Steric effects on control of endo/exo-selectivity in asymmetric cycloaddition reaction of 3,4-dimethyl-1-phenylarsole

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Supporting information

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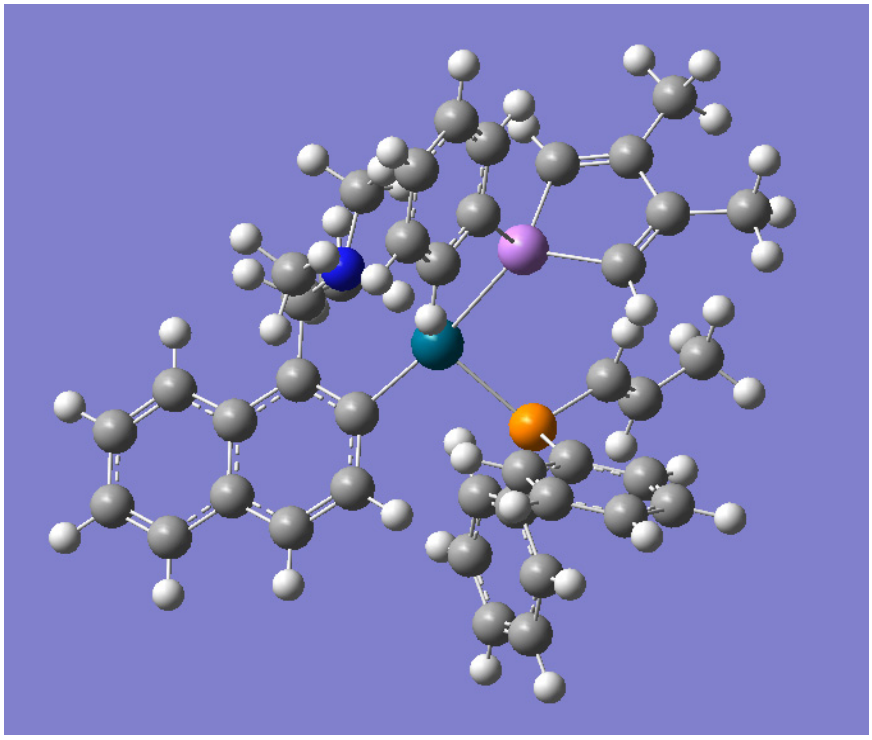
Table S1 Selected bond lengths (Å) and angles (deg) for *endo*-(–)-**7**

	Exp. data	Calc. data		Exp. data	Calc. data
Pd1–C1	2.042(2)	2.056	Pd1–N1	2.114(2)	2.191
Pd1–P1	2.253(1)	2.360	Pd1–As1	2.472(1)	2.547
As1–C35	1.986(2)	2.013	As1–C40	1.978(2)	2.003
As1–C41	1.930(2)	1.937	P1–C27	1.844(2)	1.886
P1–C15	1.823(2)	1.837	P1–C21	1.817(2)	1.835
C27–C28	1.571(3)	1.576	C28–C29	1.517(3)	1.522
C28–C35	1.569(3)	1.577	C35–C36	1.517(3)	1.521
C36–C38	1.341(3)	1.349	C36–C37	1.495(3)	1.500
C38–C39	1.494(3)	1.500	C38–C40	1.509(3)	1.520
C27–C40	1.564(3)	1.565			
C1–Pd1–N1	81.6(1)	79.9	C1–Pd1–P1	94.6(1)	97.0
N1–Pd1–P1	175.9(1)	174.1	C1–Pd1–As1	172.2(1)	173.5
N1–Pd1–As1	99.9(1)	101.2	P1–Pd1–As1	83.6(1)	82.4
C40–As1–C35	76.6(1)	75.4	C41–As1–C40	106.5(1)	109.0
C41–As1–C35	106.2(1)	108.8	C41–As1–Pd1	129.2(1)	126.5
C40–As1– Pd1	101.2(1)	102.6	C35–As1– Pd1	121.4(1)	120.5
C21–P1–C15	109.8(1)	108.0	C21–P1–C27	104.3(1)	104.7
C15–P1–C27	105.1(1)	104.2	C21–P1– Pd1	114.7(1)	117.2
C15–P1– Pd1	114.3(1)	115.0	C27–P1– Pd1	107.6(1)	106.4
C40–C27–C28	107.5(2)	107.0	C35–C28–C27	105.4(2)	105.3
C35–C28–C29	114.4(2)	112.6	C27–C28–C29	115.0(2)	116.1
C36–C35–C28	110.3(2)	109.3	C28–C35–As1	97.2(1)	98.6
C36–C35–As1	101.9(1)	102.4	C38–C36–C35	111.3(2)	111.1
C36–C38–C40	112.0(2)	111.6	C38–C40–C27	109.5(2)	110.5
C38–C40–As1	103.0(1)	103.2	C27–C40–As1	95.6(1)	96.3

Cartesian coordinates of complexes calculated at the UB3LYP/6-31G*/ LANL2DZ(Pd) level.



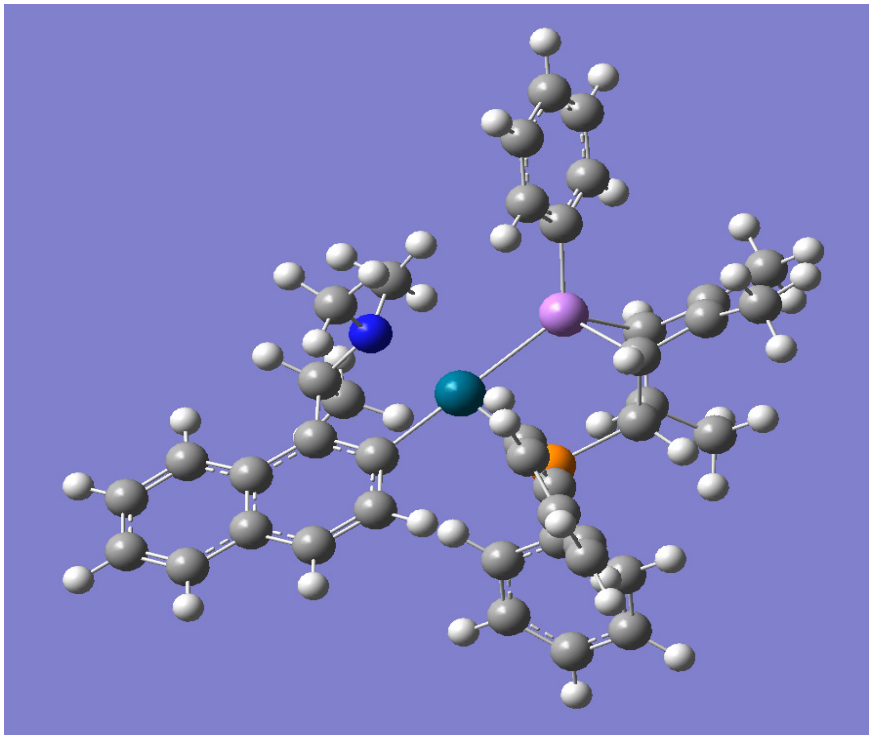
Optimized Structure of *trans*-Me-2

Gas phase energy: -4344.92639799 hartrees
Solvation (CH_2Cl_2) energy: -4344.97642209 hartrees
Gibbs free energy: -4344.268342 hartrees

Pd	0.28082000	-0.46734900	-0.17314500
As	-2.32724700	-0.75683600	-0.30522600
C	2.28129000	-0.55114300	0.22837500
C	2.96453200	0.20673300	1.21224900
H	2.45626000	0.99104800	1.76235800
C	4.29082400	-0.04100600	1.48926800
H	4.80403400	0.53969600	2.25235900
C	5.01499800	-1.03690900	0.78562000
C	4.33387900	-1.82930700	-0.19839100
C	2.94230900	-1.57882000	-0.43283800
C	6.39260600	-1.27236500	1.04166800
H	6.89274300	-0.66495600	1.79194000
C	7.08446100	-2.24445900	0.35650500
H	8.13772900	-2.41462400	0.55916300
C	6.41997800	-3.02595600	-0.61812500
H	6.97021300	-3.78966400	-1.16054600
C	5.08360300	-2.82600600	-0.88782400

H	4.60777900	-3.43445000	-1.65036000
C	2.12016600	-2.44060800	-1.36619400
H	2.53195800	-3.45792500	-1.42553800
C	2.07651100	-1.85750400	-2.78634200
H	1.61226300	-2.53481400	-3.50960200
H	3.10317900	-1.67406100	-3.11717700
H	1.54432000	-0.89956100	-2.79879200
C	0.83930400	-3.44146700	0.47021700
H	-0.12920900	-3.46730600	0.97196600
H	1.58996200	-3.04539600	1.15271900
H	1.12004400	-4.46371200	0.17849100
C	-0.21903200	-3.20420100	-1.66869100
H	0.17698600	-4.15890200	-2.04480500
H	-0.42384700	-2.54487900	-2.51168400
H	-1.15010900	-3.40736400	-1.13519500
C	-0.69640500	2.40935700	1.53810800
C	-1.49250600	3.56572100	1.57134200
H	-1.62729300	4.15708800	0.67042000
C	-2.11368400	3.95678000	2.75902100
H	-2.72870300	4.85206400	2.77578700
C	-1.94349300	3.20159000	3.92189000
H	-2.42736000	3.50846100	4.84462600
C	-1.15176600	2.05091500	3.89703900
H	-1.01716700	1.46202500	4.79979900
C	-0.53469600	1.65303700	2.71032800
H	0.07431900	0.75283500	2.69121700
C	1.68596300	2.86967700	-0.12339200
C	2.60802200	2.56638700	-1.13938900
H	2.43177800	1.72070200	-1.79749500
C	3.76011100	3.33443200	-1.29619200
H	4.46650000	3.09118800	-2.08455400
C	4.01251700	4.40337800	-0.43165800
H	4.91543500	4.99564100	-0.54887800
C	3.10568400	4.70474700	0.58476000
H	3.29870800	5.53251700	1.26104300
C	1.94336800	3.94518900	0.73918700
H	1.24528800	4.19398500	1.53167400
C	-0.89802500	2.49894200	-1.35339600
H	-1.88848100	2.04877700	-1.39775300
C	-0.54280000	3.41718500	-2.26410000
H	0.44735800	3.86723000	-2.21499300
C	-3.23272400	-1.12088700	-1.96830900
H	-2.92731200	-1.87104800	-2.68808400
C	-4.25859700	-0.26302600	-2.16194000

C	-5.11781800	-0.24985000	-3.39787700
H	-6.17332800	-0.41527000	-3.14897700
H	-4.81005000	-1.02527700	-4.10411700
H	-5.06313700	0.71842600	-3.91124600
C	-4.50742600	0.70565500	-1.05042300
C	-5.65127200	1.68227500	-1.12256000
H	-5.68093900	2.32133500	-0.23628000
H	-6.61386500	1.16089000	-1.19582400
H	-5.57372300	2.32770700	-2.00655400
C	-3.65536900	0.61910700	-0.00702100
H	-3.69981500	1.23836500	0.88107400
C	-2.92543000	-2.16116800	0.91905700
C	-3.99827800	-3.00371800	0.60212400
H	-4.50649500	-2.90240800	-0.35157900
C	-4.41908700	-3.97203900	1.51540300
H	-5.24952600	-4.62501500	1.26205400
C	-3.77976500	-4.09922300	2.75081900
H	-4.11087900	-4.85258400	3.45964600
C	-2.71460200	-3.25615900	3.07359300
H	-2.21643000	-3.34813300	4.03464800
C	-2.28497100	-2.29188900	2.15869200
H	-1.45375900	-1.63934000	2.41437700
N	0.74400900	-2.57342800	-0.73646500
P	0.14889800	1.87340200	-0.00034700
C	-1.42172100	3.88894200	-3.38429200
H	-1.56418700	4.97601400	-3.33135400
H	-0.95065100	3.68507900	-4.35486300
H	-2.40462800	3.40822000	-3.36939800



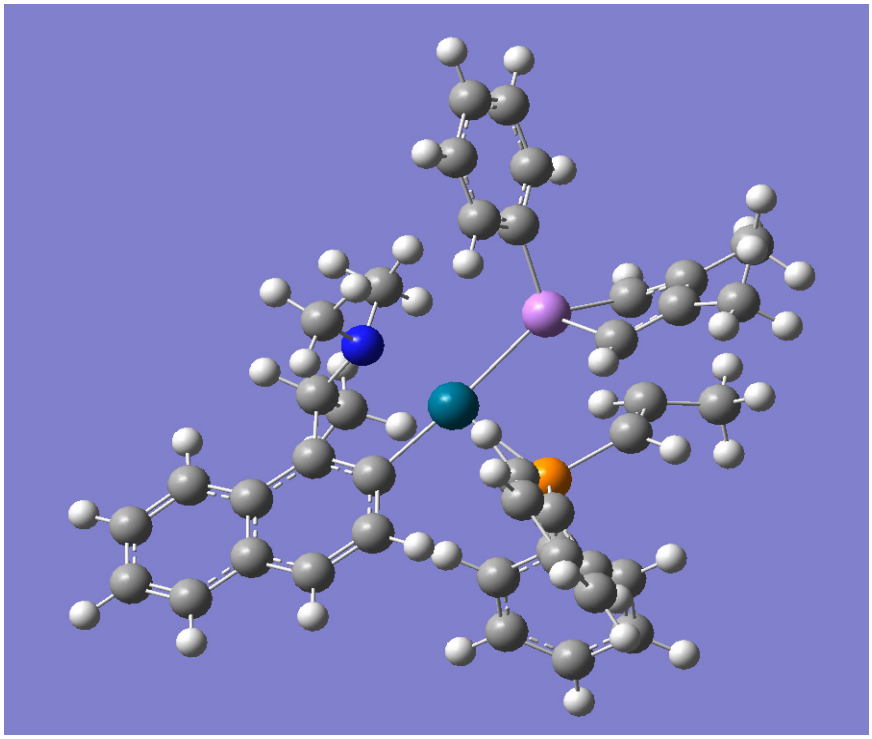
Optimized Structure of *endo*-(–)-**2**

Gas phase energy: -4344.95125703 hartrees
Solvation (CH_2Cl_2) energy: -4345.00385257 hartrees
Gibbs free energy: -4344.282160 hartrees

Pd	0.42897100	-0.59407100	-0.09162800
As	-2.10923200	-0.73950100	-0.25626900
C	2.45541700	-0.46464800	0.22783200
C	3.14201500	0.51390000	0.99178300
H	2.60440200	1.34423400	1.43609800
C	4.50121900	0.42194800	1.19461900
H	5.01604000	1.17624000	1.78550900
C	5.25594800	-0.64338600	0.64111900
C	4.58114100	-1.65141700	-0.12664900
C	3.16264400	-1.53978500	-0.30329400
C	6.66043600	-0.73456700	0.83552600
H	7.15459100	0.03591700	1.42214600
C	7.38468300	-1.77160600	0.29457700
H	8.45803700	-1.83089200	0.44882500
C	6.72706200	-2.76559700	-0.46821300
H	7.30229600	-3.58106200	-0.89754300
C	5.36579400	-2.70802800	-0.67383200
H	4.89509700	-3.48101500	-1.27264800
C	2.37755100	-2.57471900	-1.08259200
H	2.83747700	-3.56937800	-0.99816600

C	2.30460400	-2.20218700	-2.57112000
H	1.87065900	-2.99496500	-3.18778700
H	3.32040500	-2.01908700	-2.93334800
H	1.72925300	-1.27995700	-2.71071100
C	1.13296300	-3.37408100	0.87482000
H	0.16208300	-3.37518400	1.37515300
H	1.86216900	-2.85783100	1.49791400
H	1.45530200	-4.41425200	0.72376900
C	0.06360300	-3.46131200	-1.27395600
H	0.49020600	-4.44471100	-1.51943600
H	-0.16185300	-2.92719100	-2.19631400
H	-0.86295200	-3.61151000	-0.71724900
C	0.17580200	2.33361800	1.85906700
C	0.44697800	3.68024400	2.15071000
H	0.60112000	4.39651700	1.35125300
C	0.54563700	4.10748100	3.47587600
H	0.76099400	5.15080800	3.68747700
C	0.37704900	3.20019500	4.52334400
H	0.45728800	3.53644100	5.55294300
C	0.12172700	1.85597400	4.24387800
H	0.00919400	1.14138800	5.05414100
C	0.02976700	1.42329400	2.92122000
H	-0.13018200	0.36958700	2.70830500
C	0.81828300	2.86443500	-0.99812900
C	1.96410800	2.45170100	-1.69566700
H	2.35272100	1.45008700	-1.54848200
C	2.61114500	3.32677600	-2.57077200
H	3.49855600	2.99437600	-3.10143900
C	2.12215100	4.61895100	-2.76332100
H	2.62692800	5.29750800	-3.44477400
C	0.97759600	5.03811500	-2.08044900
H	0.58872500	6.04126900	-2.22942800
C	0.32676000	4.16788700	-1.20625200
H	-0.56565600	4.51218900	-0.69232500
C	-1.85803100	1.92172400	-0.25414900
H	-2.13732000	2.96042700	-0.04743700
C	-2.14061800	1.54184900	-1.76100900
H	-1.20265900	1.26349500	-2.25756700
C	-3.05762100	0.27126000	-1.71165400
H	-3.14597000	-0.21874500	-2.68307500
C	-4.37779900	0.64416300	-1.04967700
C	-5.65334100	0.61939100	-1.84003000
H	-6.51879600	0.90361900	-1.23593600
H	-5.84653700	-0.38181200	-2.24804800

