Electronic Supplementary Material (ESI) for Dalton Transactions

Coordination of a DiPhosphine-Phosphine Oxide to Au, Ag and Rh: When Polyfunctionality Rhymes with Versatility

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SUPPLEMENTARY INFORMATION

Contents

NMR spectra

Figure 1. Room temperature ^{31}P NMR spectrum of (DPPO)AuCl complex **3** in C_6D_6 (121.49 MHz).

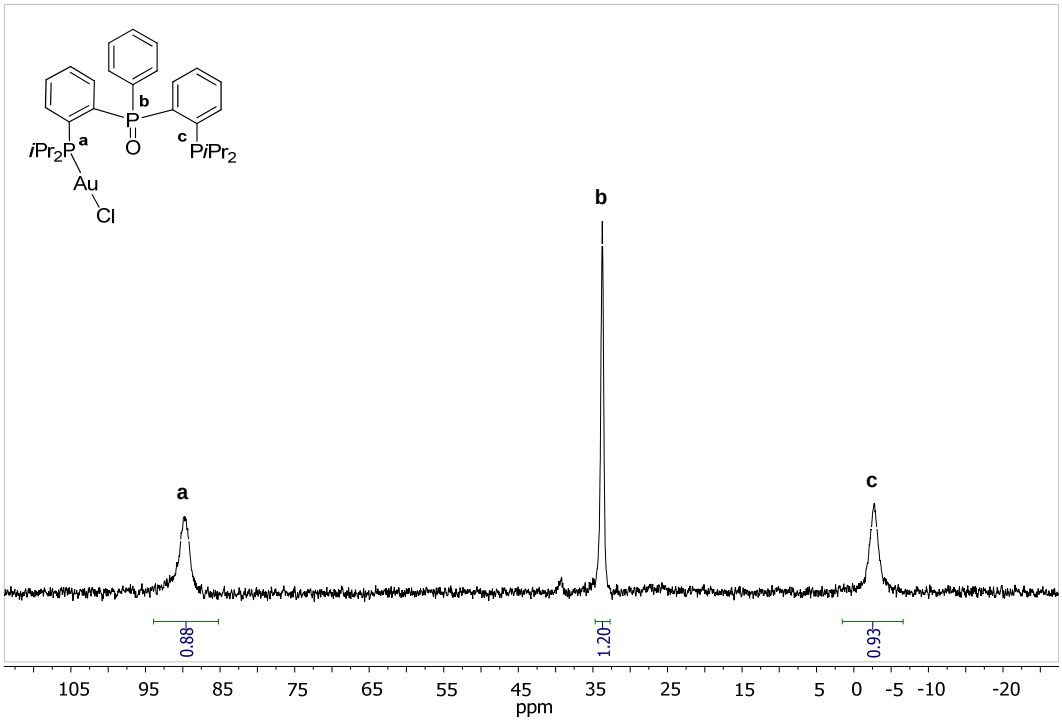


Figure 2. ^{31}P NMR spectrum of (DPPO)AuCl complex **3** at 60ºC in C_6D_6 (121.49 MHz).

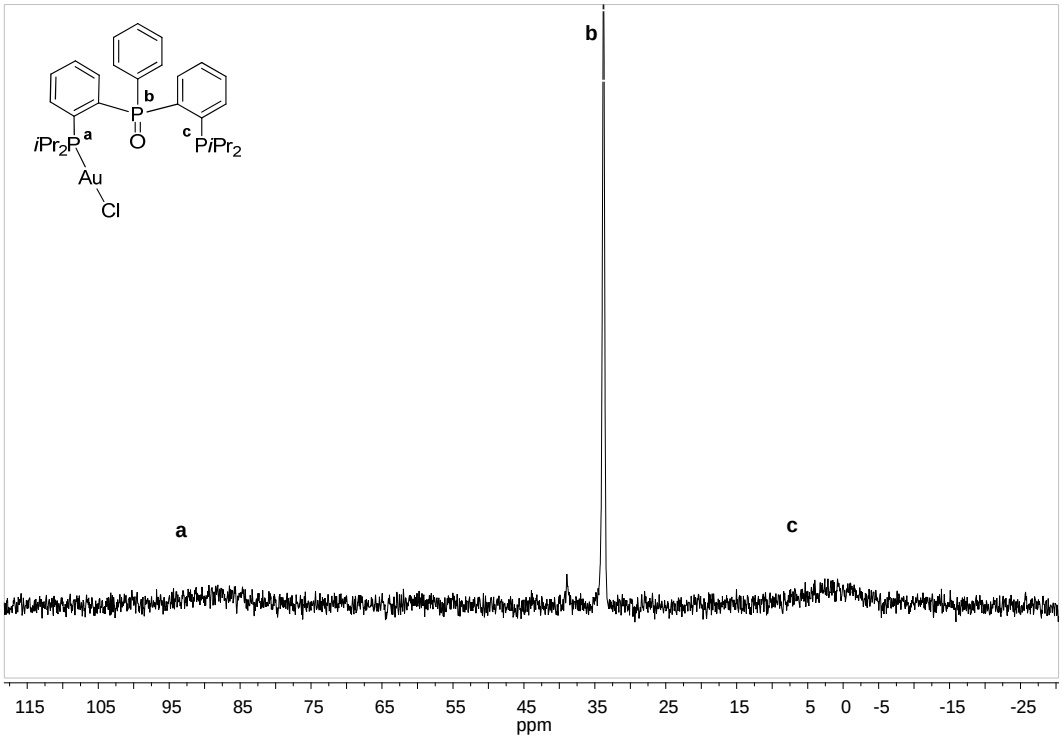


Figure 3. Room temperature ^{1}H NMR spectrum of (DPPO)AuCl complex **3** in C_6D_6 (300.18 MHz).

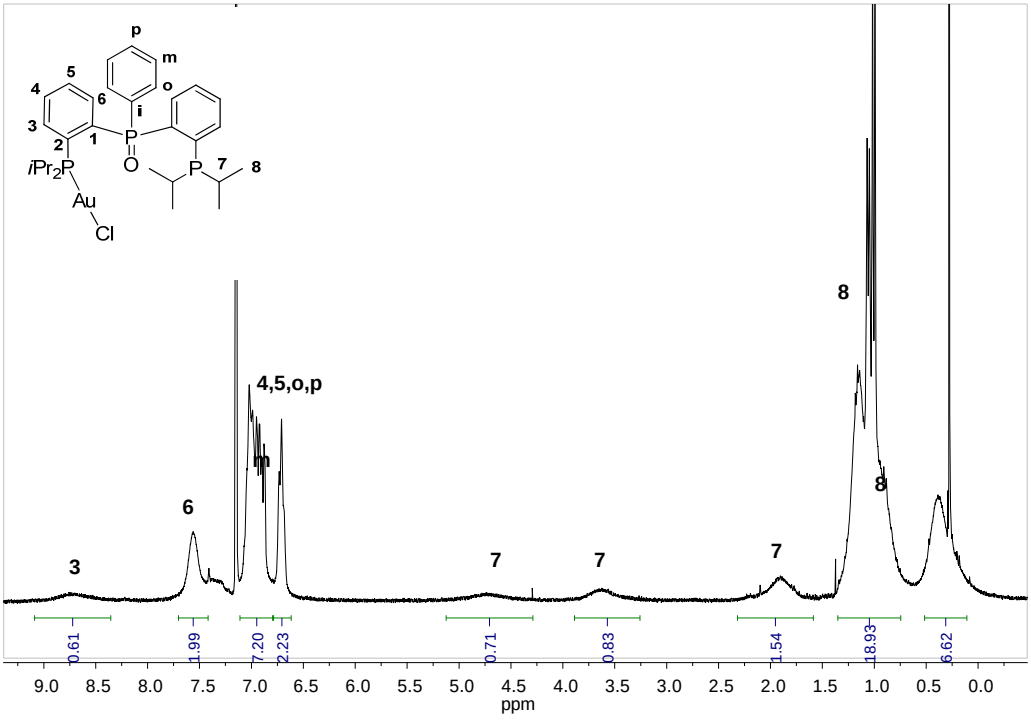


Figure 4. ^{1}H NMR spectrum of (DPPO)AuCl complex **3** at 60ºC in C_6D_6 (300.18 MHz).

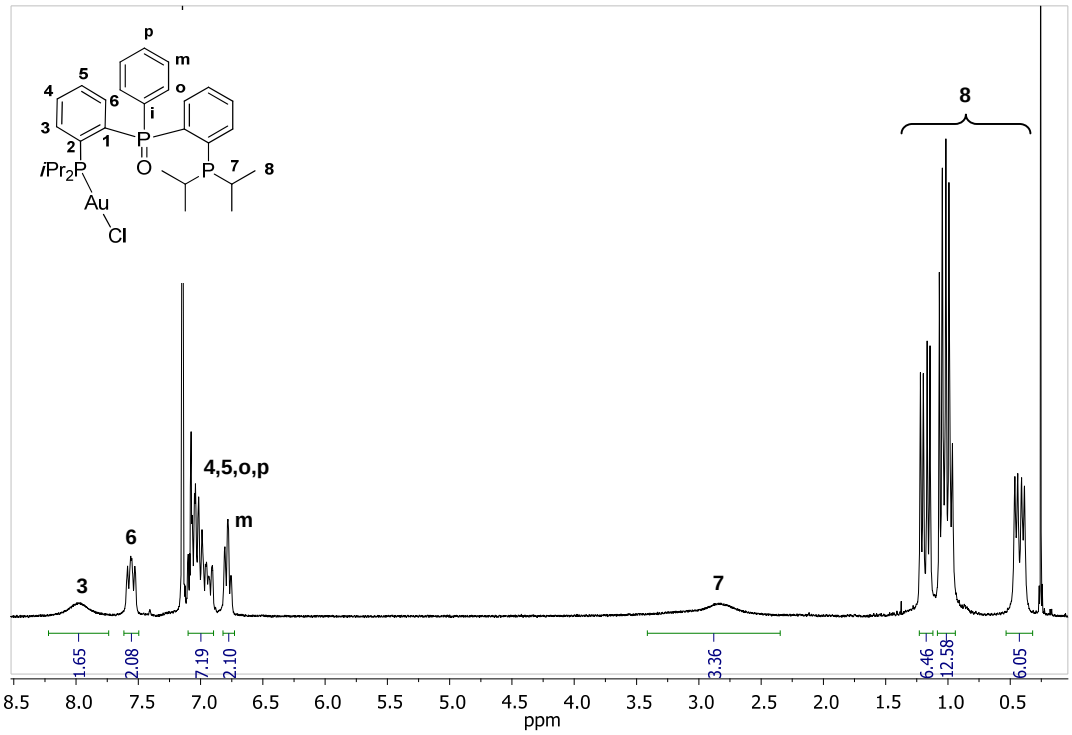


Figure 5. Room temperature ^{1}H NMR spectrum of [(DPPO)Au]OTf complex **4** in $CDCl_3$ (500.33 MHz).

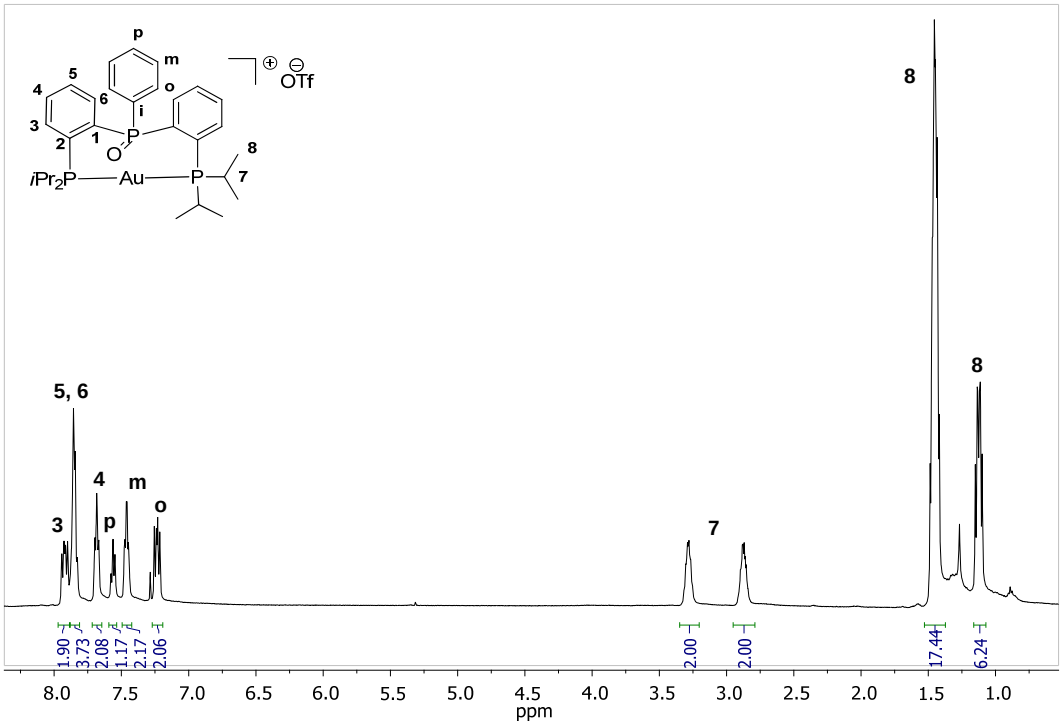


Figure 6. Room temperature ^{31}P NMR spectrum of [(DPPO)Au]OTf complex **4** in $CDCl_3$ (202.54 MHz).

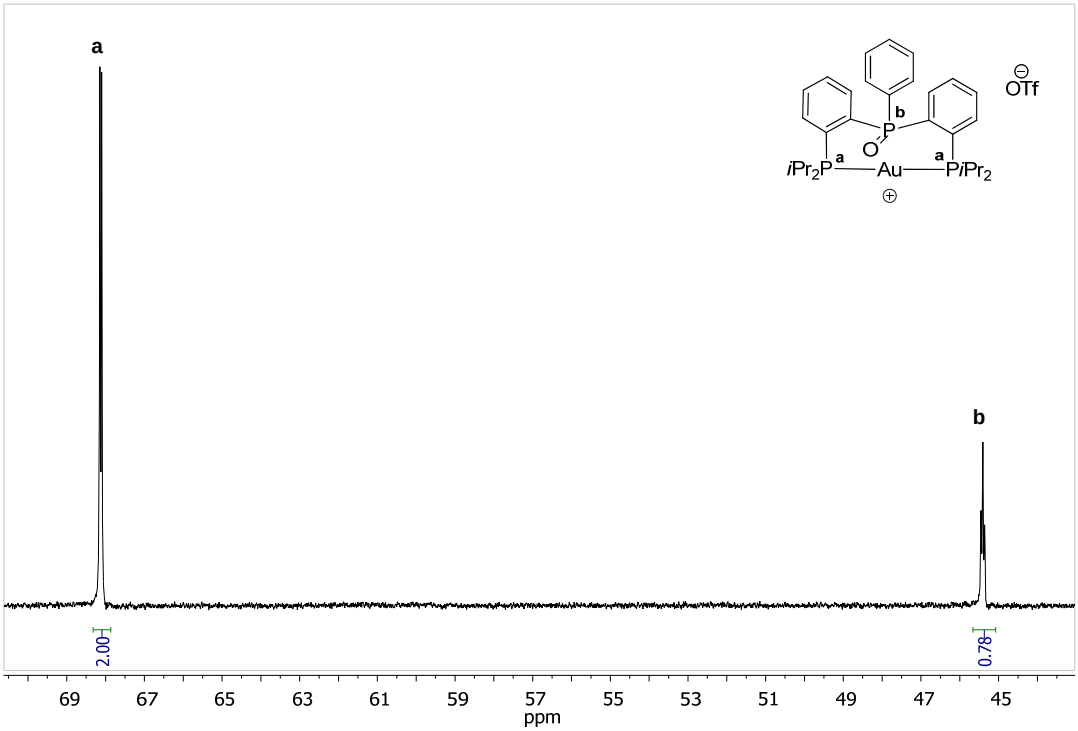


Figure 7. Room temperature ^{13}C NMR spectrum of [(DPPO)Au]OTf complex **4** in $CDCl_3$ (125.81 MHz).