H	-5.60546100	1.30281300	-2.69822800
C	-4.18482300	1.04974300	0.22237900
C	-5.18909300	1.57596100	1.20452200
H	-4.94689200	2.60289700	1.51090000
H	-5.19701100	0.96894700	2.11982400
H	-6.20380600	1.58184500	0.79848300
C	-2.72042200	0.95731100	0.62298900
H	-2.53431300	1.05853300	1.69251900
C	-3.23789900	-2.20455100	0.32052600
C	-4.19826800	-2.77501600	-0.52480100
H	-4.36231700	-2.37274700	-1.51970800
C	-4.95480300	-3.86563700	-0.09122400
H	-5.70019700	-4.30032700	-0.75098600
C	-4.75587000	-4.39383000	1.18593200
H	-5.34704800	-5.24061500	1.52195600
C	-3.79301700	-3.83519100	2.03016900
H	-3.63504500	-4.24367000	3.02419400
C	-3.02989900	-2.75038900	1.59617000
H	-2.28119600	-2.32316700	2.25977800
N	1.00780900	-2.68075000	-0.43757300
P	-0.02820000	1.70388700	0.14287700
C	-2.76167500	2.69083400	-2.56473900
H	-3.68865600	3.04809500	-2.10466500
H	-2.06547100	3.53314900	-2.62905100
H	-2.98730700	2.37062200	-3.58842100



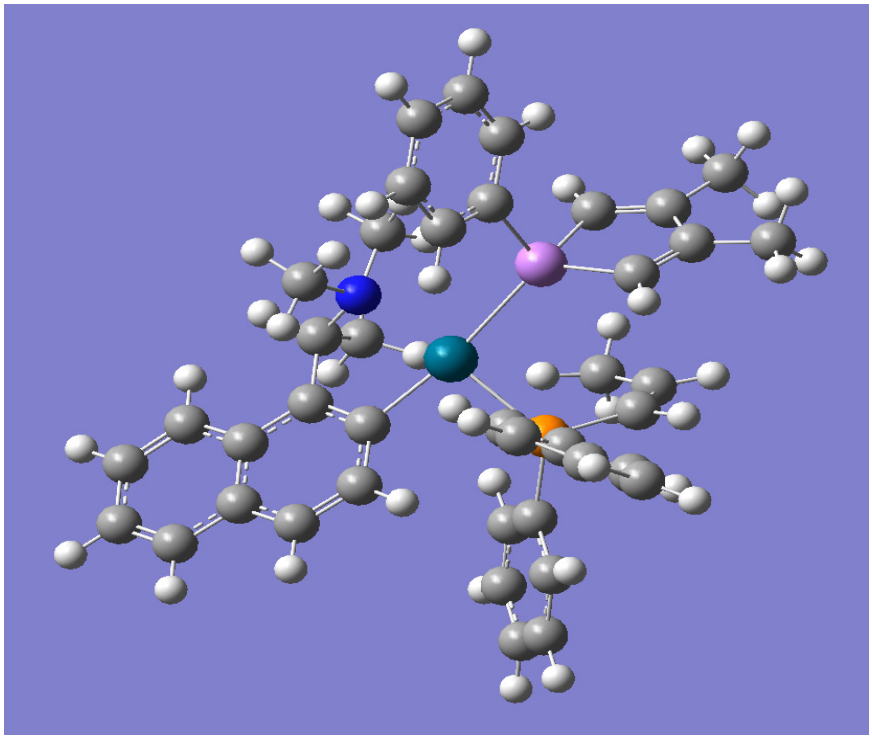
Transition state structure for TS-*trans*-Me

Imaginary frequencies: -452.9106 cm^{-1}
Gas phase energy: -4344.88079528 hartrees
Solvation (CH_2Cl_2) energy: -4344.93333816 hartrees
Gibbs free energy: -4344.218083 hartrees

Pd	0.39096400	-0.51252700	-0.17609800
As	-2.16614600	-0.66448500	-0.22270400
C	2.40030700	-0.48382200	0.23792800
C	3.06746200	0.40361600	1.12129900
H	2.53366600	1.22503700	1.58603300
C	4.40368900	0.23341500	1.41049000
H	4.90407500	0.91717500	2.09253500
C	5.15342600	-0.81972800	0.82771900
C	4.49530700	-1.73662700	-0.05953400
C	3.09839600	-1.54927400	-0.32155300
C	6.53634800	-0.98742800	1.10745600
H	7.01836900	-0.28578500	1.78371100
C	7.25529400	-2.01209500	0.53664600
H	8.31221300	-2.13014200	0.75662500
C	6.61426300	-2.91604500	-0.34339700
H	7.18603700	-3.72117000	-0.79622900
C	5.27395700	-2.78318800	-0.63388800
H	4.81622100	-3.48607400	-1.32245500

C	2.32201200	-2.49233700	-1.21520600
H	2.74723000	-3.50539200	-1.18906100
C	2.33402000	-2.00281800	-2.67125400
H	1.90244900	-2.72752800	-3.36807200
H	3.37274000	-1.83414200	-2.97039500
H	1.80185400	-1.04946400	-2.76423700
C	0.96528900	-3.40284300	0.61465300
H	-0.02929700	-3.41726300	1.06504500
H	1.67487800	-2.95806600	1.31154500
H	1.27157200	-4.43569800	0.39489800
C	-0.00309100	-3.27868600	-1.58094400
H	0.40755900	-4.24952200	-1.89477100
H	-0.16996600	-2.65924400	-2.46193800
H	-0.95688500	-3.45147300	-1.08027400
C	0.15517000	2.45960300	1.72305100
C	0.36520100	3.82289400	1.98277600
H	0.51265200	4.52105600	1.16524500
C	0.40669500	4.29017100	3.29755500
H	0.57327500	5.34677100	3.48624200
C	0.24444600	3.40480200	4.36479000
H	0.28224400	3.77145200	5.38647000
C	0.04905900	2.04431800	4.11646300
H	-0.05890300	1.34824600	4.94341700
C	0.01033800	1.57331500	2.80392200
H	-0.10877400	0.50960900	2.61310200
C	1.03482600	2.89684400	-1.07355600
C	2.29760800	2.49786300	-1.53494700
H	2.69433100	1.52899200	-1.25711900
C	3.04948500	3.34366200	-2.35356200
H	4.02590500	3.02038700	-2.70284300
C	2.55050000	4.59236500	-2.72428300
H	3.13674900	5.24726800	-3.36239700
C	1.28894700	4.99512800	-2.27906000
H	0.89016700	5.96291000	-2.56966000
C	0.53273800	4.15261300	-1.46490000
H	-0.45341100	4.47313400	-1.14272700
C	-1.69392600	2.15984200	-0.49191300
H	-2.16670700	3.00564700	0.00080000
C	-2.12606800	1.80154900	-1.78661200
H	-1.40983400	1.25517600	-2.40106300
C	-3.37732600	0.09052600	-1.55183900
H	-3.45664600	-0.30160400	-2.56196200
C	-4.50656700	0.59524300	-0.88365200
C	-5.81060900	0.88383800	-1.57922000

H	-6.63727300	0.35950700	-1.08298500
H	-5.79043400	0.56368600	-2.62430400
H	-6.05951900	1.95279300	-1.55709400
C	-4.26509300	0.97040200	0.46709400
C	-5.27251000	1.73591600	1.28738500
H	-5.55869900	2.68171700	0.80928500
H	-4.88370900	1.96494700	2.28316700
H	-6.19447800	1.15495200	1.41500200
C	-2.97659300	0.68949700	0.90984100
H	-2.63856500	0.91541900	1.91507900
C	-3.06520800	-2.30511300	0.35767400
C	-3.91942400	-3.03188800	-0.48198900
H	-4.14443000	-2.67279200	-1.48174400
C	-4.50078200	-4.22123900	-0.03520400
H	-5.16590300	-4.77443700	-0.69229900
C	-4.23274600	-4.69501900	1.25031500
H	-4.68842200	-5.61813600	1.59625100
C	-3.37662400	-3.97932300	2.09074900
H	-3.16686400	-4.34103600	3.09338300
C	-2.79012900	-2.79407800	1.64373700
H	-2.12811100	-2.24396000	2.30924400
N	0.92148500	-2.60277400	-0.63999200
P	0.02328600	1.79986000	0.01129500
C	-3.01789000	2.74206900	-2.57030900
H	-3.78886600	3.18956200	-1.93469000
H	-2.41311800	3.56234700	-2.97919000
H	-3.50881900	2.24423100	-3.41210300



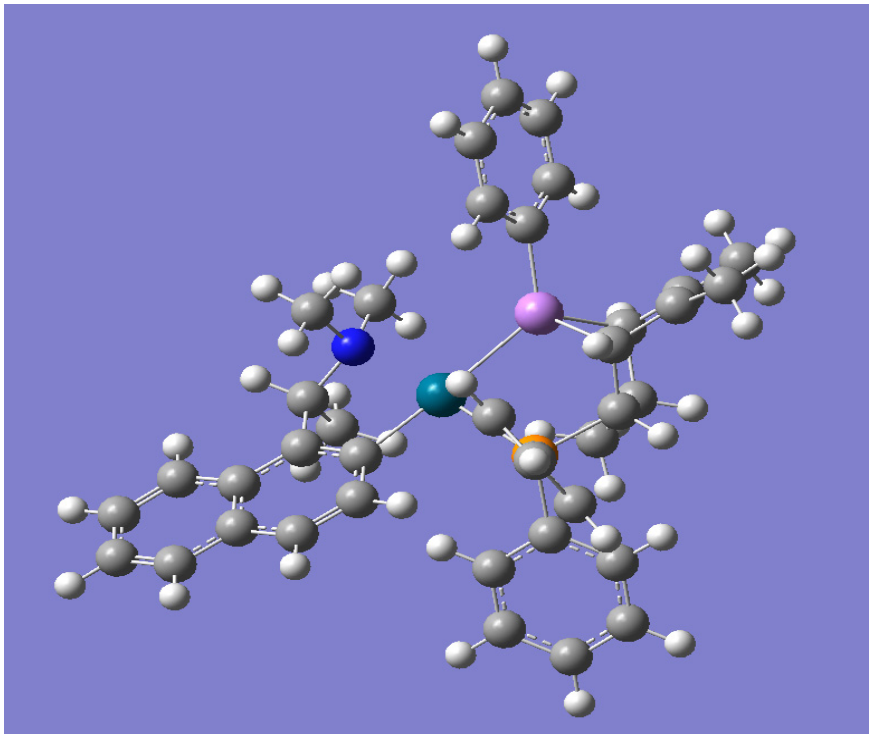
Optimized Structure of *cis*-Me-2

Gas phase energy: -4344.91780673 hartrees
Solvation (CH_2Cl_2) energy: -4344.97070738 hartrees
Gibbs free energy: -4344.258424 hartrees

Pd	0.26112700	-0.42086100	-0.15577700
As	-2.36467900	-0.60309900	-0.29736500
C	2.26298900	-0.51981000	0.25057700
C	2.97510200	0.34261300	1.12135600
H	2.49247800	1.20478700	1.56735300
C	4.29700900	0.09877900	1.42111300
H	4.83266300	0.76288100	2.09552500
C	4.98711100	-1.00383300	0.85639300
C	4.27681600	-1.90121000	-0.00935900
C	2.89156600	-1.64324300	-0.27298200
C	6.35904300	-1.24305700	1.13778300
H	6.88193700	-0.55468000	1.79706300
C	7.01737200	-2.31951500	0.58932600
H	8.06658500	-2.49199200	0.81025100
C	6.32379000	-3.20613500	-0.26807100
H	6.84768100	-4.05290600	-0.70249400
C	4.99217600	-3.00431300	-0.55924500
H	4.49294300	-3.69598800	-1.23028200
C	2.05002900	-2.58901700	-1.10074400
H	2.41748800	-3.62107800	-1.01121900

C	2.06884500	-2.20639500	-2.58709300
H	1.57674400	-2.94750600	-3.22412100
H	3.11121500	-2.13127700	-2.91070000
H	1.60123400	-1.22894700	-2.74474400
C	0.69109000	-3.30736500	0.80560500
H	-0.28839600	-3.24210100	1.28168100
H	1.44195500	-2.86049400	1.45596200
H	0.93915000	-4.36587900	0.64121400
C	-0.31792800	-3.27443500	-1.37167600
H	0.04078300	-4.28245600	-1.62631200
H	-0.47585100	-2.70942200	-2.29019500
H	-1.26620000	-3.37333100	-0.83996000
C	-0.52894700	2.51933600	1.50707700
C	-1.09803400	3.79594900	1.66246200
H	-1.14915500	4.48450400	0.82418400
C	-1.59280600	4.20328200	2.90201000
H	-2.02990700	5.19203000	3.00731900
C	-1.52132800	3.34683000	4.00338500
H	-1.90622000	3.66735100	4.96706800
C	-0.95193800	2.08038100	3.86247600
H	-0.89005900	1.41178300	4.71627300
C	-0.46115300	1.66831400	2.62206300
H	-0.02184200	0.68001600	2.51367900
C	1.68351200	2.90397200	-0.40444600
C	2.51164500	2.52968400	-1.47509200
H	2.28262800	1.64363200	-2.05772100
C	3.65002300	3.27270100	-1.78007400
H	4.28319300	2.97072600	-2.60940300
C	3.98394000	4.39178300	-1.01272400
H	4.87481900	4.96700300	-1.24747600
C	3.17473800	4.76092300	0.06131200
H	3.43258200	5.62391400	0.66851600
C	2.02814600	4.02311100	0.36645900
H	1.41491200	4.32236900	1.20919000
C	-1.03586800	2.59770900	-1.32528000
H	-1.72171300	3.33735600	-0.91965500
C	-1.13117200	2.30436100	-2.63049600
H	-1.89081300	2.84956000	-3.19266400
C	-3.27600500	-0.88624700	-1.97064900
H	-3.00512700	-1.63471100	-2.70623200
C	-4.25856900	0.02529800	-2.14635800
C	-5.11284800	0.10541500	-3.38333700
H	-6.17485700	-0.02345100	-3.14045100
H	-4.83580600	-0.66341400	-4.10936800

H	-5.01854300	1.08421100	-3.87040200
C	-4.46646200	0.97872900	-1.01481500
C	-5.56438300	2.00780400	-1.06798300
H	-5.57499600	2.62031100	-0.16257900
H	-6.54946400	1.53500600	-1.16692200
H	-5.44665200	2.67644900	-1.93020400
C	-3.62184600	0.83132400	0.02591600
H	-3.64162100	1.42919200	0.92938100
C	-3.06779800	-1.98037500	0.90473100
C	-4.11123400	-2.83357700	0.52471700
H	-4.54133000	-2.75803400	-0.46886800
C	-4.60659200	-3.77727400	1.42713600
H	-5.41404800	-4.43798800	1.12431300
C	-4.07265000	-3.86873900	2.71428700
H	-4.46214600	-4.60209800	3.41433200
C	-3.03778400	-3.01419400	3.10045800
H	-2.62240200	-3.07684100	4.10238900
C	-2.53348100	-2.07601300	2.19716100
H	-1.72776100	-1.41347200	2.50437100
N	0.65690500	-2.58257000	-0.49620000
P	0.14654800	1.92806900	-0.09594500
C	-0.32294500	1.34017200	-3.44370800
H	0.35372100	1.88146500	-4.11876700
H	0.27689400	0.67002500	-2.82113200
H	-0.97969300	0.72996400	-4.07485700



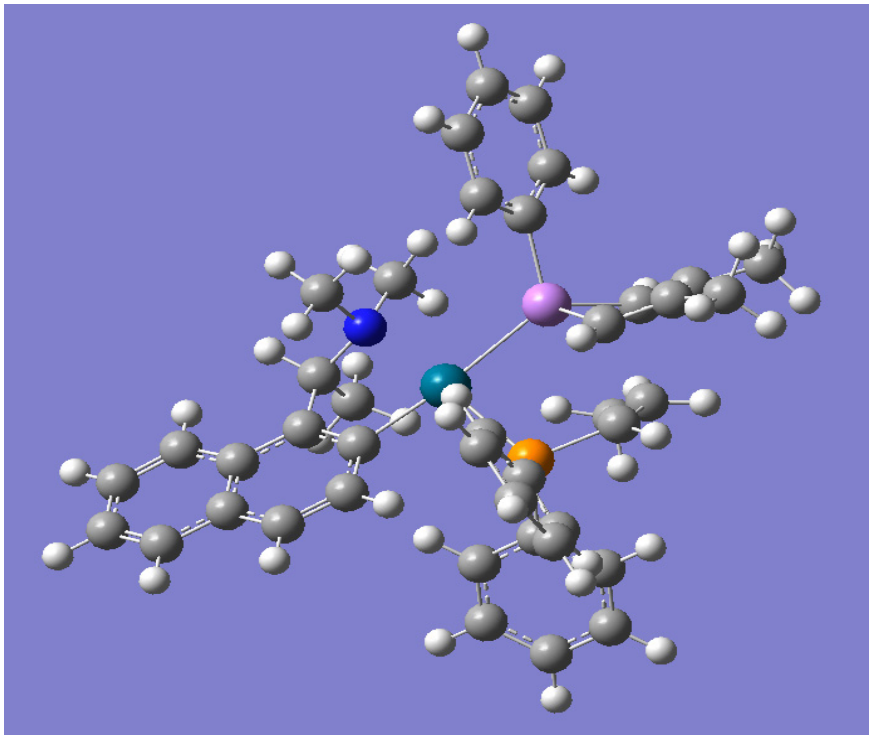
Optimized Structure of *exo*-(–)-**2**

Gas phase energy: -4344.94410006 hartrees
Solvation (CH_2Cl_2) energy: -4344.99706649 hartrees
Gibbs free energy: -4344.276002 hartrees

Pd	0.41051700	-0.56765600	-0.15520700
As	-2.13514600	-0.69973400	-0.31594000
C	2.41761800	-0.47736200	0.26511200
C	3.06875300	0.45867900	1.10979300
H	2.51705100	1.28272800	1.54955100
C	4.41008500	0.33111400	1.39751400
H	4.89808000	1.05217200	2.04951200
C	5.18054600	-0.72788100	0.85350500
C	4.53894200	-1.69550600	0.00882300
C	3.13709800	-1.54996500	-0.25329800
C	6.56804400	-0.85321600	1.13268800
H	7.03727700	-0.11329700	1.77634800
C	7.30706700	-1.88508600	0.60194900
H	8.36725700	-1.97051200	0.82119500
C	6.68221700	-2.83946500	-0.23543700
H	7.26952000	-3.65060900	-0.65651000
C	5.33803000	-2.74838800	-0.52424100
H	4.89288500	-3.49030000	-1.17935900
C	2.37838900	-2.54855200	-1.10247800
H	2.81857100	-3.55253700	-1.02462200

C	2.38613500	-2.13269000	-2.58087300
H	1.96598200	-2.89742400	-3.24096500
H	3.42255300	-1.96352900	-2.88736500
H	1.84039900	-1.19304600	-2.72182400
C	1.02842700	-3.39131600	0.76552800
H	0.03494000	-3.39462800	1.21901100
H	1.73436300	-2.90782700	1.43973700
H	1.34380300	-4.43032800	0.59327600
C	0.05800300	-3.38152300	-1.43318100
H	0.47551000	-4.36458700	-1.69509000
H	-0.11249800	-2.80820600	-2.34369400
H	-0.89627000	-3.53176700	-0.92497300
C	-0.00951100	2.34670200	1.77763500
C	0.04741000	3.71368400	2.09584100
H	0.12126100	4.45897700	1.31115800
C	0.03328400	4.12752600	3.42827400
H	0.08199900	5.18736900	3.66083300
C	-0.03477600	3.18652600	4.45785800
H	-0.04149200	3.51316100	5.49366900
C	-0.07906900	1.82480200	4.15288300
H	-0.11455700	1.08714000	4.94940500
C	-0.06054800	1.40690600	2.82191300
H	-0.06501900	0.34578500	2.58695500
C	0.88620600	2.95884100	-0.96299500
C	2.17188000	2.64358200	-1.42833000
H	2.60661700	1.67628400	-1.20431200
C	2.89735500	3.57052100	-2.17920400
H	3.89220100	3.31274400	-2.53058400
C	2.34820200	4.81702600	-2.48090000
H	2.91328100	5.53512200	-3.06794400
C	1.06520400	5.13745600	-2.03075600
H	0.62801000	6.10314100	-2.26757000
C	0.33677400	4.21602600	-1.27860500
H	-0.66357700	4.48343600	-0.95194500
C	-1.86880700	1.94986000	-0.45511200
H	-2.12999100	2.99913500	-0.28410300
C	-2.24388600	1.52213600	-1.94059900
H	-2.91484700	2.30271300	-2.31872900
C	-3.12106500	0.22826500	-1.79643300
H	-3.23050400	-0.31090100	-2.73874700
C	-4.42593700	0.63891500	-1.12886900
C	-5.70909100	0.59789900	-1.90501800
H	-6.55843100	0.95818000	-1.31908700
H	-5.94055800	-0.42336100	-2.23620900

H	-5.64522300	1.21389000	-2.81266900
C	-4.20338500	1.11870100	0.11123700
C	-5.18250100	1.71482100	1.07884800
H	-4.92586400	2.75660200	1.31549000
H	-5.17672600	1.16632500	2.03033300
H	-6.20525400	1.70416400	0.69345600
C	-2.73286100	1.03985400	0.48448300
H	-2.52531400	1.19205100	1.54313900
C	-3.24225000	-2.13685300	0.36082500
C	-4.22167700	-2.75657100	-0.42611400
H	-4.41562200	-2.41020500	-1.43667800
C	-4.96009200	-3.82518000	0.08668600
H	-5.72024000	-4.29839400	-0.52821400
C	-4.72495300	-4.28149200	1.38517000
H	-5.30245500	-5.11089600	1.78267700
C	-3.74393000	-3.67267000	2.17197100
H	-3.55830800	-4.02449200	3.18274900
C	-2.99839800	-2.61063300	1.65887400
H	-2.23562800	-2.14285400	2.27765000
N	0.97662400	-2.65135700	-0.52597200
P	-0.05314500	1.73894000	0.03944900
C	-1.12362000	1.36190300	-2.97787400
H	-0.38708800	0.60332200	-2.68842200
H	-1.56341000	1.04998200	-3.93201700
H	-0.59170800	2.29969600	-3.15147200



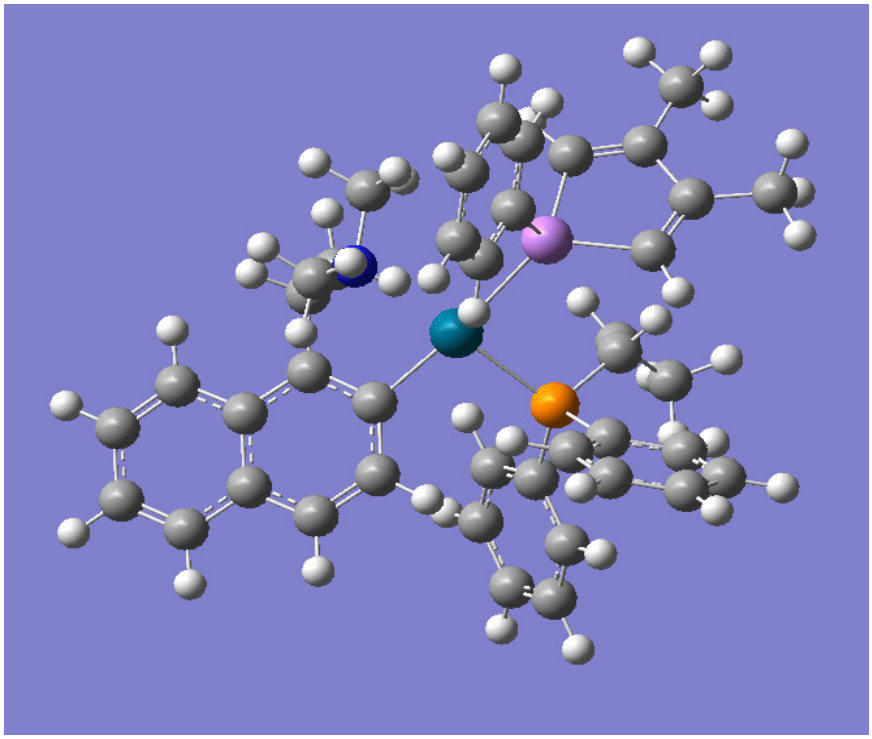
Transition state structure for TS-*cis*-Me

Imaginary frequencies: -477.1279 cm^{-1}
Gas phase energy: -4344.87745701 hartrees
Solvation (CH_2Cl_2) energy: -4344.93030865 hartrees
Gibbs free energy: -4344.214312 hartrees

Pd	0.36739700	-0.48440300	-0.15902400
As	-2.20148200	-0.64616700	-0.26235700
C	2.36009400	-0.45073100	0.31788300
C	2.99642500	0.44709700	1.21361400
H	2.44655800	1.27301400	1.65125200
C	4.32266900	0.28176800	1.54852700
H	4.79960700	0.97379300	2.23898000
C	5.09205800	-0.77693600	1.00264900
C	4.46396100	-1.70510100	0.10537700
C	3.07634400	-1.52245400	-0.20511100
C	6.46526000	-0.93954900	1.32932000
H	6.92439700	-0.22920100	2.01237100
C	7.20321800	-1.97029300	0.79489700
H	8.25249400	-2.08439600	1.05058900
C	6.59176200	-2.88580000	-0.09418900
H	7.17847500	-3.69589700	-0.51811000
C	5.26157300	-2.75796300	-0.42991300
H	4.82690500	-3.46982200	-1.12416900
C	2.32999200	-2.47823100	-1.11100100

H	2.75353800	-3.49079900	-1.05543700
C	2.39237600	-2.01137400	-2.57297300
H	1.98240900	-2.74575500	-3.27271300
H	3.44103500	-1.84970000	-2.83948900
H	1.86689900	-1.05822800	-2.69896000
C	0.91305100	-3.36698500	0.68288200
H	-0.09599300	-3.37863300	1.09991800
H	1.59835200	-2.91364700	1.39840300
H	1.22771500	-4.40175200	0.48476400
C	0.01503500	-3.26337000	-1.54409600
H	0.43240400	-4.23819600	-1.83575700
H	-0.12275200	-2.65126500	-2.43509700
H	-0.95481600	-3.42821500	-1.07262800
C	0.03468100	2.51061600	1.69198000
C	0.14605800	3.88731700	1.94243400
H	0.26482100	4.58689000	1.12121500
C	0.12453500	4.36789400	3.25271900
H	0.21452000	5.43500100	3.43427600
C	-0.00290000	3.48278100	4.32514300
H	-0.01411800	3.86007100	5.34358500
C	-0.10109100	2.11033000	4.08623900
H	-0.18270900	1.41566100	4.91740400
C	-0.07719700	1.62628800	2.77781100
H	-0.12423900	0.55564800	2.59463000
C	1.03755500	2.94291000	-1.05704200
C	2.34344500	2.58231200	-1.41981800
H	2.75296600	1.63174600	-1.10028000
C	3.12321200	3.44329700	-2.19505900
H	4.13333100	3.15060600	-2.46692400
C	2.60918800	4.66791900	-2.62246700
H	3.21733400	5.33428300	-3.22735600
C	1.30487600	5.03037900	-2.27796800
H	0.89358800	5.97764300	-2.61504400
C	0.52166700	4.17325000	-1.50504400
H	-0.49846800	4.45803700	-1.26478000
C	-1.71911200	2.17445800	-0.56448100
H	-2.22104800	2.97034100	-0.02449400
C	-2.21295000	1.81291100	-1.84727500
H	-3.02881300	2.44444200	-2.19391400
C	-3.40020300	0.14659500	-1.59083100
H	-3.49670500	-0.25453400	-2.59564500
C	-4.53561700	0.64061600	-0.91455700
C	-5.81064800	0.99484200	-1.63130800
H	-6.68512200	0.60928000	-1.09356100

H	-5.83127300	0.58749500	-2.64575500
H	-5.94338300	2.08395300	-1.70362300
C	-4.29995100	0.98985900	0.44035100
C	-5.29538200	1.77075100	1.26085500
H	-5.53974100	2.73547700	0.79714100
H	-4.91646300	1.96577400	2.26758900
H	-6.23870400	1.21972300	1.36049700
C	-3.01836400	0.68301700	0.88633500
H	-2.67245000	0.90958500	1.88842200
C	-3.12072300	-2.29542900	0.26009500
C	-3.93403700	-3.01560300	-0.62479700
H	-4.11593200	-2.64662400	-1.62978200
C	-4.53086200	-4.21144500	-0.21771300
H	-5.16485800	-4.75861800	-0.90969100
C	-4.31889100	-4.69888600	1.07320500
H	-4.78678100	-5.62689500	1.38836900
C	-3.50294000	-3.99051900	1.95852900
H	-3.33639300	-4.36301400	2.96532300
C	-2.90126400	-2.79853200	1.55132700
H	-2.27149300	-2.25377000	2.25148700
N	0.91097900	-2.58041100	-0.58109200
P	-0.01228800	1.83460400	-0.01861800
C	-1.31024500	1.36737900	-2.98778300
H	-0.59100900	0.60139500	-2.67858600
H	-1.89591300	0.96879200	-3.82175700
H	-0.73603500	2.22212200	-3.36360400



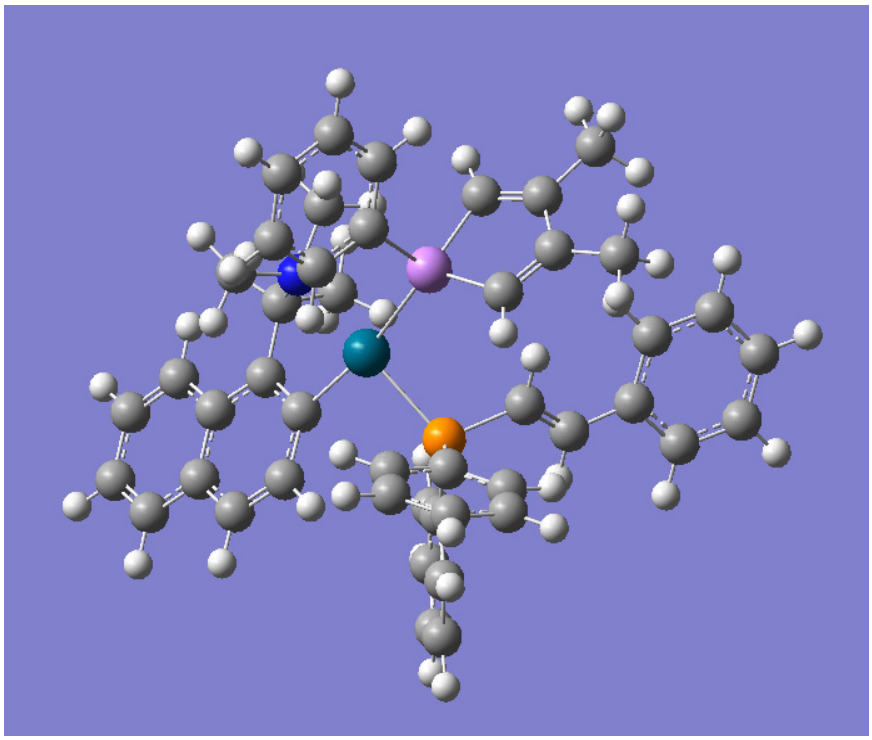
Transition state structure for TS-Me-1

Imaginary frequencies: -979.5280 cm^{-1}
Gas phase energy: -4344.83127659 hartrees
Solvation (CH_2Cl_2) energy: -4344.84499900 hartrees
Gibbs free energy: -4344.181364 hartrees

Pd	0.23521400	-0.48276200	-0.10445900
As	-2.39553200	-0.67042800	-0.17552400
C	2.24647300	-0.61431400	0.22791700
C	2.99678200	0.19900100	1.11336600
H	2.53853000	1.04444700	1.61418500
C	4.32542300	-0.07196200	1.35491700
H	4.89132900	0.55233200	2.04254400
C	4.98398600	-1.14999700	0.71040500
C	4.23460200	-1.99720000	-0.17330100
C	2.84292500	-1.71689600	-0.37097000
C	6.36310700	-1.41299800	0.92877700
H	6.91549500	-0.76309800	1.60290000
C	6.99188900	-2.46381000	0.30160000
H	8.04690800	-2.65454900	0.47469100
C	6.26001800	-3.29977600	-0.57464000
H	6.76067300	-4.12578300	-1.07192000
C	4.92031700	-3.07482700	-0.80532000
H	4.39166600	-3.72739400	-1.49283800

C	1.95443500	-2.62066300	-1.19819700
H	2.33042000	-3.65359800	-1.19099600
C	1.87257800	-2.15052900	-2.65783900
H	1.35742700	-2.86557400	-3.30649200
H	2.89022400	-2.02915100	-3.04080800
H	1.37128100	-1.17822800	-2.72438300
C	0.71444700	-3.41383500	0.76456400
H	-0.23634800	-3.36570200	1.29796300
H	1.49938400	-2.98246000	1.38413400
H	0.95565300	-4.46605700	0.55589000
C	-0.41718200	-3.32696400	-1.34768600
H	-0.06942800	-4.32618300	-1.64873400
H	-0.63054200	-2.73981500	-2.24047000
H	-1.33427100	-3.44490600	-0.76657400
C	-0.61516700	2.54610900	1.39323800
C	-1.33843400	3.74999800	1.34974800
H	-1.43222100	4.29461200	0.41449600
C	-1.93785300	4.25162300	2.50611200
H	-2.49660100	5.18214000	2.46297100
C	-1.81517000	3.56259500	3.71536400
H	-2.28046900	3.95641300	4.61430000
C	-1.09325500	2.36807500	3.76796000
H	-0.99444500	1.83159300	4.70722100
C	-0.49988600	1.85829600	2.61216700
H	0.05339100	0.92372400	2.65472700
C	1.74567100	2.80211400	-0.36559400
C	2.59365500	2.42270300	-1.41852500
H	2.36261100	1.54664900	-2.01622800
C	3.74802700	3.15563400	-1.68775600
H	4.39835300	2.85491100	-2.50404700
C	4.07564700	4.26268300	-0.90015900
H	4.98031800	4.82749100	-1.10590100
C	3.24283400	4.63679400	0.15474800
H	3.49522700	5.49345400	0.77301200
C	2.07790700	3.91323400	0.42221000
H	1.43588900	4.21873600	1.24170600
C	-0.85807800	2.36982800	-1.49325100
H	-1.93202800	2.29909400	-1.29335100
C	-0.37183600	2.65616700	-2.83253500
H	-0.28009300	1.83395000	-3.54495600
C	-3.32110300	-1.07138000	-1.81830200
H	-3.05434600	-1.87045800	-2.49997000
C	-4.30039000	-0.17146700	-2.05785800
C	-5.15426000	-0.17272100	-3.29752200