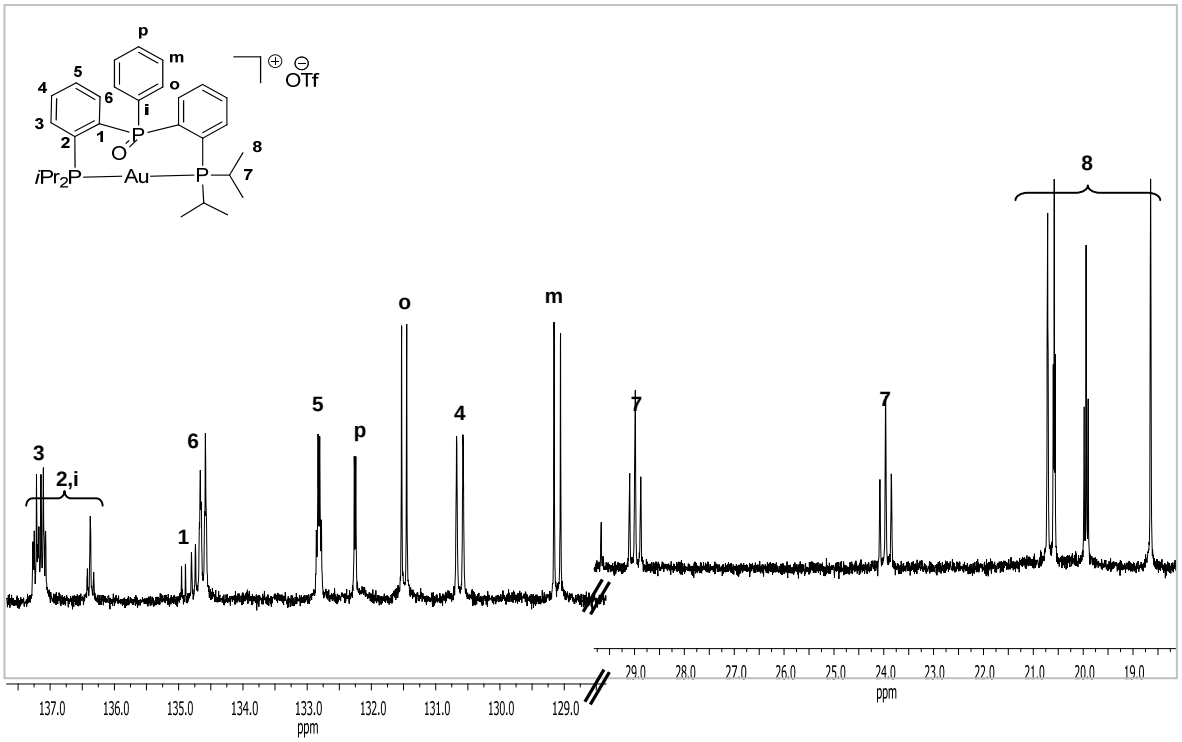


Figure 8. Room temperature ^{1}H NMR spectrum of (DPPO)AgCl complex **5** in $CDCl_3$ (300.18 MHz).

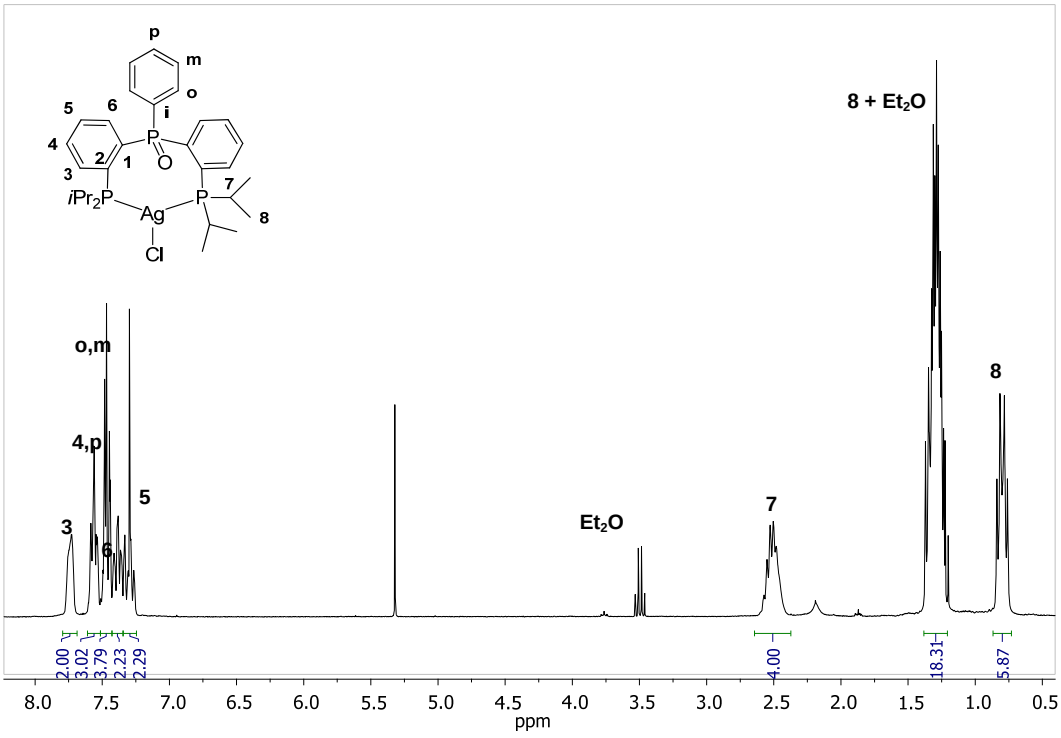


Figure 9. Room temperature ^{31}P NMR spectrum of (DPPO)AgCl complex **5** in $CDCl_3$ (121.49 MHz).

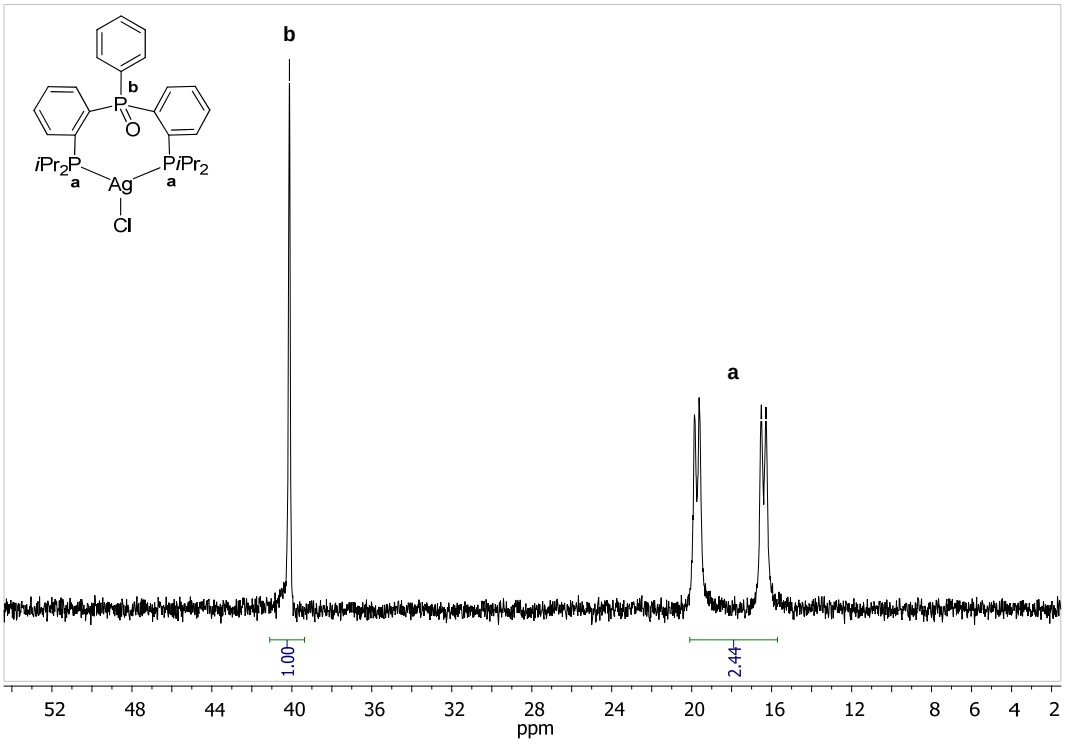


Figure 10. Room temperature ^{13}C NMR spectrum of (DPPO)AgCl complex **5** in $CDCl_3$ (75.47 MHz).

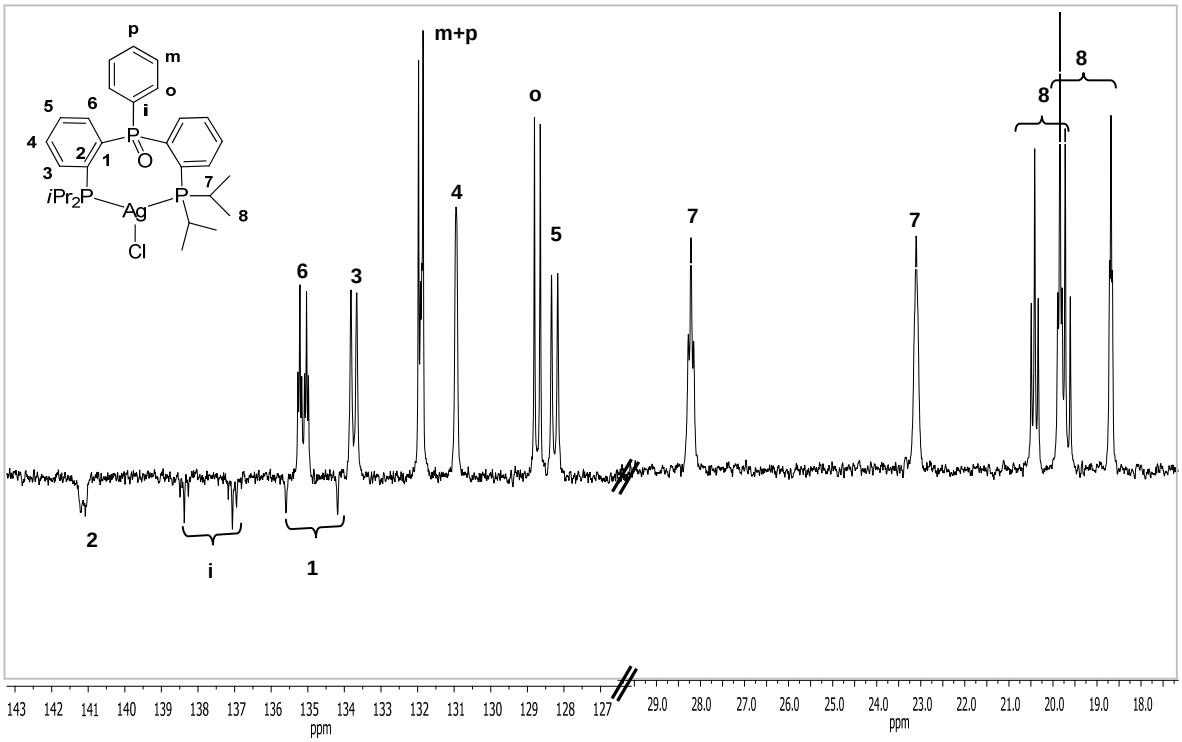


Figure 11. Room temperature ^{1}H NMR spectrum of (DPPO)Rh(nbd)Cl complex **6** in $CDCl_3$ (300.18 MHz).

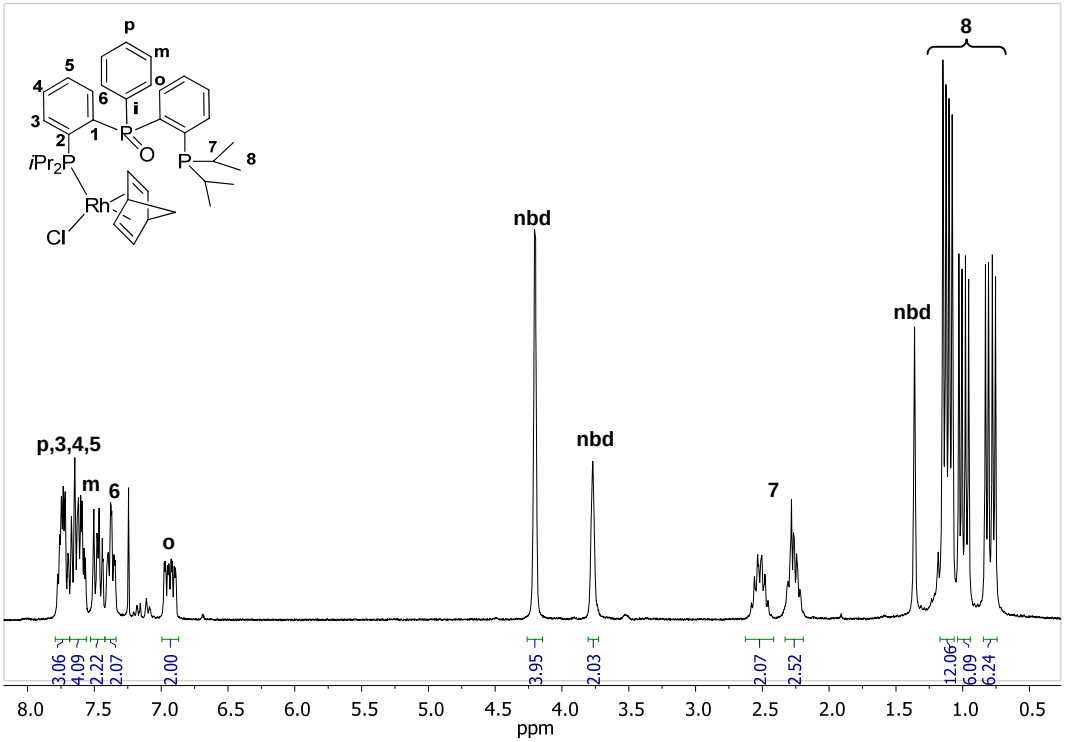


Figure 12. Room temperature ^{31}P NMR spectrum of (DPPO)Rh(nbd)Cl complex **6** in $CDCl_3$ (121.49 MHz).

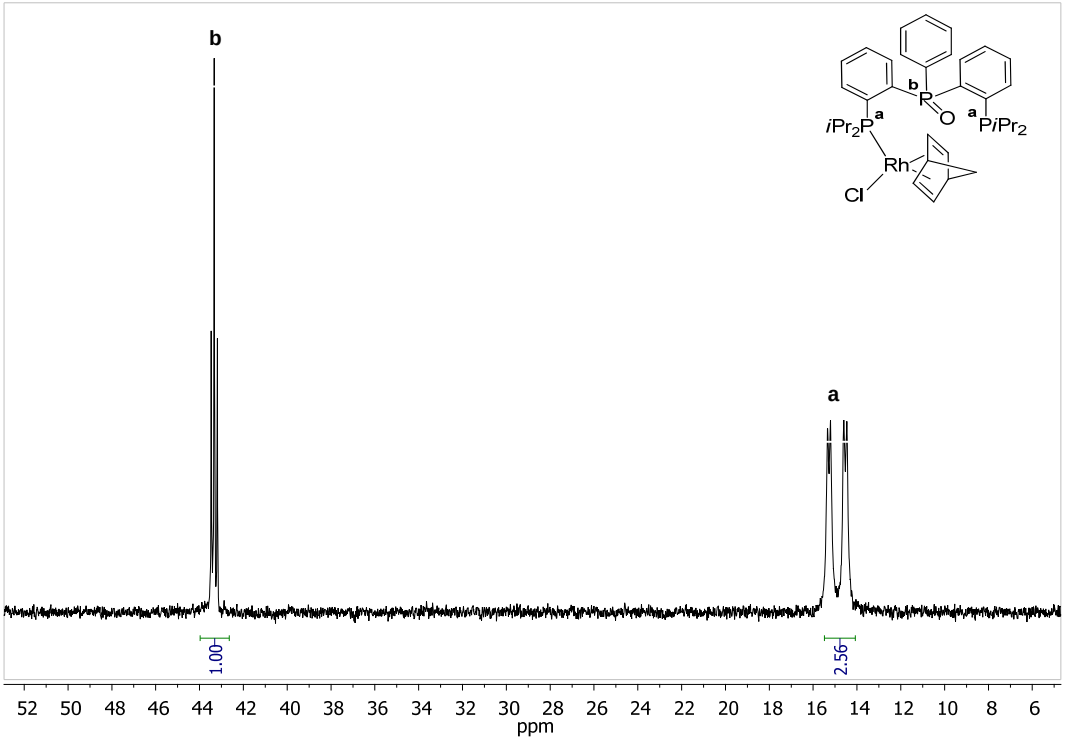


Figure 13. Room temperature ^{1}H NMR spectrum of [(DPPO)Rh(CO)]Cl complex **7** in $CDCl_3$ (500.33 MHz).