H	-6.21826000	-0.26421200	-3.04690200
H	-4.88949800	-0.99981300	-3.96131900
H	-5.04170200	0.76326400	-3.85912900
C	-4.50127200	0.86046200	-0.99529800
C	-5.59572200	1.88744000	-1.11778400
H	-5.59996600	2.56423800	-0.25940400
H	-6.58197700	1.41042700	-1.17694700
H	-5.48081800	2.48996900	-2.02758600
C	-3.65548300	0.78130000	0.05421600
H	-3.67365500	1.44064500	0.91400100
C	-3.05345400	-1.98195100	1.11801800
C	-4.16305200	-2.79219400	0.84672900
H	-4.67046900	-2.71749000	-0.10989000
C	-4.62083800	-3.69395400	1.80909600
H	-5.47966500	-4.32260300	1.59136000
C	-3.98204400	-3.78550500	3.04798000
H	-4.34204900	-4.48696700	3.79495200
C	-2.88036100	-2.97369200	3.32533700
H	-2.38272900	-3.03809300	4.28892300
C	-2.41381100	-2.07691100	2.36123100
H	-1.55397200	-1.44819000	2.57991300
N	0.60138100	-2.65261400	-0.51043600
P	0.18883300	1.86405900	-0.10662400
C	-0.17648600	4.05780100	-3.33348300
H	0.33980000	4.68244900	-2.59435100
H	0.40357000	4.06809900	-4.26142600
H	-1.14138900	4.54884700	-3.54520100



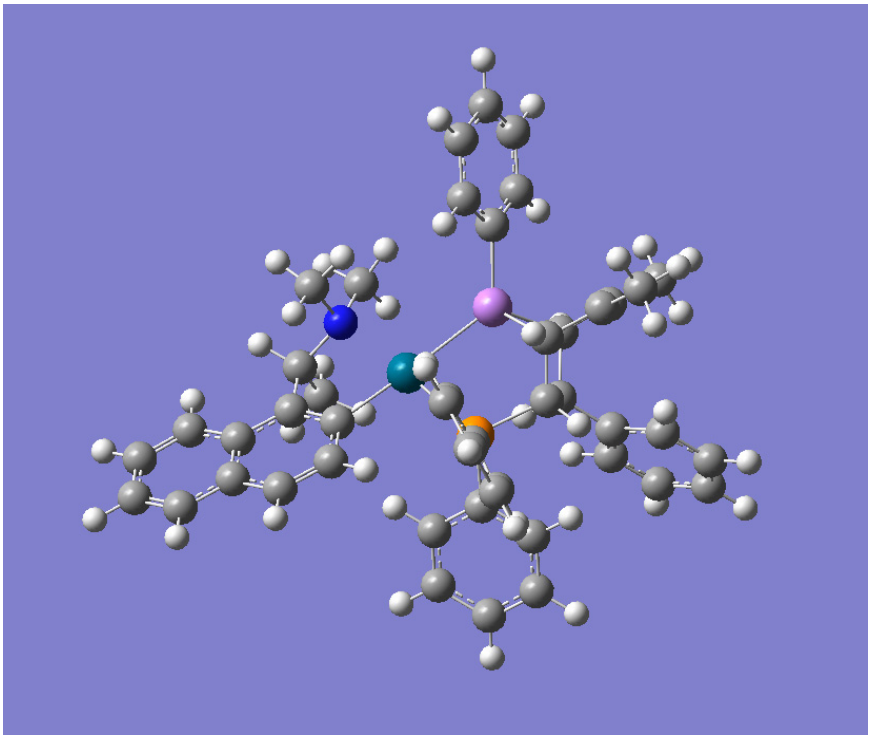
Optimized structure of *trans*-Ph-2

Gas phase energy: -4536.66379466 hartrees
Solvation (CH_2Cl_2) energy: -4536.71579234 hartrees
Gibbs free energy: -4535.957484 hartrees

Pd	0.72450400	-0.59759400	-0.18043000
As	-1.62055600	-1.79008200	-0.22605200
C	2.68123300	-0.03988000	0.00094000
C	3.27757500	0.54018900	1.14811500
H	2.67316300	0.83225300	1.99954800
C	4.63899300	0.74232300	1.20140100
H	5.08951700	1.17944200	2.08956500
C	5.47535300	0.40231900	0.10768500
C	4.89179300	-0.20584300	-1.05425900
C	3.47866600	-0.44485000	-1.06222800
C	6.87568800	0.64036000	0.14323700
H	7.30226300	1.09913800	1.03181100
C	7.67910300	0.30210100	-0.92121200
H	8.74805500	0.49017400	-0.88364300
C	7.10921600	-0.29300300	-2.07163800
H	7.74580400	-0.55443900	-2.91226300
C	5.75542500	-0.54110200	-2.13712500
H	5.34862200	-0.98702600	-3.03919300
C	2.79625600	-1.18398500	-2.19284000

H	3.49275300	-1.87589600	-2.68689000
C	2.24659400	-0.21670400	-3.25097100
H	1.87377800	-0.72914900	-4.14309300
H	3.05598500	0.44882100	-3.56574200
H	1.44652500	0.40362100	-2.83153200
C	2.35394000	-3.15535300	-0.79951700
H	1.58109300	-3.72544100	-0.28136600
H	3.05425200	-2.75121700	-0.06992200
H	2.89312400	-3.82333900	-1.48667700
C	0.83529200	-2.65084200	-2.58487800
H	1.43134600	-3.18221100	-3.34124000
H	0.23403500	-1.88591700	-3.07567700
H	0.17391800	-3.37346700	-2.10180300
C	-0.76793700	0.91030400	2.58307000
C	-1.88617400	1.57604800	3.11027100
H	-2.39421800	2.33312700	2.52015700
C	-2.34936100	1.26415200	4.39002700
H	-3.21578400	1.78295100	4.79028800
C	-1.70026400	0.29101400	5.15388200
H	-2.06243600	0.05092100	6.14935400
C	-0.58624900	-0.37430200	4.63626200
H	-0.07963300	-1.13134500	5.22799800
C	-0.12471800	-0.07107000	3.35469600
H	0.73566100	-0.59787400	2.94990600
C	0.95203400	2.78094400	1.11060900
C	1.65977700	3.25746800	-0.00617100
H	1.59871400	2.73028100	-0.95375600
C	2.45246500	4.39837000	0.09811300
H	2.99479900	4.75876600	-0.77116700
C	2.56043500	5.06731900	1.32101600
H	3.18590000	5.95155400	1.40325000
C	1.86714900	4.59528700	2.43557600
H	1.94910100	5.11029700	3.38840400
C	1.06199500	3.45790100	2.33355900
H	0.52436800	3.10385200	3.20677100
C	-1.54562700	1.90685800	-0.03984500
H	-2.28009700	1.13864500	-0.26638000
C	-1.72785900	3.17289300	-0.46743300
H	-0.99331000	3.92737400	-0.19261200
C	-2.84704800	3.67153100	-1.27468400
C	-3.74640200	2.82369900	-1.94975700
H	-3.60352600	1.74731200	-1.91467000
C	-4.79813000	3.35315600	-2.69079800
H	-5.47861400	2.68812300	-3.21578500

C	-4.97555100	4.73856900	-2.77536300
H	-5.79679700	5.14763600	-3.35663400
C	-4.08570000	5.59204600	-2.12131100
H	-4.21197100	6.66861000	-2.18890900
C	-3.02808200	5.06233300	-1.38410700
H	-2.33511100	5.72998400	-0.87782200
C	-2.69826600	-1.88326200	-1.82355900
H	-2.33437200	-2.18098400	-2.79969600
C	-3.95998300	-1.46107300	-1.58525400
C	-5.02576700	-1.36722200	-2.64453000
H	-4.64247900	-1.67089500	-3.62210400
H	-5.41289000	-0.34424100	-2.73311500
H	-5.88301900	-2.00716700	-2.40113200
C	-4.25739700	-1.08540800	-0.16883000
C	-5.63399100	-0.62672800	0.23383300
H	-6.39067100	-1.38723600	0.00482000
H	-5.92447900	0.28447800	-0.30433900
H	-5.68050200	-0.41547400	1.30520300
C	-3.22052000	-1.19799300	0.68789600
H	-3.26759800	-0.97434000	1.74686700
C	-1.46517400	-3.64066600	0.38860400
C	-0.55652300	-3.93398400	1.41409100
H	0.06375000	-3.14562500	1.83311600
C	-0.44814300	-5.23696000	1.90592300
H	0.25491400	-5.45572600	2.70473900
C	-1.24076300	-6.25357800	1.36948300
H	-1.15338000	-7.26794000	1.74772900
C	-2.14627300	-5.96429200	0.34588300
H	-2.76566300	-6.75275500	-0.07230500
C	-2.26325600	-4.66177400	-0.14239800
H	-2.97639800	-4.44162500	-0.93063200
N	1.71683300	-2.04449200	-1.56029400
P	-0.12120600	1.30557400	0.90995700



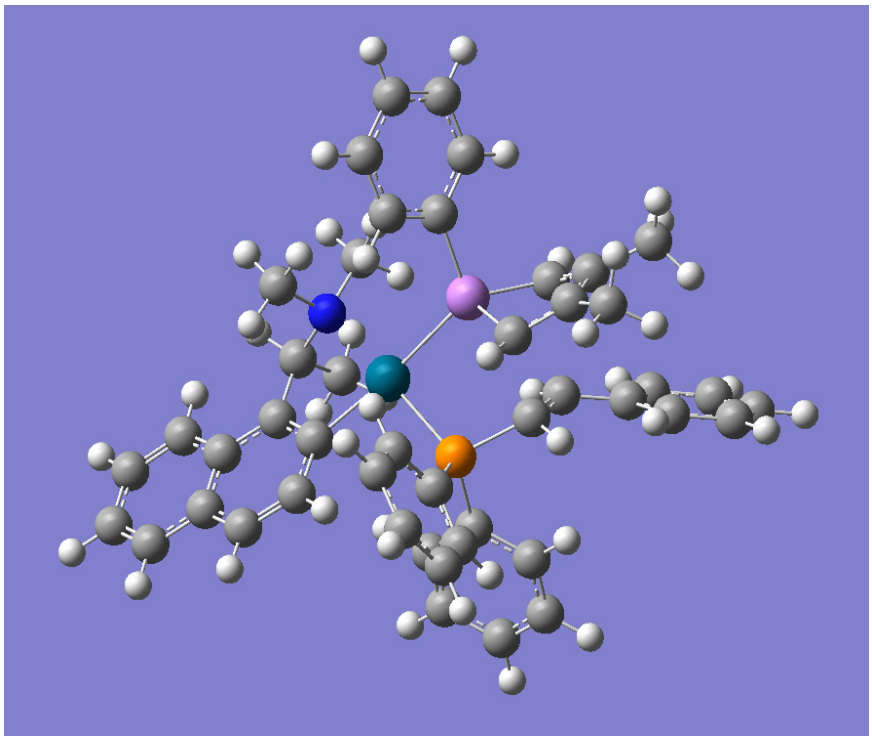
Optimized structure of *endo*-(–)-**7**

Gas phase energy: -4536.68178426 hartrees
Solvation (CH_2Cl_2) energy: -4536.73538077 hartrees
Gibbs free energy: -4535.965145 hartrees

Pd	-0.93905700	0.64273600	-0.12997100
As	1.44414200	1.54119400	-0.12402800
C	-2.87532300	-0.01377600	0.08809800
C	-3.37130500	-0.92265200	1.05824500
H	-2.69751700	-1.40705500	1.75636600
C	-4.71835600	-1.19933700	1.14018500
H	-5.08630700	-1.89504800	1.89105000
C	-5.64760500	-0.59585000	0.25528500
C	-5.17066800	0.33620600	-0.72674200
C	-3.76618700	0.62046800	-0.77337400
C	-7.03583700	-0.89035200	0.32517100
H	-7.37970400	-1.59634500	1.07702600
C	-7.92969100	-0.29972200	-0.53788600
H	-8.98853200	-0.53305000	-0.47628300
C	-7.46596300	0.61576600	-1.51210400
H	-8.17355500	1.07741500	-2.19505700
C	-6.12646900	0.92506400	-1.60507500
H	-5.80432700	1.62286500	-2.37140300
C	-3.19284400	1.61224300	-1.76399500
H	-3.91702700	2.40589900	-1.99549200

C	-2.80328800	0.91663300	-3.07718900
H	-2.52514000	1.62227600	-3.86577900
H	-3.66347200	0.34266600	-3.43389500
H	-1.97811300	0.21414500	-2.91351200
C	-2.51478200	3.22297800	-0.03968100
H	-1.66371300	3.64151900	0.50205100
H	-3.15875100	2.68510600	0.65488600
H	-3.08249700	4.04421900	-0.50020500
C	-1.21554400	3.08676800	-2.05485200
H	-1.86137000	3.78832900	-2.60257600
H	-0.71239600	2.43172500	-2.76530000
H	-0.46507700	3.66040600	-1.50818300
C	-0.15483300	-1.56878500	2.53359900
C	0.02740100	-2.82859000	3.12672300
H	0.27709900	-3.69147400	2.51772300
C	-0.13203600	-2.98529700	4.50423200
H	0.00663500	-3.96502800	4.95213000
C	-0.47568400	-1.89205800	5.30239600
H	-0.60210000	-2.01949100	6.37357800
C	-0.67180800	-0.63836800	4.71933500
H	-0.95710400	0.21104300	5.33330800
C	-0.51903500	-0.47809400	3.34204200
H	-0.70615000	0.49015700	2.88449300
C	-0.16729700	-2.86435700	-0.13931500
C	-1.34649100	-3.05109700	-0.87907500
H	-2.08015800	-2.25515300	-0.93709300
C	-1.58168200	-4.25928100	-1.53726600
H	-2.49954700	-4.39102400	-2.10284400
C	-0.64296100	-5.28976300	-1.47302000
H	-0.82697700	-6.22796500	-1.98852300
C	0.53852900	-5.10951800	-0.75073700
H	1.27946300	-5.90224200	-0.70658000
C	0.77840200	-3.90582100	-0.08839000
H	1.71183200	-3.78439500	0.45097500
C	1.97345300	-0.97911900	0.59764900
H	2.48871900	-1.78883800	1.12156700
C	2.40037500	-0.89731500	-0.91716800
H	1.51455500	-1.03043300	-1.54936100
C	3.41536100	-1.93084900	-1.38435800
C	3.31279100	-2.42248700	-2.69478800
H	2.49608900	-2.08471200	-3.32951500
C	4.23416500	-3.34204800	-3.19554900
H	4.13089000	-3.70974300	-4.21257800
C	5.27980400	-3.79384800	-2.38810900

H	5.99730900	-4.51307700	-2.77232900
C	5.39328000	-3.31740900	-1.08122800
H	6.20209800	-3.66378900	-0.44371500
C	4.47071300	-2.39410800	-0.58356900
H	4.58712000	-2.03120400	0.43300500
C	2.90127600	0.58320500	-1.13013200
H	3.02706000	0.82568500	-2.18618200
C	4.12128100	0.83223200	-0.25621500
C	5.45803900	1.09091700	-0.88553000
H	6.23583200	1.27781500	-0.14042800
H	5.41759600	1.96334600	-1.55150200
H	5.77623500	0.23754900	-1.49777500
C	3.81568400	0.70191000	1.05162800
C	4.72393100	0.79033000	2.24215400
H	4.74913600	-0.15766500	2.79773800
H	4.37317200	1.55608900	2.94700200
H	5.75092200	1.03841600	1.96253000
C	2.34067000	0.39450200	1.25256300
H	1.99062900	0.48904400	2.28117000
C	1.98028400	3.38329000	0.14559400
C	2.83610400	4.04233500	-0.74643900
H	3.26024100	3.51297400	-1.59449800
C	3.15483400	5.38725100	-0.54725400
H	3.82282000	5.89064400	-1.24024700
C	2.61994100	6.08137200	0.53977900
H	2.87138500	7.12657700	0.69400900
C	1.75856700	5.43181400	1.42757900
H	1.34081200	5.96853500	2.27452600
C	1.43219600	4.08993700	1.22660400
H	0.76034200	3.59205900	1.92248100
N	-2.01529200	2.29258500	-1.09021700
P	0.11734400	-1.27960300	0.73982700