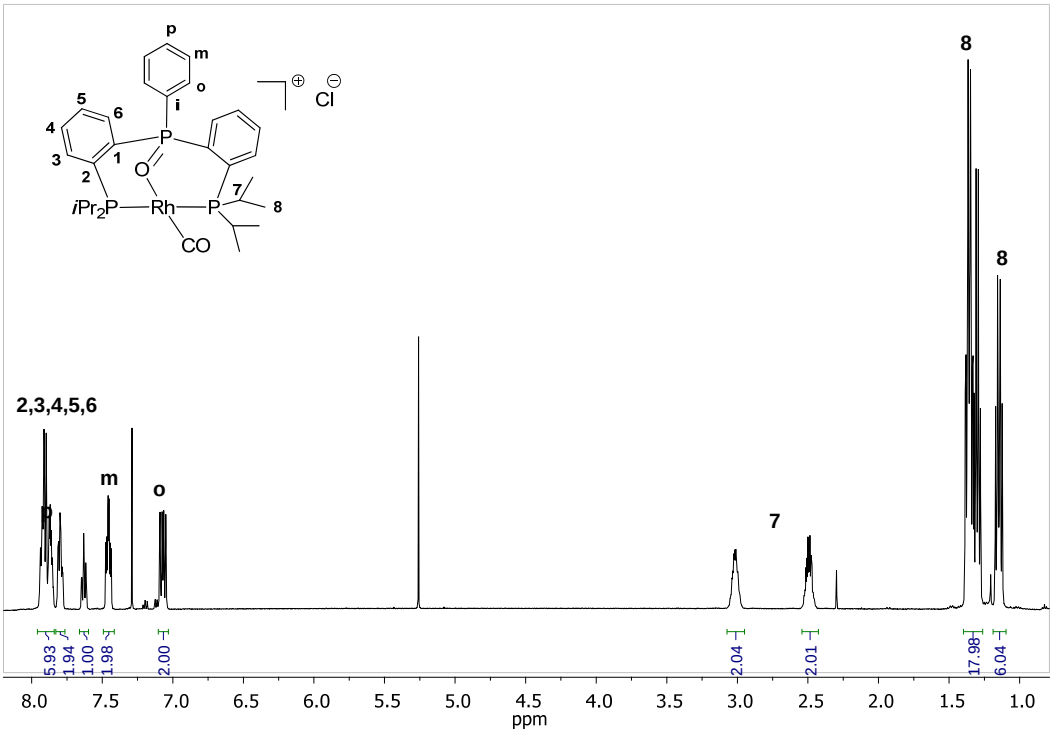


Figure 14. Room temperature ^{31}P NMR spectrum of [(DPPO)Rh(CO)]Cl complex **7** in $CDCl_3$ (202.54 MHz).

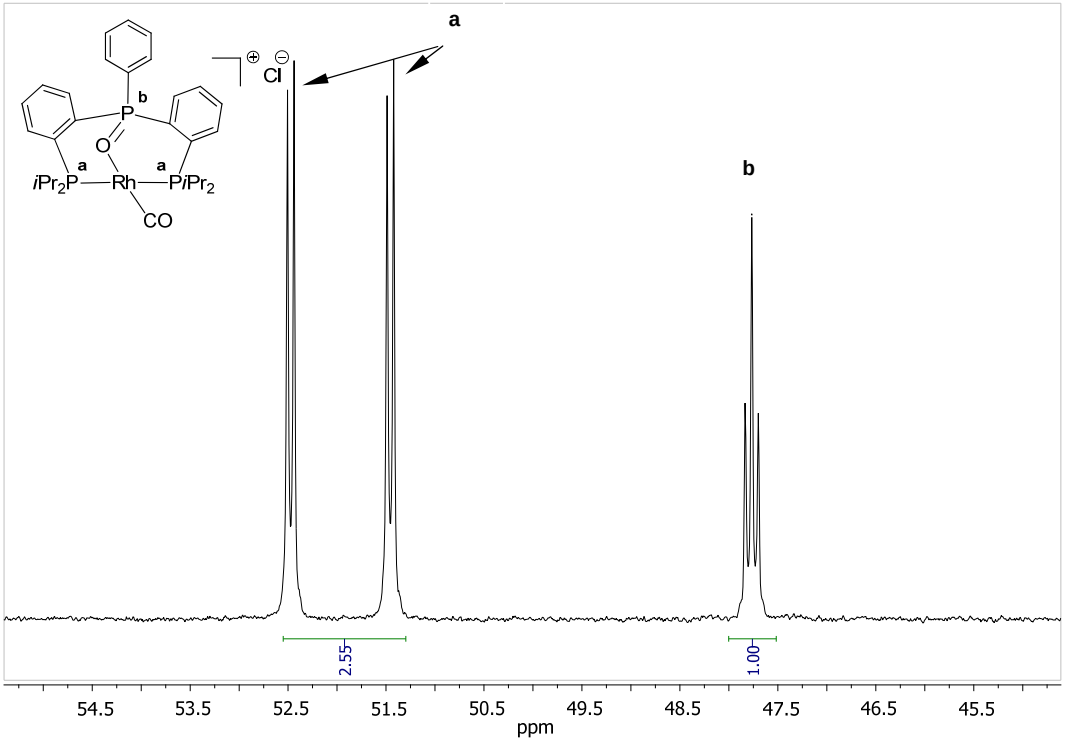


Figure 15. Room temperature ^{13}C NMR spectrum of [(DPPO)Rh(CO)]Cl complex **7** in $CDCl_3$ (125.81 MHz).

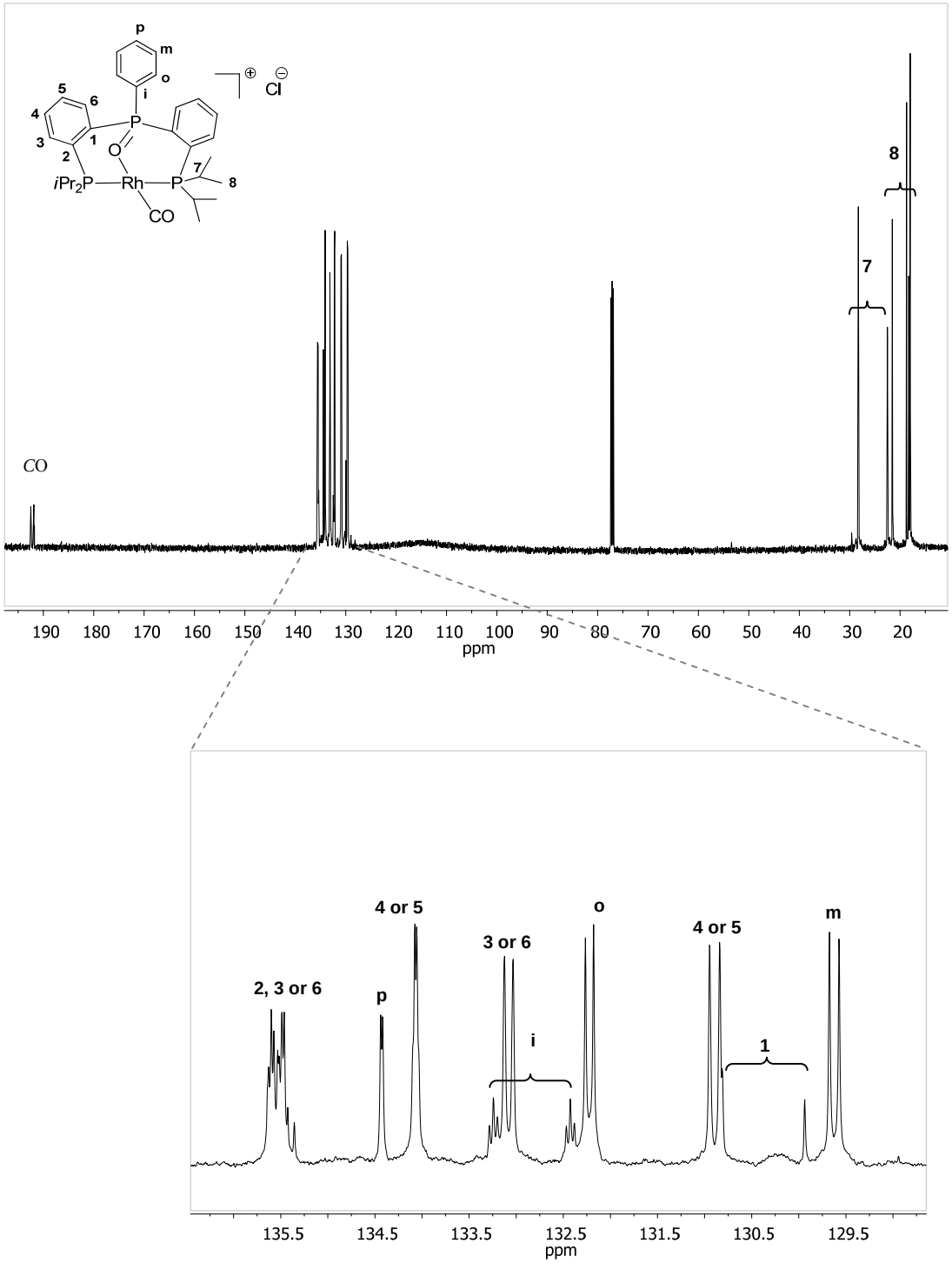


Figure 16. Room temperature ^{1}H NMR spectrum of [(DPPO)Rh(CO)]OTf complex **8** in $CDCl_3$ (300.18 MHz).

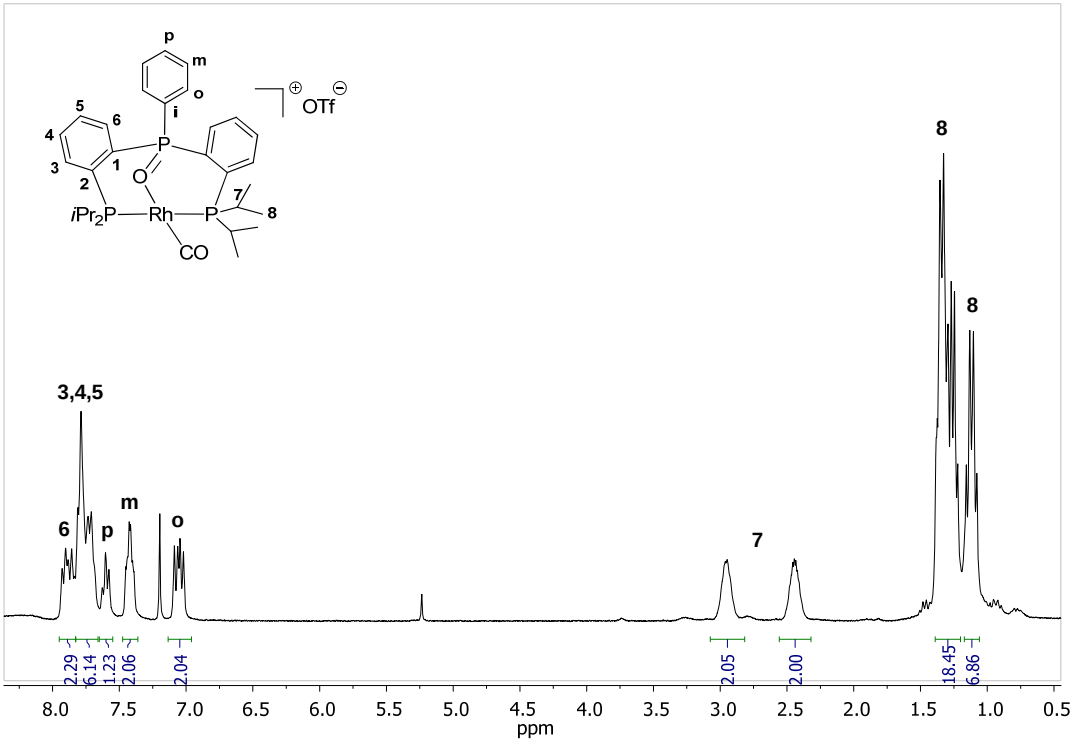
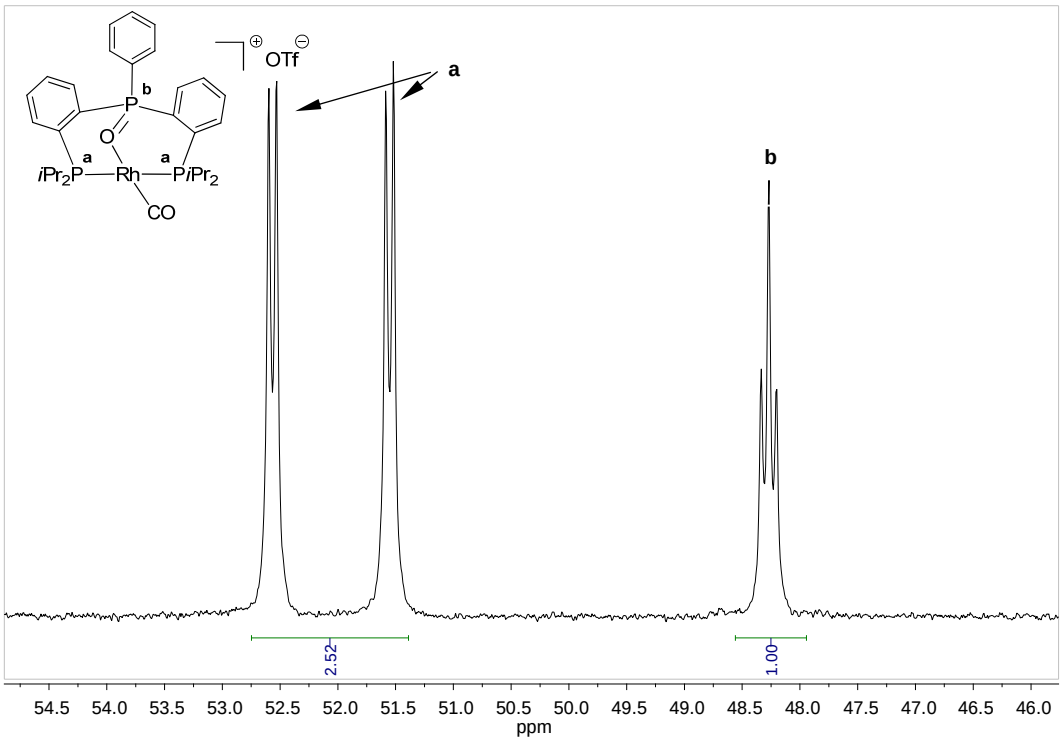


Figure 17. Room temperature ^{31}P NMR spectrum of [(DPPO)Rh(CO)]OTf complex **8** in $CDCl_3$ (121.49 MHz).



Theoretical results:

For the compounds **4***, **5*** and **7***, three minima (**a**, **b** and **c**) have been found on the potential energy surface (see for example Figure 18 for complex **4***). The forms **a** and **b** differ in the position of the Phenyl group and O atom around the P1 centre. The isomer **c** corresponds to the oxidative addition of (O)P-Ph bond on the metal. For all the complexes, form **a** (**4a***, **5a*** or **7a***) is the more stable (Table S1).

Figure 18: three minima localized for complex **4***

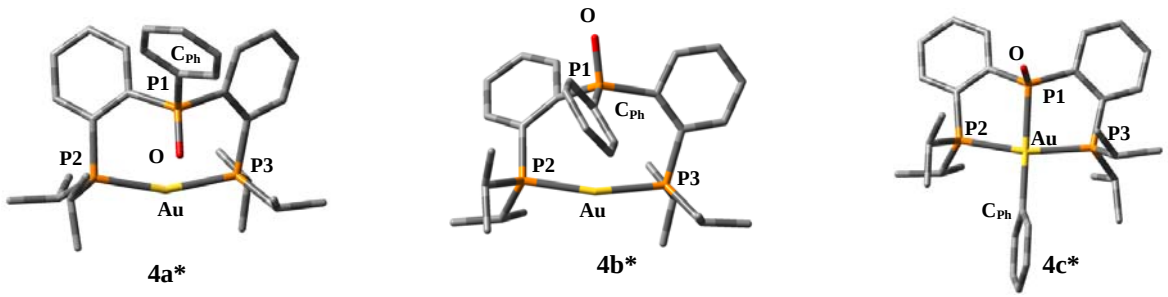


Table S1. Relative stability (ΔG in kcal/mol) of the different isomers for compounds **4***, **5*** and **7*** as optimized computationally at the B3PW91/SDD+f(Pd),6-31G**(other atoms) level of theory.