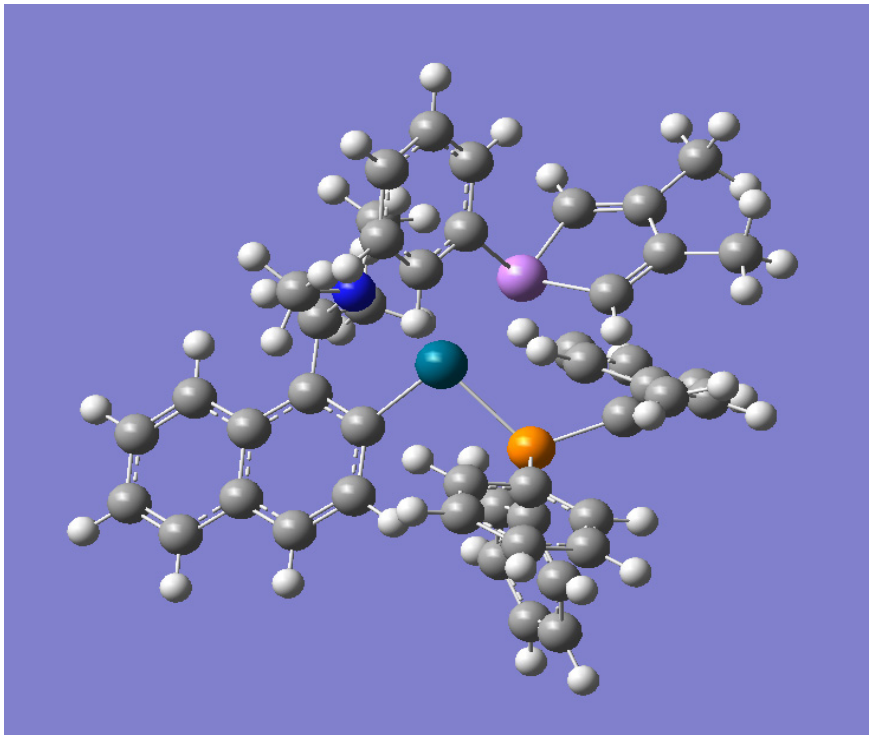
Transition state structure for TS-*trans*-Ph

Imaginary frequencies: -443.3753 cm^{-1}
Gas phase energy: -4536.61766136 hartrees
Solvation (CH_2Cl_2) energy: -4536.67091834 hartrees
Gibbs free energy: -4535.906873 hartrees

Pd	0.01749000	-0.07607000	0.07490900
As	2.56439400	-0.00426000	0.11517200
C	-2.00672300	0.23001800	-0.04505400
C	-2.77793200	1.10331500	0.76454600
H	-2.32503400	1.62132400	1.60312200
C	-4.11335000	1.31234100	0.49664100
H	-4.69498300	1.98639100	1.12152800
C	-4.75757500	0.65526000	-0.58259000
C	-3.99168800	-0.22039600	-1.42407600
C	-2.59882200	-0.39723400	-1.13628300
C	-6.13946600	0.85055700	-0.84951300
H	-6.70387700	1.51852700	-0.20359200
C	-6.75563400	0.20957500	-1.89936900
H	-7.81278600	0.36511700	-2.09334600
C	-6.00771400	-0.65809900	-2.73012200
H	-6.49823200	-1.16593300	-3.55579100
C	-4.66534100	-0.86741900	-2.50058800
H	-4.12444000	-1.54777100	-3.15050400

C	-1.70716400	-1.26284800	-2.00158100
H	-2.06410100	-1.28768100	-3.04072300
C	-1.65810800	-2.70508200	-1.47582300
H	-1.13156900	-3.38614400	-2.15117000
H	-2.68440600	-3.06952300	-1.37171800
H	-1.19027100	-2.74274700	-0.48561600
C	-0.41637400	0.63260600	-2.87070500
H	0.54112500	1.15508400	-2.82930200
H	-1.20412400	1.28553400	-2.49669600
H	-0.63201600	0.36649600	-3.91539100
C	0.69031400	-1.48585200	-2.62167800
H	0.37374100	-1.84317000	-3.61241800
H	0.86966100	-2.34228900	-1.97217900
H	1.61934000	-0.92396900	-2.73603100
C	0.00245200	1.84893300	3.04805000
C	-0.26739800	2.10446400	4.40204300
H	-0.40793100	1.28323800	5.09767000
C	-0.37716300	3.41804600	4.86035300
H	-0.58975300	3.60455800	5.90905200
C	-0.22433400	4.48758000	3.97540800
H	-0.31561200	5.50826700	4.33535200
C	0.03148800	4.24280400	2.62454300
H	0.13455000	5.07098500	1.92926600
C	0.13900300	2.93078900	2.16190000
H	0.30850600	2.73903800	1.10522100
C	-0.80597300	-0.96472200	3.46326100
C	-2.06046600	-1.41263000	3.02259400
H	-2.42684300	-1.12493800	2.04491600
C	-2.84366900	-2.23259100	3.83753200
H	-3.81239300	-2.57091900	3.48115100
C	-2.38479500	-2.61958100	5.09665000
H	-2.99478600	-3.25970000	5.72748900
C	-1.13212900	-2.18906100	5.53966000
H	-0.76140400	-2.49514600	6.51365000
C	-0.34459600	-1.37191100	4.72934400
H	0.63534800	-1.07069100	5.08460000
C	1.95288100	-0.31207800	2.86630700
H	2.27676600	0.12287700	3.80803600
C	2.32570700	-1.65202800	2.59236100
H	1.66931100	-2.23018400	1.94561700
C	3.16752500	-2.46388000	3.48250900
C	3.21254100	-3.86015900	3.29567000
H	2.63014000	-4.30644300	2.49241700
C	3.98102600	-4.67358100	4.12270000

H	3.99367500	-5.74781600	3.96145900
C	4.73051900	-4.11166200	5.16087300
H	5.32871800	-4.74507100	5.80914800
C	4.69620600	-2.73050200	5.36342300
H	5.26744700	-2.28559800	6.17360400
C	3.92258900	-1.91503700	4.53696400
H	3.90521200	-0.84517500	4.72303100
C	3.81356300	-1.33186400	0.76421800
H	3.92755600	-2.32001600	0.33142000
C	4.84757700	-0.69406300	1.45662100
C	6.16072000	-1.36655300	1.76330500
H	6.99968900	-0.75939500	1.40063400
H	6.22700700	-2.34980400	1.29042400
H	6.30003600	-1.50245100	2.84207200
C	4.50749000	0.58637900	1.96622400
C	5.43267300	1.39276900	2.84077100
H	5.77405600	0.82797000	3.71749900
H	4.95021900	2.30850200	3.19404200
H	6.33411700	1.68713000	2.28744100
C	3.18015600	0.96750400	1.69456800
H	2.82157500	1.96231000	1.94173300
C	3.49208300	0.86916500	-1.37063100
C	4.57944400	0.28158100	-2.02941300
H	4.96514300	-0.67783500	-1.69954300
C	5.18271300	0.93269200	-3.10820500
H	6.02674000	0.46988400	-3.61183200
C	4.70684900	2.17344900	-3.53584200
H	5.17968500	2.67879600	-4.37286500
C	3.62015500	2.76375900	-2.88585400
H	3.24806500	3.73097200	-3.21178800
C	3.01033900	2.11035700	-1.81366600
H	2.16458800	2.57926800	-1.31486000
N	-0.34150600	-0.59728000	-2.03478000
P	0.22350500	0.14035500	2.40648800



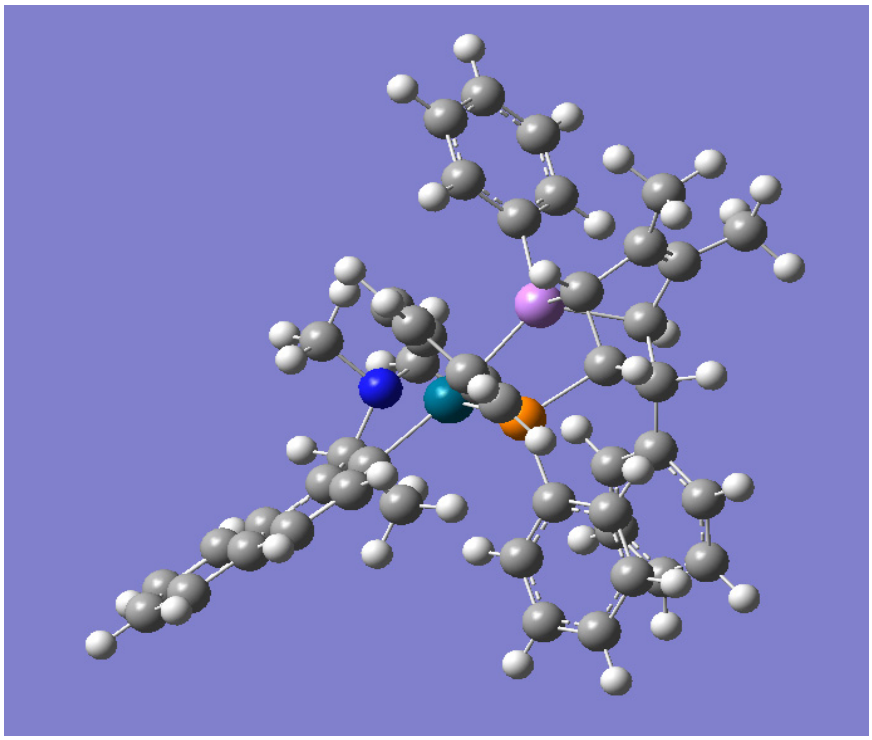
Optimized structure of *cis*-Ph-2

Gas phase energy: -4536.64980154 hartrees
Solvation (CH_2Cl_2) energy: -4536.70365579 hartrees
Gibbs free energy: -4535.941465 hartrees

Pd	0.16798100	-0.62695700	-0.09035000
As	-2.46164700	-0.60564600	-0.32526500
C	2.15636700	-1.02808800	0.21495400
C	2.90776900	-0.70506400	1.37438900
H	2.47864800	-0.10379800	2.16755000
C	4.20315500	-1.14896300	1.51940500
H	4.76484200	-0.89932700	2.41662800
C	4.83354600	-1.91981000	0.51033700
C	4.08833900	-2.26879600	-0.66495600
C	2.72902400	-1.82395600	-0.77081500
C	6.17897100	-2.35660800	0.64238600
H	6.72762000	-2.08460000	1.54067700
C	6.78038100	-3.10503700	-0.34302200
H	7.80996700	-3.43240700	-0.23269400
C	6.05336800	-3.44839200	-1.50729100
H	6.53217300	-4.03581500	-2.28569200
C	4.74578700	-3.04311500	-1.66475700
H	4.22176000	-3.31463400	-2.57549800
C	1.85985500	-2.21495000	-1.94524700
H	2.16342900	-3.19006500	-2.35108500

C	1.94995700	-1.18043300	-3.07586700
H	1.44677900	-1.50463200	-3.99169400
H	3.00565400	-1.02176300	-3.31529900
H	1.53244500	-0.22030400	-2.75530400
C	0.40097000	-3.64926300	-0.60576800
H	-0.58585900	-3.74920100	-0.15207400
H	1.15862300	-3.61270500	0.17609500
H	0.58881300	-4.52035300	-1.24990200
C	-0.52896300	-2.53196100	-2.51684400
H	-0.21560000	-3.32075700	-3.21618000
H	-0.62656100	-1.59163000	-3.05910300
H	-1.49904100	-2.81044600	-2.10122400
C	-0.30965300	1.05827200	2.87339200
C	-0.87445300	2.04882200	3.69684900
H	-1.04473700	3.05089900	3.31457100
C	-1.22570100	1.75825900	5.01600700
H	-1.66012900	2.53467300	5.63919000
C	-1.01932600	0.47760700	5.53294000
H	-1.29326400	0.25460000	6.56000000
C	-0.46353800	-0.51476700	4.72399300
H	-0.30207300	-1.51389400	5.11856400
C	-0.11499300	-0.22843400	3.40281500
H	0.31119400	-1.00830200	2.77812800
C	1.73746800	2.38103800	1.19085400
C	2.65822300	2.31547100	0.13511300
H	2.49299100	1.63282800	-0.68924400
C	3.80394800	3.11107400	0.14823500
H	4.50788500	3.04986500	-0.67661600
C	4.05062400	3.96986300	1.21984200
H	4.94713200	4.58309000	1.23215200
C	3.14582800	4.03138700	2.28132600
H	3.33551000	4.68932600	3.12455200
C	1.99469500	3.24378200	2.26868200
H	1.31126800	3.29696400	3.10876400
C	-1.11184000	2.57703700	0.61311500
H	-1.94857400	2.57920800	1.30611200
C	-1.19527700	3.44686100	-0.41469300
H	-2.05928300	4.11305700	-0.37518000
C	-0.33846000	3.67550600	-1.58487100
C	0.33613000	2.63817200	-2.25094700
H	0.23183400	1.61730100	-1.89179100
C	1.09717700	2.90082400	-3.38888700
H	1.60276300	2.08677000	-3.90144400
C	1.20361200	4.20472500	-3.87868400

H	1.79831000	4.40746700	-4.76469200
C	0.52699400	5.24419800	-3.23503400
H	0.59608400	6.25870900	-3.61656100
C	-0.24967300	4.97838100	-2.11020500
H	-0.78571000	5.78762300	-1.62036500
C	-3.29061300	-0.03531000	-1.96742200
H	-2.97172800	-0.33419400	-2.95906200
C	-4.26457600	0.87086000	-1.72952600
C	-5.04805800	1.56039300	-2.81389300
H	-6.12217600	1.36007700	-2.71612600
H	-4.72968800	1.22979900	-3.80590800
H	-4.92346200	2.64932200	-2.76265600
C	-4.53783400	1.16277300	-0.29000200
C	-5.64622500	2.10142100	0.10752100
H	-5.71696100	2.19190300	1.19469200
H	-6.61683300	1.75215700	-0.26598300
H	-5.49007700	3.10477400	-0.30885100
C	-3.74228100	0.52098300	0.58964900
H	-3.82265400	0.59860600	1.66773300
C	-3.23386800	-2.36605400	0.05354700
C	-4.22837100	-2.92919100	-0.75581100
H	-4.58128100	-2.39845200	-1.63446100
C	-4.77535600	-4.17186800	-0.42835000
H	-5.54402500	-4.60435200	-1.06269800
C	-4.34325500	-4.85290900	0.71150300
H	-4.77290500	-5.81771600	0.96475600
C	-3.35880700	-4.29005800	1.52690800
H	-3.02344700	-4.81229100	2.41858500
C	-2.80139300	-3.05280000	1.19665700
H	-2.03382700	-2.62122000	1.83516300
N	0.45122000	-2.39781100	-1.41340500
P	0.18098800	1.38890500	1.12746700



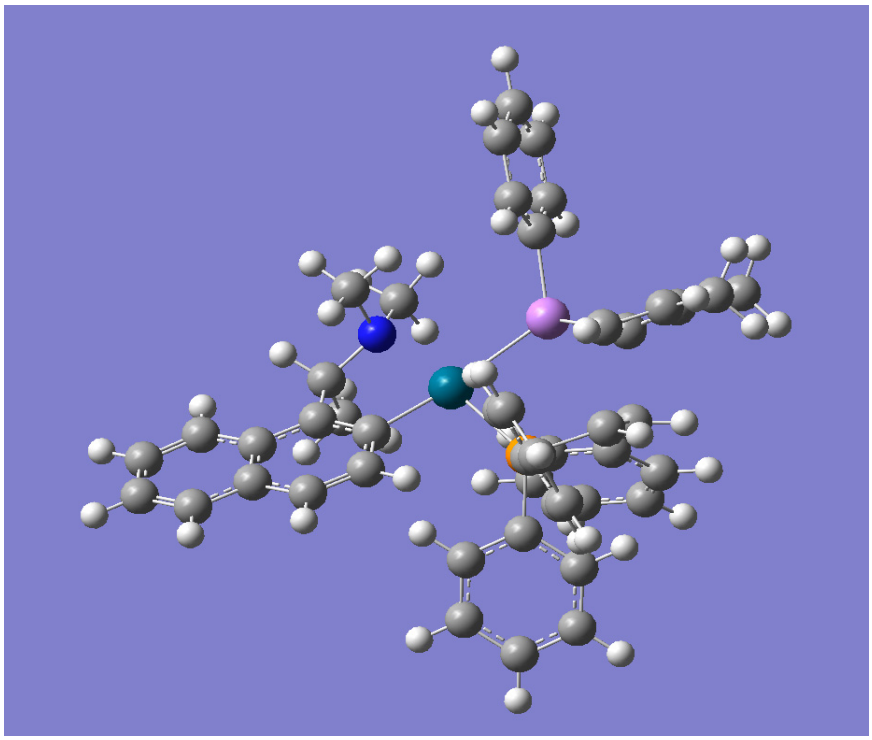
Optimized structure of *exo*-(–)-**7**

Gas phase energy: -4536.67167416 hartrees
Solvation (CH_2Cl_2) energy: -4536.72673908 hartrees
Gibbs free energy: -4535.954409 hartrees

Pd	0.43543800	-0.68787400	-0.07532000
As	-2.11792300	-0.78783400	-0.20771600
C	2.45073000	-0.68247100	0.32659200
C	3.11888800	0.06574900	1.33013400
H	2.57777200	0.78388200	1.93615500
C	4.46442800	-0.11217500	1.56422400
H	4.96317800	0.46733000	2.33793400
C	5.22474500	-1.04154500	0.80994500
C	4.56796800	-1.82063000	-0.20065900
C	3.16295400	-1.62489100	-0.40967200
C	6.61564100	-1.21973400	1.03870500
H	7.09562700	-0.62240800	1.80996800
C	7.34432300	-2.12556600	0.30296000
H	8.40722900	-2.25308900	0.48565900
C	6.70449900	-2.89447500	-0.69765300
H	7.28270400	-3.60698800	-1.27924300
C	5.35670600	-2.74697900	-0.94335400
H	4.90111300	-3.34649600	-1.72486100
C	2.40311800	-2.41716100	-1.45260400
H	2.83410900	-3.41944600	-1.58468600

C	2.43411300	-1.69753600	-2.80885400
H	2.01071700	-2.29841400	-3.61972100
H	3.47721900	-1.48736500	-3.06289200
H	1.90729600	-0.73884200	-2.75137800
C	1.02699000	-3.63357600	0.17143200
H	0.02847200	-3.72639000	0.60472500
H	1.72984600	-3.31629700	0.94100400
H	1.33557000	-4.61278600	-0.22198300
C	0.07986300	-3.12938000	-1.97801200
H	0.49229700	-4.03377300	-2.44846300
H	-0.07867500	-2.36904500	-2.74227100
H	-0.88019300	-3.37908500	-1.52301500
C	0.05629700	1.44154000	2.63348700
C	0.17385800	2.61157400	3.40150300
H	0.26175200	3.58003500	2.92287500
C	0.20869300	2.54206200	4.79519800
H	0.30530200	3.45608500	5.37398600
C	0.12907200	1.30789700	5.44238100
H	0.16029000	1.25815500	6.52689600
C	0.02634200	0.13656300	4.68946000
H	-0.01623100	-0.82934300	5.18469900
C	-0.00281800	0.20233400	3.29655000
H	-0.04792200	-0.71333600	2.71257700
C	0.86112800	2.93395500	0.21014100
C	2.05953400	2.78391000	-0.50214200
H	2.43323900	1.79159900	-0.72764800
C	2.77397200	3.90726600	-0.92287000
H	3.70149500	3.77619800	-1.47249800
C	2.30118200	5.18885200	-0.64074100
H	2.86103700	6.06099400	-0.96599500
C	1.10057300	5.34885200	0.05537600
H	0.72064900	6.34380500	0.26928100
C	0.38109700	4.23050600	0.47347100
H	-0.56025000	4.37903100	0.99424900
C	-1.88052200	1.78546400	0.46175500
H	-2.12619600	2.72867000	0.96066300
C	-2.33835200	1.84873900	-1.06825800
H	-3.07675600	2.65747600	-1.09572200
C	-1.32970600	2.18455300	-2.15904200
C	-0.63710700	1.21051400	-2.89267300
H	-0.77922500	0.15720600	-2.67106000
C	0.22484000	1.57056600	-3.93201400
H	0.73942800	0.79720200	-4.49595700
C	0.41100900	2.91332700	-4.25923400

H	1.07673700	3.19234300	-5.07082100
C	-0.28264400	3.89424200	-3.54737900
H	-0.16097600	4.94305900	-3.80231800
C	-1.14852500	3.52905800	-2.51799000
H	-1.69774400	4.30159200	-1.98508400
C	-3.16016500	0.52955900	-1.31144700
H	-3.29066200	0.30575300	-2.37014100
C	-4.44900900	0.67228900	-0.51424600
C	-5.75833400	0.81416300	-1.23219700
H	-6.59427800	0.96030200	-0.54338300
H	-5.97440600	-0.07682100	-1.83672900
H	-5.74262900	1.66676800	-1.92496900
C	-4.19246200	0.76388500	0.80619800
C	-5.14995400	1.00297600	1.93574000
H	-4.90754100	1.92880800	2.47537800
H	-5.10031800	0.18876100	2.67119400
H	-6.18468500	1.07984800	1.59213100
C	-2.70886700	0.61746700	1.09753400
H	-2.46808000	0.44395500	2.14572300
C	-3.22434400	-2.36349500	0.02038100
C	-4.09582300	-2.79608600	-0.98793500
H	-4.20762100	-2.22122000	-1.90286400
C	-4.83408600	-3.96978700	-0.82120200
H	-5.51179000	-4.29549900	-1.60513600
C	-4.70463600	-4.71927100	0.34968400
H	-5.28193300	-5.63004900	0.47861300
C	-3.83012800	-4.29788400	1.35444400
H	-3.72736700	-4.87762200	2.26728100
C	-3.08550000	-3.12931600	1.18750700
H	-2.40830400	-2.81019900	1.97676400
N	0.99524600	-2.62664100	-0.92571200
P	-0.04547900	1.44983000	0.78884500



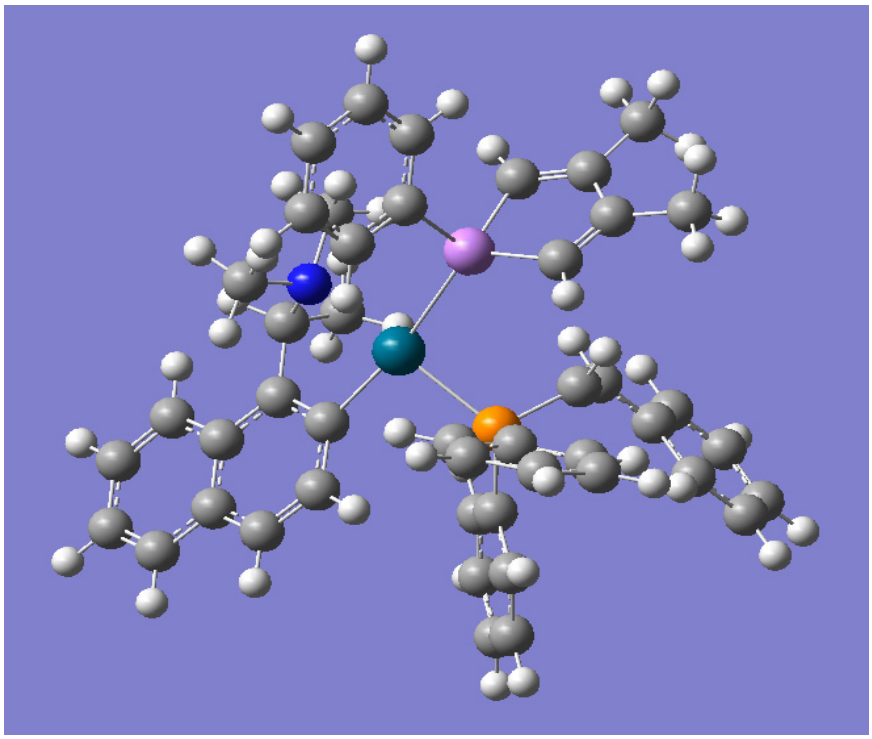
Transition state structure for TS-*cis*-Ph

Imaginary frequencies: -487.3538 cm^{-1}
Gas phase energy: -4536.60601774 hartrees
Solvation (CH_2Cl_2) energy: -4536.66016035 hartrees
Gibbs free energy: -4535.894345 hartrees

Pd	0.47335400	-0.63889000	-0.01112000
As	-2.09917900	-0.69824000	-0.20476600
C	2.45208500	-0.79288400	0.50881200
C	3.08424600	-0.18276800	1.62329000
H	2.54178200	0.51017500	2.25588700
C	4.39851700	-0.46201200	1.92717200
H	4.87024600	0.01190300	2.78506500
C	5.16151500	-1.35776300	1.13638800
C	4.53952200	-1.99574000	0.01112200
C	3.16489500	-1.69938900	-0.26948400
C	6.52153100	-1.63760800	1.43746500
H	6.97535600	-1.14643300	2.29463000
C	7.25322000	-2.50892500	0.66419400
H	8.29242800	-2.71510400	0.90279000
C	6.64789000	-3.13880000	-0.44894900
H	7.22907400	-3.82381200	-1.05984700
C	5.33055300	-2.89009400	-0.76737100
H	4.90183400	-3.38283500	-1.63402400
C	2.43678600	-2.34488500	-1.42862500

H	2.83128800	-3.34913200	-1.63736300
C	2.58416200	-1.49887500	-2.70224900
H	2.18069600	-1.99246600	-3.59129300
H	3.64954800	-1.32133500	-2.87612100
H	2.10191900	-0.52295200	-2.57802800
C	0.91730500	-3.64619000	-0.01433000
H	-0.10647100	-3.72992700	0.35595200
H	1.59048900	-3.44376300	0.81818800
H	1.20254800	-4.59636800	-0.48847000
C	0.12811900	-2.88849500	-2.15576800
H	0.54390100	-3.74981100	-2.69851800
H	0.03862700	-2.04314700	-2.83760300
H	-0.86354200	-3.15638900	-1.78930000
C	0.18254800	1.64689900	2.67826700
C	0.29653600	2.88522000	3.32924000
H	0.40549500	3.79880000	2.75357000
C	0.29055000	2.94968900	4.72348700
H	0.38238200	3.91319500	5.21648500
C	0.17716300	1.78249000	5.48164100
H	0.17815400	1.83637900	6.56645800
C	0.07760400	0.54479700	4.84258400
H	0.00727600	-0.36798400	5.42734200
C	0.08455500	0.47664100	3.44877200
H	0.03760800	-0.48974900	2.95282000
C	1.14970000	2.89225700	0.18078800
C	2.45544600	2.64870100	-0.26909600
H	2.85556100	1.64174100	-0.25593700
C	3.24535200	3.70005400	-0.73761000
H	4.25568700	3.49808800	-1.08172200
C	2.74044400	5.00055700	-0.76966900
H	3.35660100	5.81608600	-1.13724300
C	1.43610200	5.24948700	-0.33723700
H	1.03205200	6.25723800	-0.37076700
C	0.64252600	4.20266900	0.13056000
H	-0.37802000	4.40636900	0.44025600
C	-1.62298200	2.02117100	0.50522600
H	-2.06410600	2.57690800	1.32611200
C	-2.22689800	2.21440700	-0.77743300
H	-3.09724800	2.86185800	-0.69861100
C	-1.57436800	2.42220700	-2.10759900
C	-0.47397200	1.70047000	-2.59930200
H	-0.01597800	0.92298800	-1.99483000
C	0.05207500	1.96711400	-3.86325100
H	0.90924400	1.39964100	-4.21598200

C	-0.51153400	2.95459500	-4.67323600
H	-0.09873500	3.15933900	-5.65665100
C	-1.61145700	3.67458500	-4.20518000
H	-2.06376700	4.44572700	-4.82225700
C	-2.13634000	3.40631300	-2.94187300
H	-2.99413600	3.97535100	-2.59074100
C	-3.34856800	0.48931000	-1.14021600
H	-3.46337400	0.47718500	-2.21929900
C	-4.46191600	0.69046400	-0.29578400
C	-5.77724100	1.21870100	-0.80372600
H	-6.61114000	0.60668600	-0.43859700
H	-5.81590000	1.22290400	-1.89623000
H	-5.96550300	2.24351400	-0.45409200
C	-4.16860800	0.57252000	1.08376100
C	-5.13558700	0.99627600	2.15974700
H	-5.41301300	2.05479100	2.06659900
H	-4.71553300	0.84407000	3.15760900
H	-6.06685800	0.41970100	2.09821700
C	-2.85228600	0.18299900	1.34666500
H	-2.47316000	0.05682300	2.35436500
C	-3.04410500	-2.41424100	-0.24955900
C	-3.69535600	-2.85634800	-1.40925400
H	-3.73647000	-2.22397200	-2.29192900
C	-4.30963100	-4.11055200	-1.43841600
H	-4.81858300	-4.43986100	-2.33991000
C	-4.27531500	-4.93465100	-0.31174200
H	-4.75573300	-5.90838800	-0.33464400
C	-3.62183800	-4.50376700	0.84508200
H	-3.59527400	-5.13911300	1.72589700
C	-3.00401300	-3.25178900	0.87454200
H	-2.50548100	-2.92566100	1.78426500
N	0.99267800	-2.53602800	-1.00412000
P	0.10508400	1.52556400	0.84223700



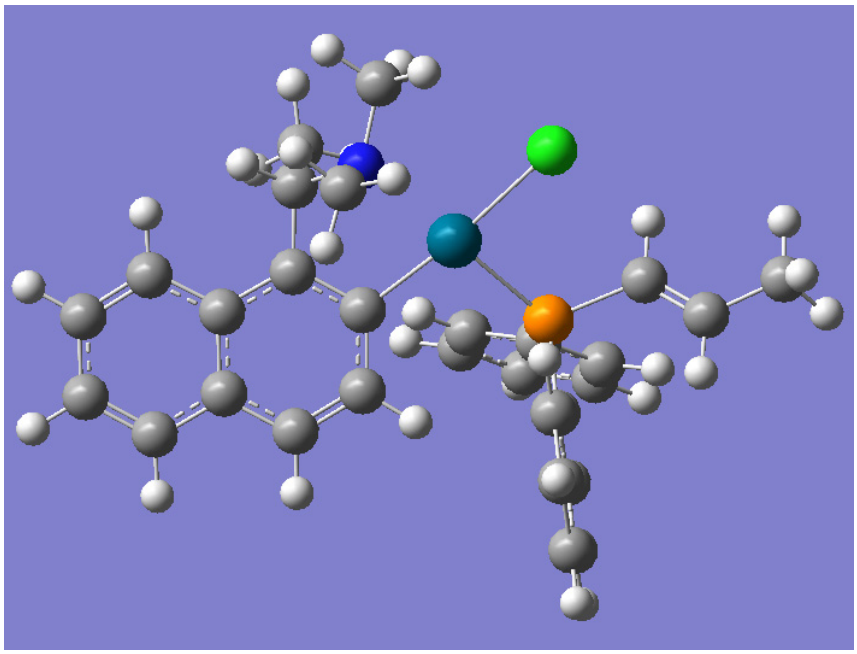
Transition state structure for TS-Ph-1

Imaginary frequencies: -922.5814 cm^{-1}
Gas phase energy: -4536.58084019 hartrees
Solvation (CH_2Cl_2) energy: -4536.60222339 hartrees
Gibbs free energy: -4535.881383 hartrees

Pd	0.12042600	-0.67149000	-0.04361900
As	-2.51506400	-0.74554100	-0.12935300
C	2.12750100	-0.99696800	0.13380200
C	2.90025300	-0.78268600	1.30191800
H	2.46532400	-0.31114100	2.17598500
C	4.22083800	-1.17151400	1.34656100
H	4.80431600	-1.01210400	2.25042700
C	4.84871400	-1.76919200	0.22412000
C	4.07568500	-2.01202700	-0.96078100
C	2.69221900	-1.63761500	-0.96183000
C	6.22000700	-2.14003300	0.25214500
H	6.79072400	-1.95155500	1.15809100
C	6.81893800	-2.72273000	-0.84085700
H	7.86831800	-3.00054600	-0.80864300
C	6.06369000	-2.96013100	-2.01369200
H	6.54087300	-3.41610700	-2.87660100
C	4.73074500	-2.61616400	-2.07279300
H	4.18345500	-2.79999300	-2.99185800
C	1.77674900	-1.95624900	-2.12413200

H	2.12363700	-2.84922900	-2.66286500
C	1.70433300	-0.79139400	-3.12213200
H	1.16857500	-1.05050000	-4.04044600
H	2.72392000	-0.51005200	-3.40206800
H	1.23015200	0.08358600	-2.66311000
C	0.51982500	-3.63129800	-0.84614100
H	-0.42836500	-3.84759300	-0.35139200
H	1.31763000	-3.60661300	-0.10507700
H	0.73139200	-4.42351300	-1.57882800
C	-0.61735000	-2.42244700	-2.57645700
H	-0.30653700	-3.13019200	-3.35914500
H	-0.81052700	-1.45049800	-3.02970600
H	-1.53707900	-2.79710100	-2.12187800
C	-0.66726100	1.18267800	2.80203400
C	-1.35865300	2.25344700	3.39331400
H	-1.42974900	3.20726900	2.87840300
C	-1.95739800	2.09786900	4.64450900
H	-2.49154700	2.93048400	5.09324500
C	-1.86595400	0.87793100	5.31953200
H	-2.33062400	0.76065900	6.29422400
C	-1.17656200	-0.18997600	4.74070700
H	-1.10309600	-1.13923000	5.26343300
C	-0.58415600	-0.04082900	3.48583200
H	-0.05694500	-0.87585100	3.03176500
C	1.71830400	2.23776400	1.42532600
C	2.56844900	2.45219600	0.32873100
H	2.31442600	2.05063200	-0.64690900
C	3.75221500	3.16896700	0.49011200
H	4.40167900	3.33334300	-0.36463200
C	4.10763900	3.66331700	1.74778900
H	5.03481000	4.21518000	1.87264200
C	3.27277500	3.44233900	2.84339300
H	3.54662600	3.81989700	3.82440000
C	2.07872600	2.73505000	2.68630500
H	1.43739700	2.57346500	3.54623400
C	-0.90248500	2.50334300	0.23455700
H	-1.97121900	2.40617300	0.44475900
C	-0.46369700	3.24518400	-0.94214200
H	-0.49472800	2.71748000	-1.89928300
C	-0.07267600	4.61052900	-0.97413700
C	-0.01463400	5.42108700	0.19525500
H	-0.26390800	4.98075600	1.15629800
C	0.36036800	6.75388100	0.11962600
H	0.39807800	7.35428200	1.02444600