	4a*	**4b***	**4c***	**5a***	**5b***	**5c***	**7a***	**7b***	**7c***
ΔG	0	22.1	12.7	0	12.5	36.6	0	43.6	25.3

Table S2. Selected bond lengths and angles (in Å and °, respectively) for compounds **4***, **5*** and **7*** as optimized computationally at the B3PW91/SDD+f(Pd),6-31G**(other atoms) level of theory.

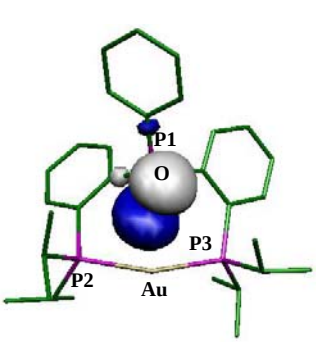
	4a*	**5a***	**7a***	**4b***	**5b***	**7b***	**4c***	**5c***	**7c***
P1-O	1.511 (1.510)[#]	1.506	1.542	1.506	1.508	1.500	1.511	1.515	1.512
P1-C_{Ph}	1.825 (1.824)[#]	1.835	1.811	1.826	1.827	1.825	4.482	3.084	3.222
P1-M	3.174	3.569	3.021	3.394	3.842	3.103	2.385	2.357	2.339
O-M	2.613	2.732	2.096	4.886	5.315	4.519	3.309	3.258	3.439
M-P2/ M-P3	2.335/ 2.324	2.465/ 2.495	2.322/ 2.322	2.331/ 2.318	2.452/ 2.496	2.354/ 2.345	2.381/ 2.369	3.514/ 2.453	2.392/ 2.399
P2-M-P3	159.49	125.54	160.37	159.12	121.91	146.01	163.18	94.81	160.04
M-Cl		2.447			2.444			2.397	
M-C_{CO}			1.804			1.810			1.963
M-C_{Ph}	4.943	5.248	4.666	3.457	3.463	2.393	2.110	2.097	2.040
ΣM	/	/	361.6	359.5	358.6	360.1	355.5	329.7	358.4

[#] Values for the ligand

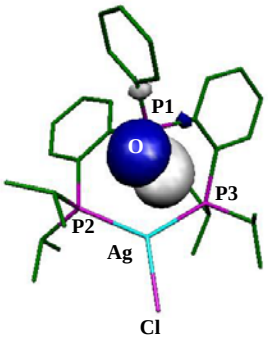
Table S3. NBO analyses: stabilizing energies ΔE(2) (in kcal/mol) for the donor-acceptor interactions accounting for the interaction of the Oxygen atom of P=O fragment with the metal centre (Au, Ag, Rh) for forms **4a***, **5a*** and **7a*** at the B3PW91/SDD+f(M),6-31G**(other atoms) level of theory.

	4a*	**5a***	**7a***
LP(O) →(M)	3.1	1.3	55.6

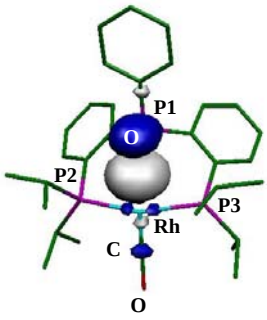
Figure 19: NBO analyses: Natural Localized Molecular Orbitals (cutoff : 0.04) associated with the O→Metal interaction in **4a***, **5a*** and **7a***.



4a*



5a*



7a*

Z-matrices :

Compound 4*

- **4a***

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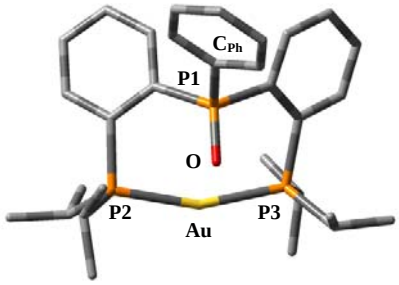
Sum of electronic and thermal Free Energies= -2401.800034



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C	1.62391100	1.68970600	0.95440400	H	-0.75952100	-2.76165200	2.86974000
C	2.41428900	2.36123200	1.89740700	H	0.04558500	3.45699600	4.06419100
C	1.86768800	3.01131900	3.00086000	H	-1.39110900	2.39487900	2.39122700
C	0.49318500	2.98588100	3.19467500	H	-2.50985600	-2.32430200	-3.54506200
C	-0.31596600	2.36822500	2.24459800	H	0.14242700	-4.27939200	2.97635200
P	2.50709100	0.62027900	-0.27780200	H	6.22824200	0.37956100	0.72911300
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C	3.92436800	-0.65894600	1.80759400	H	2.23904400	3.18406400	-3.07219000
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H	4.83376200	-1.19867100	2.08996100	C	-3.52131200	4.95775800	-1.30784400
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H	-3.22790200	-4.45439800	-2.39189700	H	-4.08821300	5.82265400	-1.63917100
H	3.10130700	-1.37997400	1.77693700	O	-0.57366400	0.68700000	-1.44890600

- **4b***

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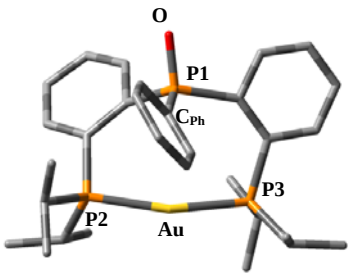
Sum of electronic and thermal Free Energies= -2401.764767



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C	2.01619700	0.44467600	4.17715700	H	-3.57489500	-0.26367200	-3.79613800
C	1.02016300	0.88555900	3.31246000	H	-2.12228000	-3.42699600	2.60394200
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C	-4.02095200	2.16892500	2.35292500	H	-2.69945600	-2.14992000	-2.38778000
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C	4.52725500	-2.64137600	0.00963400	H	2.56322200	2.00559500	-1.88321300
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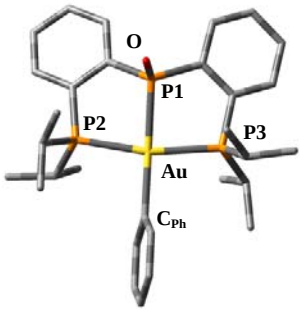
H	-5.82763800	1.03774600	2.01274900	C	0.93917500	3.76481700	-0.47163900
H	-4.48455700	2.90819300	2.99894500	C	-0.16791100	2.86979400	-2.87065400
H	-4.71664300	-0.60507500	0.58788100	H	-1.06414400	1.31135000	-1.70639900
H	-2.07486500	3.05818800	2.51891300	C	1.16597700	4.46843000	-1.65121300
H	-5.25694700	-0.73458900	-1.46665100	H	1.31954000	4.13559600	0.47432500
H	2.50923000	-4.28582700	0.82595000	C	0.62234100	4.01793500	-2.85405300
H	-3.35560700	0.84268000	-2.43818300	H	-0.62570700	2.53555500	-3.79717800
H	2.44131300	-2.88746200	1.90783700	H	1.75700600	5.37904400	-1.62744300
H	-5.07149000	-1.93555200	-2.73827300	H	0.79316800	4.57346600	-3.77147900
H	1.15147600	-3.15670600	0.72453400	O	-0.08183300	3.09220800	2.12020300

- **4c***

Sum of electronic and zero-point Energies= -2401.708449
Sum of electronic and thermal Free Energies= -2401.779827