C	0.69095900	7.33154300	-1.11447200
H	0.98282500	8.37609900	-1.16736100
C	0.64247100	6.55329100	-2.28005300
H	0.89713700	6.99659600	-3.23865700
C	0.26931800	5.21993700	-2.21614000
H	0.23068800	4.62145200	-3.12324900
C	-3.48236700	-0.23591600	-1.71752500
H	-3.25274400	-0.58003000	-2.71908700
C	-4.43525900	0.67960500	-1.43435200
C	-5.30848000	1.32957400	-2.47385900
H	-6.37030700	1.13351600	-2.27987800
H	-5.07354200	0.96225600	-3.47623200
H	-5.18329800	2.41966900	-2.47271500
C	-4.58538500	1.02697400	0.01181100
C	-5.64840800	1.99282800	0.46427700
H	-5.61945200	2.13257900	1.54803500
H	-6.65001600	1.63386100	0.19665300
H	-5.52683300	2.97472000	-0.01013800
C	-3.72567200	0.40616100	0.84736300
H	-3.70915100	0.53294900	1.92335100
C	-3.18991500	-2.52180900	0.33677400
C	-4.35196600	-3.04317600	-0.24598700
H	-4.89000200	-2.47000700	-0.99447100
C	-4.82322900	-4.29947400	0.13881800
H	-5.72314000	-4.69954000	-0.31978600
C	-4.14484700	-5.03826800	1.11121200
H	-4.51520500	-6.01491400	1.40891900
C	-2.99029700	-4.51917000	1.70013300
H	-2.46107400	-5.08757900	2.45982200
C	-2.51153500	-3.26560100	1.31156000
H	-1.61165600	-2.86642000	1.77320200
N	0.42532700	-2.31238900	-1.53096200
P	0.13587200	1.34659000	1.16289000

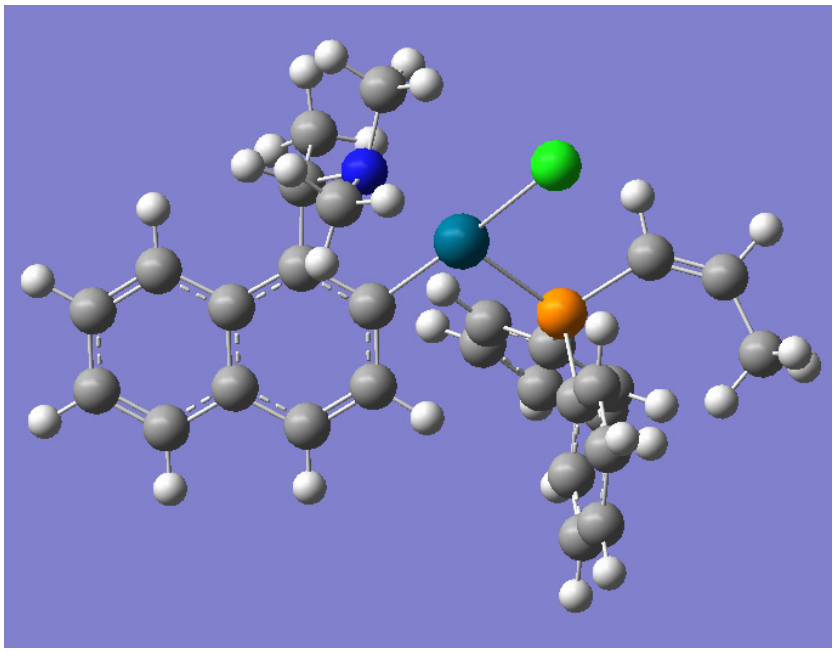


Optimized structure of *trans*-(+)-**11**

Gas phase energy: -2106.83566401 hartrees
Solvation (CH_2Cl_2) energy: -2106.86501579 hartrees
Gibbs free energy: -2106.373446 hartrees

Pd	0.00000000	0.00000000	0.00000000
Cl	2.45334555	0.00000000	0.00000000
N	-0.08557930	2.19667276	0.00000000
P	-0.02138420	-2.32967976	-0.15214540
C	-2.01645914	0.27967946	0.19274516
C	-2.97394177	-0.63622851	0.70822354
H	-2.67116371	-1.63779848	0.99063403
C	-4.29469553	-0.28368893	0.87143354
H	-5.00708119	-1.00366890	1.26988100
C	-4.75515872	1.01115969	0.52433684
C	-6.11845209	1.38183897	0.67263181
H	-6.81559619	0.64414555	1.06404476
C	-6.55504644	2.64091713	0.32922069
H	-7.60091955	2.91162918	0.44581353
C	-5.63347861	3.58632142	-0.17970843
H	-5.97824379	4.58004346	-0.45391468
C	-4.30363846	3.25858447	-0.33315299
H	-3.62520162	4.00440761	-0.73466807
C	-3.81217684	1.96530213	0.01360623
C	-2.44178354	1.56915332	-0.12775992
C	-1.39863369	2.52852872	-0.66480199
H	-1.63586944	3.56839871	-0.39372736

C	-1.32679599	2.43642656	-2.19786089
H	-0.95104836	1.45396230	-2.50379594
H	-0.69625424	3.21374421	-2.64005597
H	-2.33693155	2.55321991	-2.60242178
C	-0.11097649	2.63423786	1.41932750
H	0.80279736	2.29035284	1.90798097
H	-0.97589389	2.20405262	1.92413205
H	-0.16361690	3.73254626	1.47832217
C	1.05818638	2.86508858	-0.66174789
H	1.19769068	2.47444672	-1.66791128
H	1.96261595	2.64701846	-0.09612551
H	0.88640668	3.95232491	-0.70078260
C	3.53139881	-4.61365655	0.19842980
H	4.05565087	-4.13462377	-0.63389682
H	3.50426597	-5.69681636	0.01817050
H	4.12611814	-4.46042744	1.10889332
C	2.14640985	-4.06097550	0.37753862
H	1.55786430	-4.49980251	1.18237999
C	1.63045858	-3.06938780	-0.35891013
H	2.22459407	-2.59346793	-1.13517446
C	-0.69596232	-3.17169086	1.34246216
C	-0.29600201	-2.67599112	2.59552646
H	0.36660028	-1.81562873	2.64504216
C	-0.74813887	-3.27789200	3.76888960
H	-0.43043362	-2.88681731	4.73157318
C	-1.61538717	-4.37223303	3.70652202
H	-1.97446316	-4.83544265	4.62162943
C	-2.02341981	-4.86460020	2.46648897
H	-2.70124737	-5.71232478	2.41198203
C	-1.56475007	-4.27042905	1.28767710
H	-1.89054247	-4.66039024	0.32862296
C	-0.94692225	-3.00885438	-1.59989436
C	-0.67138903	-4.30193516	-2.07805523
H	0.09830517	-4.90016405	-1.60015596
C	-1.36630597	-4.81529322	-3.17339841
H	-1.14165147	-5.81609692	-3.53266552
C	-2.33863524	-4.04176491	-3.81144827
H	-2.87553926	-4.44003473	-4.66832615
C	-2.61038854	-2.75267566	-3.35119208
H	-3.35955458	-2.14210765	-3.84787666
C	-1.91786556	-2.23618886	-2.25422207
H	-2.12888375	-1.23175162	-1.90447039

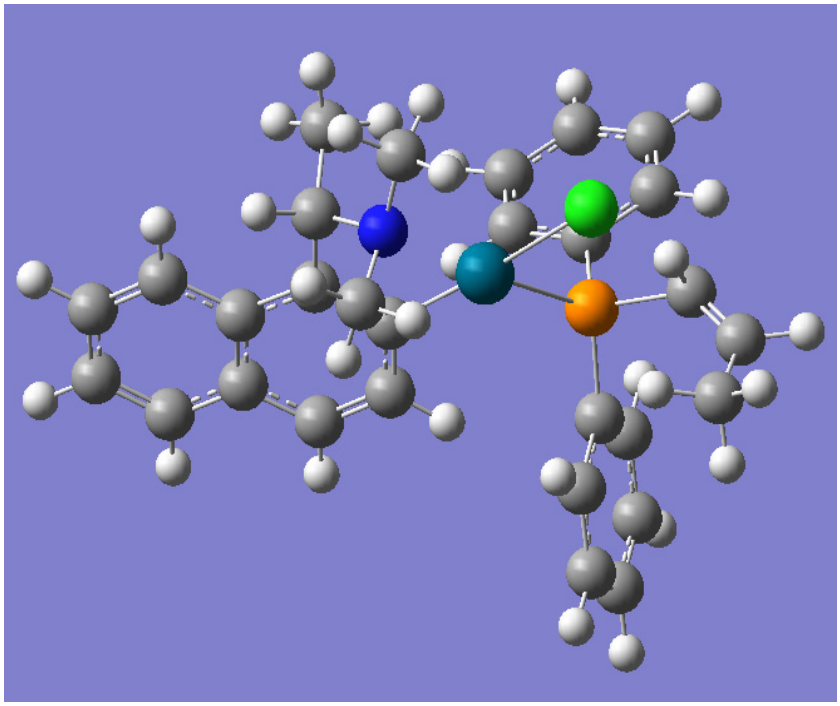


Optimized structure of *cis*-(+)-**11**

Gas phase energy: -2106.84313778 hartrees
Solvation (CH_2Cl_2) energy: -2106.85737766 hartrees
Gibbs free energy: -2106.382057 hartrees

Pd	0.00000000	0.00000000	0.00000000
Cl	2.46474751	0.00000000	0.00000000
N	-0.10654762	2.19201619	0.00000000
P	0.00957505	-2.32863742	-0.15582892
C	-1.98778075	0.25821130	0.34695048
C	-2.86214846	-0.66339654	0.98367328
H	-2.50860142	-1.65432513	1.24787011
C	-4.15774488	-0.32258344	1.29963040
H	-4.80857586	-1.04213011	1.79271390
C	-4.67172655	0.96305204	0.99235191
C	-6.01240362	1.32093128	1.29605780
H	-6.65111238	0.57955503	1.77126663
C	-6.49989934	2.57324802	0.99863694
H	-7.52781400	2.83390072	1.23562703
C	-5.65495975	3.52476528	0.38025761
H	-6.04038915	4.51300415	0.14291623
C	-4.34847380	3.20965199	0.07455897
H	-3.72922675	3.95931672	-0.40761883
C	-3.80634484	1.92398394	0.36875997
C	-2.45625058	1.54258134	0.07555529
C	-1.47561875	2.51365796	-0.55087900
H	-1.69911130	3.54998372	-0.25614375

C	-1.53686485	2.42825502	-2.08418276
H	-1.18547496	1.44907573	-2.42734708
H	-0.95146579	3.21113526	-2.57572809
H	-2.57914506	2.54207773	-2.39783338
C	-0.00950482	2.64054485	1.41304591
H	0.93932978	2.29248632	1.82581860
H	-0.83193360	2.22063283	1.99244716
H	-0.05085648	3.73953153	1.46790689
C	0.97884020	2.84938515	-0.76324078
H	1.01971359	2.46073253	-1.77960941
H	1.92826368	2.61819956	-0.28191711
H	0.81918128	3.93884944	-0.78700008
C	2.11191210	-5.19862976	0.10166775
H	1.22628918	-5.14234060	0.73493756
H	2.98937718	-5.27833235	0.75769908
H	2.07111223	-6.13255778	-0.47556049
C	2.26773471	-4.03026065	-0.82742119
H	3.14130993	-4.10193779	-1.47872765
C	1.53109546	-2.92052490	-0.98340513
H	1.86767311	-2.19061134	-1.71425661
C	-0.04311519	-3.06106821	1.53130512
C	0.98789468	-2.69217251	2.41505440
H	1.78070702	-2.03235812	2.07106032
C	0.98706032	-3.16362562	3.72636666
H	1.79052320	-2.87654749	4.39932388
C	-0.04408222	-3.99327574	4.17806228
H	-0.04372016	-4.35512649	5.20273611
C	-1.07635158	-4.34933383	3.31079564
H	-1.88472715	-4.98838415	3.65619125
C	-1.07909032	-3.88595991	1.99163813
H	-1.88649862	-4.17497446	1.32620719
C	-1.31852952	-3.13818153	-1.15234339
C	-1.36036889	-4.53712470	-1.29193499
H	-0.63426373	-5.15834612	-0.77734910
C	-2.32559519	-5.14070122	-2.09620649
H	-2.34857623	-6.22316593	-2.18987227
C	-3.25273435	-4.35579271	-2.78765430
H	-4.00145863	-4.82702612	-3.41882859
C	-3.20816230	-2.96716667	-2.67015763
H	-3.92168592	-2.34963474	-3.20878951
C	-2.24741812	-2.36042409	-1.85694753
H	-2.22038806	-1.28062337	-1.76196731

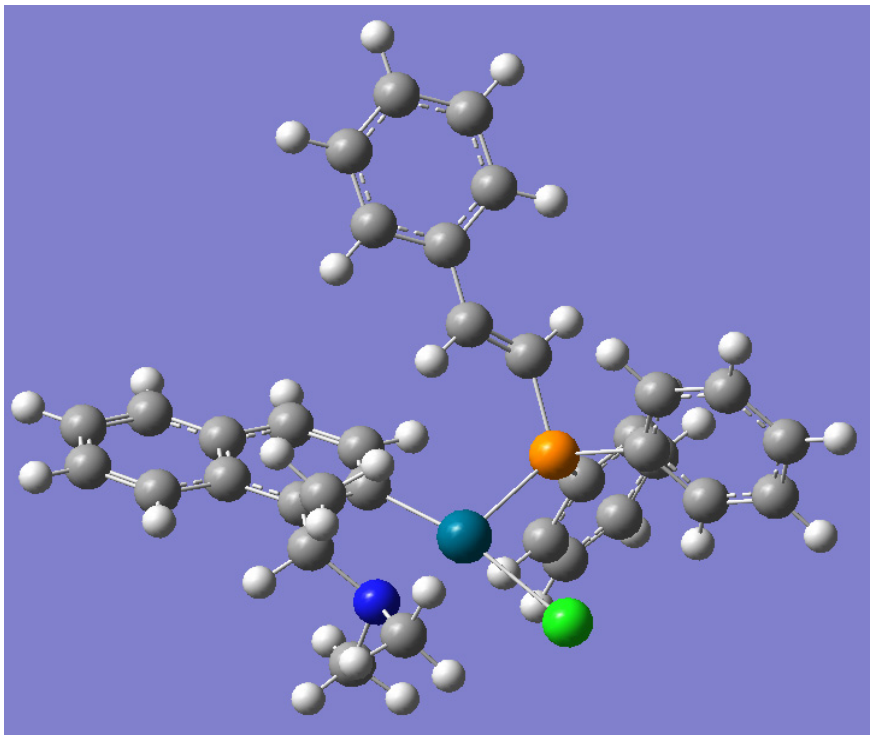


Transition state structure for TS-Me-2

Imaginary frequencies: -1027.4717 cm^{-1}
Gas phase energy: -2106.71375418 hartrees
Solvation (CH_2Cl_2) energy: -2106. 72776685 hartrees
Gibbs free energy: -2106.259998 hartrees

Pd	-0.01352300	-0.17227200	-0.07800400
Cl	2.45298200	-0.37754800	-0.53454800
N	0.02128300	2.04048300	-0.22920600
P	-0.09061300	-2.51619800	-0.10735100
C	-1.97051900	0.23623800	0.31550200
C	-2.91743500	-0.57670900	0.99489900
H	-2.63949700	-1.56860200	1.32766300
C	-4.19614600	-0.13379600	1.25155300
H	-4.90110700	-0.77673000	1.77519200
C	-4.62128100	1.15399900	0.84143000
C	-5.94090500	1.61705200	1.09164300
H	-6.63069000	0.95649300	1.61239300
C	-6.34457400	2.86838400	0.68615400
H	-7.35687000	3.21100700	0.88256100
C	-5.43319400	3.71095500	0.00665000
H	-5.75264300	4.69781000	-0.31830700
C	-4.14576400	3.29177600	-0.25001600
H	-3.47711900	3.96025800	-0.78239400
C	-3.68740300	2.00405900	0.15894600
C	-2.35934300	1.51823400	-0.07783800

C	-1.33394400	2.37276600	-0.79880100
H	-1.50389200	3.44315200	-0.60688500
C	-1.41370900	2.13851000	-2.31604800
H	-1.12278100	1.11139500	-2.56106200
H	-0.78962700	2.83488500	-2.88448900
H	-2.45065400	2.27995600	-2.63575600
C	0.14135600	2.59277400	1.14259700
H	1.07921600	2.24724200	1.58300500
H	-0.69169700	2.24858500	1.75513500
H	0.14014900	3.69399200	1.11498500
C	1.12347600	2.59652000	-1.04521500
H	1.16471100	2.10774000	-2.01692200
H	2.06777100	2.40406100	-0.53634600
H	0.99049200	3.68211400	-1.17812000
C	2.79495300	-2.87637200	2.05967100
H	2.38768900	-1.86280700	2.06739200
H	3.88113300	-2.85045300	2.21021900
H	2.36742300	-3.43520200	2.90803400
C	2.41940700	-3.62824400	0.81497800
H	3.07418700	-4.50065900	0.64517100
C	1.48754900	-3.32738900	-0.15003200
H	2.18378500	-2.31958500	-0.25235000
C	-0.94628600	-3.41822100	1.25769800
C	-0.80930300	-2.94619700	2.57387800
H	-0.27702500	-2.01627900	2.75751300
C	-1.37289300	-3.64793500	3.63913400
H	-1.26818400	-3.26766100	4.65186600
C	-2.08004300	-4.83030500	3.40240800
H	-2.52212400	-5.37576100	4.23190900
C	-2.22206400	-5.30427000	2.09754500
H	-2.77314500	-6.22161700	1.90780100
C	-1.65971100	-4.60279400	1.02808800
H	-1.77520000	-4.97608700	0.01559400
C	-0.95327500	-3.07334700	-1.64799200
C	-0.36389800	-4.03289500	-2.48151000
H	0.60845900	-4.42764600	-2.20076200
C	-1.01644600	-4.45164700	-3.64359400
H	-0.54808600	-5.19307000	-4.28617200
C	-2.26175100	-3.91972900	-3.98111900
H	-2.76783500	-4.24519900	-4.88650600
C	-2.85311000	-2.96041500	-3.15433600
H	-3.82032500	-2.53762800	-3.41375300
C	-2.20134200	-2.53223200	-1.99775000
H	-2.66270300	-1.77443100	-1.37238000



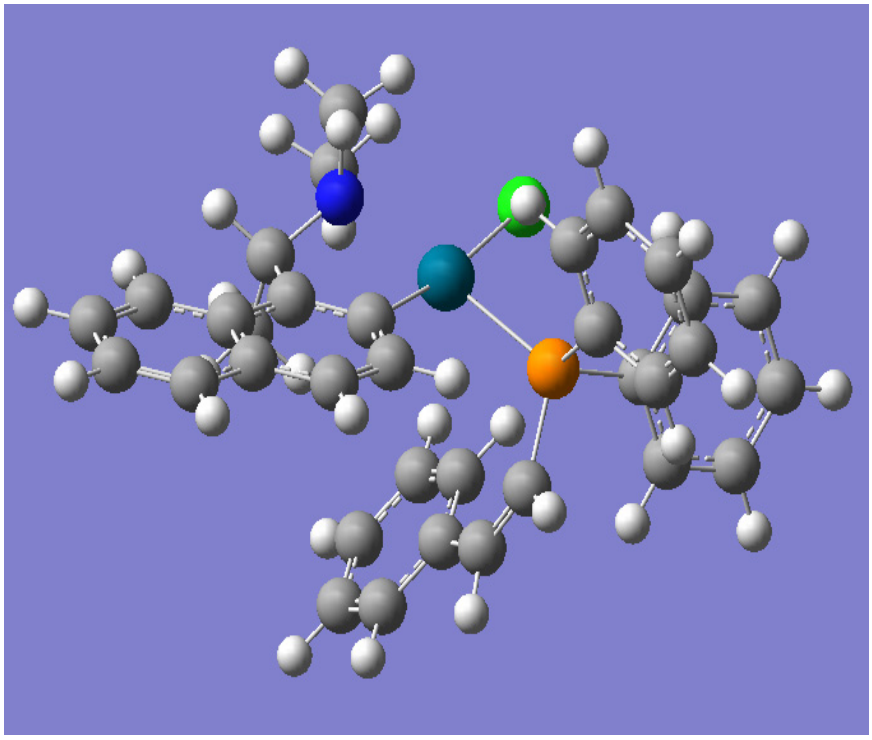
Optimized structure of *trans*-(+)-**12**

Gas phase energy: -2298.57788142 hartrees
Solvation (CH_2Cl_2) energy: -2298.60385457 hartrees
Gibbs free energy: -2298.069634 hartrees

C	1.45567200	-0.65106400	0.39150000
C	1.56187700	0.23280500	1.50088900
H	0.66549300	0.61323500	1.97917300
C	2.78691700	0.62031400	1.99447500
H	2.84523900	1.29487000	2.84647300
C	3.99239300	0.15917400	1.40570600
C	5.26245100	0.57157700	1.89001500
H	5.29665200	1.26100200	2.73078300
C	6.42653100	0.11547700	1.31424300
H	7.39168600	0.43956000	1.69393300
C	6.36261400	-0.78079200	0.22145800
H	7.28164100	-1.13974300	-0.23468600
C	5.14600200	-1.20163000	-0.27108000
H	5.13157100	-1.88231500	-1.11633800
C	3.91850500	-0.75233400	0.29892200
C	2.62619400	-1.15495400	-0.17279000
C	2.46935900	-2.13904300	-1.31513000
H	3.30907800	-2.84939800	-1.34599200
C	2.42074700	-1.40003700	-2.66216500

H	1.52042100	-0.77959500	-2.72880700
H	2.44998100	-2.07953500	-3.51934200
H	3.29166300	-0.74041200	-2.72789600
C	1.48076200	-3.92177600	0.04998700
H	0.54100800	-4.41433500	0.30713700
H	1.86757500	-3.39755500	0.92437600
H	2.21382400	-4.67713600	-0.27310200
C	0.77708500	-3.71267400	-2.23508200
H	1.59159400	-4.35719900	-2.60140700
H	0.46142800	-3.03215400	-3.02428600
H	-0.08461600	-4.31698700	-1.95452300
C	-1.11880800	1.93695300	0.09142700
H	-1.75233700	2.69175900	0.55612200
C	0.00462100	2.29017700	-0.55697300
H	0.62426400	1.49689700	-0.97136800
C	0.52937400	3.65054500	-0.74423600
C	1.85189100	3.80228900	-1.19775400
H	2.44755400	2.91489400	-1.39718100
C	2.40901400	5.06760400	-1.37646800
H	3.43511700	5.16179400	-1.72124000
C	1.64894300	6.20854300	-1.11433000
H	2.07822900	7.19649300	-1.25698300
C	0.32821000	6.07418600	-0.67370900
H	-0.27190500	6.95868100	-0.47735300
C	-0.22632200	4.81069900	-0.49181600
H	-1.25882300	4.72321000	-0.16567500
C	-3.25835600	0.30641900	-0.79944500
C	-3.29222500	1.10752900	-1.94963100
H	-2.42615800	1.70160500	-2.22486500
C	-4.43909700	1.15342000	-2.74424100
H	-4.45295000	1.77981000	-3.63231700
C	-5.56191500	0.40148100	-2.39676700
H	-6.45553100	0.43852000	-3.01424800
C	-5.53176700	-0.40262800	-1.25522100
H	-6.39843800	-0.99957500	-0.98487200
C	-4.38618600	-0.45707900	-0.46272800
H	-4.36529700	-1.10235000	0.40814200
C	-2.34919100	0.13047400	1.95309300
C	-3.28092300	1.06070300	2.44425400
H	-3.67982200	1.83173300	1.79045600
C	-3.72022500	0.98873700	3.76507400
H	-4.44171900	1.71278500	4.13411700
C	-3.23953600	-0.01634100	4.60959900
H	-3.58508600	-0.07263700	5.63839300

C	-2.32288700	-0.95050900	4.12716000
H	-1.95345500	-1.73967200	4.77618000
C	-1.87904100	-0.87851900	2.80448700
H	-1.17315400	-1.61060700	2.42291100
Cl	-2.13855000	-2.96517000	-0.86401500
N	1.22455100	-2.95229900	-1.04542400
P	-1.72521000	0.22211200	0.22269000
Pd	-0.25215600	-1.49786300	-0.32230800



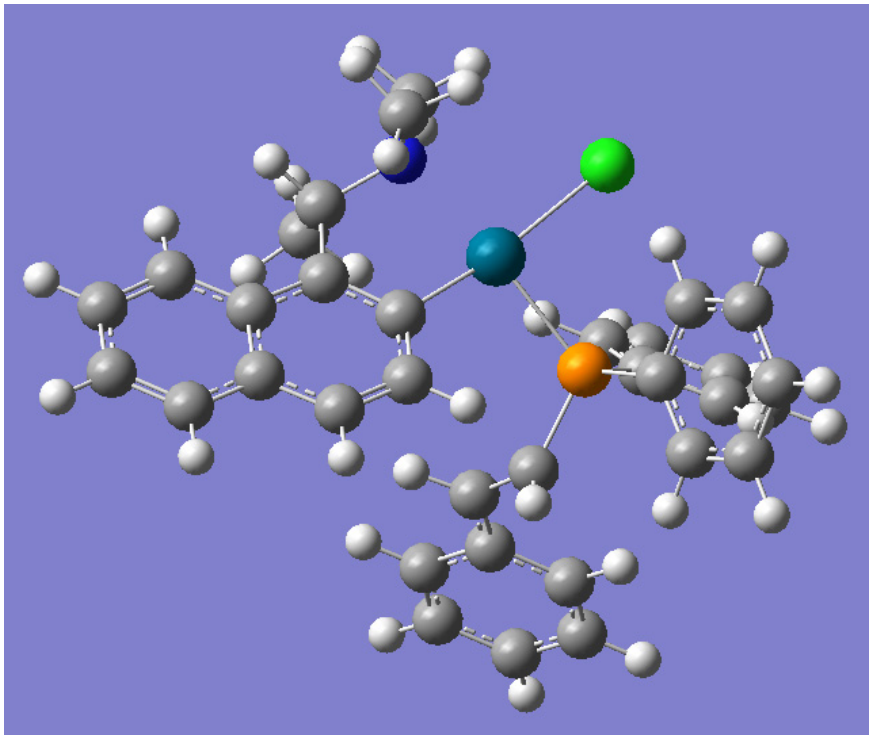
Optimized structure of *cis*-(+)-**12**

Gas phase energy: -2298.57075849 hartrees
Solvation (CH_2Cl_2) energy: -2298.59561611 hartrees
Gibbs free energy: -2298.060346 hartrees

C	1.57015100	0.65132200	0.01199900
C	1.52805800	1.68303400	-0.96575000
H	0.57792400	2.09944200	-1.27726100
C	2.67394700	2.19559500	-1.52963400
H	2.61054700	2.98921200	-2.27187800
C	3.95203600	1.70731800	-1.16029200
C	5.14261200	2.22207400	-1.73925000
H	5.05701300	3.01105500	-2.48338800
C	6.37831700	1.73857300	-1.37425100
H	7.28177400	2.14009200	-1.82519800
C	6.46855800	0.71103100	-0.40596200
H	7.44377900	0.32629800	-0.11872600
C	5.33173100	0.19186000	0.17524800
H	5.43742200	-0.60156300	0.90775900
C	4.03347800	0.66891800	-0.17330300
C	2.81906100	0.16865400	0.40283600
C	2.84860900	-0.94594800	1.42862600
H	3.74845500	-0.88376000	2.05935300
C	2.84973600	-2.31373600	0.72674500
H	1.90738800	-2.47903900	0.19543800

H	3.02255600	-3.14287400	1.41988600
H	3.65666500	-2.32237900	-0.01220200
C	1.91982900	0.38794400	3.26048700
H	1.01469400	0.58233600	3.83940100
H	2.17694900	1.27317000	2.67864100
H	2.74743600	0.15295600	3.94781500
C	1.41911600	-1.95522600	3.18547200
H	2.33154700	-2.21967300	3.74286300
H	1.10759700	-2.79434200	2.56633100
H	0.60684700	-1.73462700	3.87619700
C	-1.25739900	0.21562300	-2.19917600
H	-1.38260500	1.08562300	-2.84097700
C	-0.76731600	-0.89645000	-2.78666200
H	-0.53314000	-0.78896000	-3.84712800
C	-0.45896300	-2.23536900	-2.26999200
C	0.37536400	-3.05338000	-3.05902100
H	0.75365300	-2.66659600	-4.00253900
C	0.73232500	-4.33446000	-2.64787700
H	1.38264200	-4.94108800	-3.27226100
C	0.24664200	-4.83812700	-1.43813200
H	0.51496600	-5.84098600	-1.11673100
C	-0.59672400	-4.05035600	-0.65141700
H	-0.99263300	-4.43296900	0.28492200
C	-0.94978400	-2.76411500	-1.05952000
H	-1.63017000	-2.20060600	-0.43346900
C	-3.39210100	-0.07046900	-0.25098600
C	-4.02456500	-0.83696200	-1.23873500
H	-3.48678400	-1.11709800	-2.13836300
C	-5.35249400	-1.24128200	-1.07607800
H	-5.82975200	-1.83772900	-1.84914400
C	-6.05962800	-0.87788700	0.06901400
H	-7.09263200	-1.19133200	0.19500100
C	-5.43462500	-0.11077000	1.05605400
H	-5.97661400	0.16893400	1.95514900
C	-4.10861300	0.28676600	0.90300700
H	-3.62558200	0.85863300	1.68684800
C	-1.92387000	2.36564800	-0.42168500
C	-2.78363800	2.98350800	-1.34524900
H	-3.29598100	2.38851900	-2.09671000
C	-3.00470800	4.35891000	-1.29282700
H	-3.67057100	4.82612500	-2.01341600
C	-2.38063900	5.13198300	-0.30958000
H	-2.55746700	6.20337600	-0.26709800
C	-1.53562700	4.52476100	0.61946700

H	-1.05064900	5.12000400	1.38828500
C	-1.30639400	3.14784400	0.56344400
H	-0.64137300	2.67348500	1.27966700
Cl	-1.66305600	-1.12261100	2.57173600
N	1.66833300	-0.75832500	2.34919900
P	-1.65639800	0.53826300	-0.44675500
Pd	0.00240900	-0.15838900	1.05083100



Transition state structure for TS-Ph-2

Imaginary frequencies: -808.3883 cm^{-1}
Gas phase energy: -2298.49779319 hartrees
Solvation (CH_2Cl_2) energy: -2298.4898498 hartrees
Gibbs free energy: -2297.995251 hartrees

C	1.67985100	-0.77123900	0.54040500
C	1.81208100	0.15548300	1.61013600
H	0.92646800	0.53603000	2.10787600
C	3.04930900	0.56128400	2.05865500
H	3.12959700	1.26708600	2.88324400
C	4.23920300	0.07004800	1.46337100
C	5.52133800	0.50034900	1.89807900
H	5.57715000	1.23270600	2.70050000
C	6.67039200	0.00790900	1.32247900
H	7.64494600	0.34656400	1.66331300
C	6.57900300	-0.94535700	0.28083700
H	7.48654500	-1.33276400	-0.17495100
C	5.35044200	-1.38541500	-0.16248500
H	5.31400500	-2.11021300	-0.96971300
C	4.13775700	-0.89796200	0.40749700
C	2.83454800	-1.31678700	-0.01571100
C	2.64510100	-2.37702200	-1.08328500
H	3.47660200	-3.09795300	-1.07770400
C	2.57663900	-1.73424400	-2.47742500

H	1.68522400	-1.10340100	-2.56322000
H	2.57457300	-2.47210200	-3.28549600
H	3.45505800	-1.09491200	-2.60938000
C	1.65158100	-4.02835100	0.43905400
H	0.70834500	-4.48463000	0.74623200
H	2.05278900	-3.43910000	1.26369800
H	2.37045200	-4.81943900	0.17460700
C	0.92218300	-4.00312700	-1.84583900
H	1.71904100	-4.69505100	-2.16106600
H	0.61192700	-3.38978000	-2.69016800
H	0.05111500	-4.56277800	-1.50659300
C	-0.63097200	1.82672100	0.29004700
H	-0.39451100	2.24483100	1.27070300
C	0.06197300	2.35821000	-0.87921900
H	1.08027900	1.99660300	-1.04362900
C	-0.43319100	3.33404000	-1.78426300
C	0.38970000	3.78846200	-2.85561300
H	1.38633200	3.36720600	-2.96416400
C	-0.05976400	4.75084800	-3.74650000
H	0.58762400	5.08097100	-4.55485900
C	-1.34272900	5.30012600	-3.60911700
H	-1.69257800	6.05404600	-4.30863600
C	-2.17084200	4.86854700	-2.56339800
H	-3.16738300	5.28868300	-2.45432600
C	-1.73177800	3.90688900	-1.66550900
H	-2.38286100	3.57175000	-0.86413300
C	-2.74217300	0.39631900	-1.01206100
C	-2.41397000	0.11308100	-2.34472200
H	-1.43301700	-0.28375600	-2.58544100
C	-3.35169500	0.31447100	-3.35644500
H	-3.08803600	0.08959700	-4.38617300
C	-4.62941500	0.78403000	-3.04560000
H	-5.36277700	0.92990600	-3.83419700
C	-4.96584200	1.05489900	-1.71853100
H	-5.96253500	1.40880100	-1.46851500
C	-4.02600200	0.86632400	-0.70357900
H	-4.30024400	1.07328500	0.32609500
C	-2.32883400	0.14170400	1.90138200
C	-2.67739400	1.30324500	2.61097800
H	-2.44318600	2.28359400	2.20685000
C	-3.33735200	1.21015900	3.83767800
H	-3.59856400	2.11583600	4.37852500
C	-3.66233200	-0.04143600	4.36368900
H	-4.17550600	-0.11317200	5.31900300

C	-3.32998700	-1.19964600	3.65781800
H	-3.58712700	-2.17600200	4.05925200
C	-2.66395300	-1.11424600	2.43456300
H	-2.41862400	-2.01449700	1.87826600
Cl	-2.00796700	-3.00734400	-0.62201300
N	1.39601900	-3.15133300	-0.73190400
P	-1.45105500	0.20746300	0.28826700
Pd	-0.04966400	-1.61146500	-0.11347900