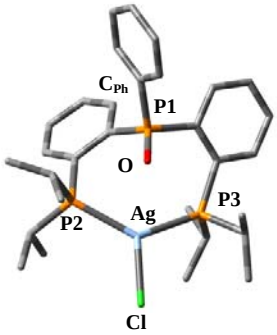


P	-0.18453300	-1.85347400	0.75033700	H	-3.98179900	0.81416100	-1.76816600
C	1.23689400	-2.66243200	-0.09705200	H	-5.13948600	1.34501000	0.34789200
C	2.42382000	-1.90540400	-0.18046600	H	-2.09924400	-0.28120500	-3.00702500
C	3.62628900	-2.53761100	-0.52276300	H	2.47423400	-5.68627300	-1.06115200
C	3.64638300	-3.89441900	-0.83448800	H	0.37145200	-4.62081900	-0.37076800
C	2.46552800	-4.63167200	-0.80327800	H	-3.15117800	0.84052900	3.49392300
C	1.27372400	-4.02298200	-0.41885700	H	-2.60933800	1.22046800	-3.78759400
P	2.36604700	-0.09314400	0.10633500	H	5.01618400	1.38698100	-2.20622300
C	3.35944100	0.29449300	1.62436900	H	-1.57697900	0.54522900	2.74409400
C	2.78611300	-0.41817000	2.85177300	H	4.58307000	-4.37155800	-1.10553400
C	-1.79866400	-2.38838800	0.05719700	H	5.02816800	-0.30667700	-1.73949700
C	-2.19018000	-3.73287600	0.06944500	H	2.85928400	1.79761600	-1.18908400
C	-3.44793400	-4.11015500	-0.39066500	H	-2.93267900	2.09081500	1.33714400
C	-4.34342800	-3.14226600	-0.84092400	H	-1.12953300	1.19702900	-2.82308400
C	-3.99199200	-1.79636500	-0.79782400	H	-3.49233200	3.15248500	-2.42573000
C	-2.72497000	-1.40572700	-0.34088300	H	-3.71476500	3.03577600	-0.68217400
P	-2.30317500	0.37128000	-0.14203800	H	4.55534400	-1.97852900	-0.54824500
C	-2.96608300	1.21682800	-1.65809700	H	5.17242300	0.96163600	-0.50526100
C	-3.06420800	2.73662100	-1.50791800	H	-2.08277100	3.19158000	-1.35921200
Au	0.04703300	0.44313000	0.14937900	H	4.35542900	-0.11890100	1.40991300
C	-3.20153600	1.02569400	1.34748900	H	3.95294300	2.32162700	0.99880400
C	-2.65369400	0.39113600	2.62873300	H	2.70815600	-1.49888900	2.71470600
C	-4.72313400	0.88672100	1.24966500	H	2.48756500	2.26159100	1.98482200
C	3.14840300	0.75216700	-1.35707400	H	4.07139100	1.99909900	2.72969900
C	4.67703700	0.68358400	-1.43875900	H	1.78807800	-0.04899400	3.10369700
C	2.49437200	0.27052900	-2.65580900	H	3.44144200	-0.22998800	3.70801300
C	-2.14898300	0.80491800	-2.88589000	O	-0.12073800	-2.11972900	2.23615300
C	3.47113500	1.80756800	1.83485100	C	0.24950300	2.53310200	-0.06171800
H	-5.32499300	-3.43124600	-1.20368800	C	0.61742800	3.18411900	-1.24668900
H	-3.73211600	-5.15800100	-0.39014400	C	-0.00053600	3.32688500	1.06874900
H	-4.71948700	-1.05574600	-1.11399900	C	0.73692800	4.57567900	-1.30215700
H	-1.52277800	-4.49036500	0.46653400	H	0.80577200	2.61463600	-2.15420900
H	-5.02912800	-0.16301500	1.28145800	C	0.12143600	4.71733400	1.01901000
H	2.85617200	0.87452300	-3.49381700	H	-0.28960500	2.86606900	2.01212600
H	-2.83472800	-0.68687800	2.66076900	C	0.49041000	5.34654900	-0.16846500
H	2.74264000	-0.77449500	-2.86394500	H	1.02025100	5.05512500	-2.23565600
H	-5.18088400	1.38654000	2.10915500	H	-0.07392200	5.30724300	1.91073800
H	1.40302300	0.35595700	-2.62805200	H	0.58294200	6.42770900	-0.20990000

Compound 5*

- **5a***

Sum of electronic and zero-point Energies= -2873.296258
Sum of electronic and thermal Free Energies= -2873.372413



C	3.37573200	-0.14306900	-0.81016300
C	3.65942400	0.16914300	-2.14892500
H	2.88118700	0.60170400	-2.77072000
C	4.91582100	-0.09880600	-2.68327300
H	5.12390800	0.14804200	-3.72039800
C	5.89921800	-0.69343400	-1.89305500
H	6.87846500	-0.90783200	-2.31182500
C	5.61913500	-1.02445800	-0.56926400
H	6.37649800	-1.50311000	0.04513000
C	4.36316600	-0.75267600	-0.02807700
H	4.15429500	-1.03176300	0.99958000
C	1.42227700	-0.70996600	1.28934400
C	2.20576400	-0.29140100	2.37470200
H	2.80781200	0.60884600	2.28443800
C	2.22450300	-0.99362700	3.57686000
H	2.83518800	-0.64246800	4.40331800
C	1.45618400	-2.14481300	3.69799800
H	1.46864900	-2.72090600	4.61905500
C	0.64725300	-2.55249300	2.63984300
H	0.03804400	-3.43962100	2.77226000
C	0.58432300	-1.84602900	1.42914100
C	-1.83361000	-3.49408100	0.99516300
H	-1.25725600	-4.31846300	1.43624600
C	-2.80272100	-4.07709700	-0.04357600
H	-3.56079400	-4.68085800	0.46835000
H	-2.30233400	-4.72711500	-0.76545300
H	-3.32063100	-3.28258000	-0.59324300
C	-2.63582600	-2.77545700	2.08768400
H	-3.25097800	-1.98500400	1.64446900
H	-2.00647700	-2.32246900	2.85903800
H	-3.31096900	-3.48561200	2.57884500
C	0.33254000	-3.24927000	-1.10107600
H	1.21788300	-2.61227300	-1.20605900
C	0.78013600	-4.62510400	-0.60675500
H	-0.06076500	-5.31990500	-0.51451500
H	1.28395500	-4.56858000	0.36380000
H	1.48623200	-5.06480100	-1.32079400
C	-0.34028500	-3.29427200	-2.47563500
H	0.34645000	-3.74200100	-3.20361900
H	-0.59450600	-2.28892100	-2.81947400
H	-1.25636000	-3.89066700	-2.47554100
C	1.65304600	2.00204500	0.21903500
C	2.89299900	2.62925000	0.41783400
H	3.80698100	2.06475700	0.26072500
C	2.97994800	3.96347500	0.80125200
H	3.95257300	4.42389600	0.94821200
C	1.81296700	4.69653800	0.98478600
H	1.85773300	5.74004700	1.28377000
C	0.57921800	4.08894100	0.77201600
H	-0.32017700	4.68211700	0.91261700
C	0.46058000	2.74425500	0.38754900
C	-2.19679400	2.68384700	1.62467600
H	-2.35053900	3.76852100	1.53364600
C	-1.41855000	2.39067700	2.91058600
H	-2.02637200	2.66574000	3.78009700
H	-0.47632700	2.94040100	2.97035400
H	-1.19204100	1.32161800	2.99313400
C	-3.56288200	1.98728500	1.67754600
H	-3.43686500	0.91157800	1.83998400
H	-4.14401100	2.10201400	0.76135200
H	-4.15148200	2.38867700	2.51096200
C	-1.77749400	3.26554100	-1.28313500
H	-1.41721600	4.26253800	-0.99396800
C	-1.07523800	2.84313800	-2.57695700
H	-1.43676700	1.86547500	-2.91058900
H	0.01088400	2.78191900	-2.46316500
H	-1.29369500	3.57177600	-3.36605700
C	-3.29287100	3.32248400	-1.48492700
H	-3.51163200	3.94646000	-2.35945300
H	-3.80881400	3.77062300	-0.63067100
H	-3.70940700	2.32578900	-1.67157700
O	0.72619900	-0.07773300	-1.41802200
P	1.65964000	0.22974100	-0.27715500
P	-0.68901600	-2.28131800	0.14762100
P	-1.26877100	2.09040200	0.09786300
Cl	-3.97212000	-0.42643500	-1.80178100
Ag	-1.86615800	-0.23813000	-0.57042400

- **5b***

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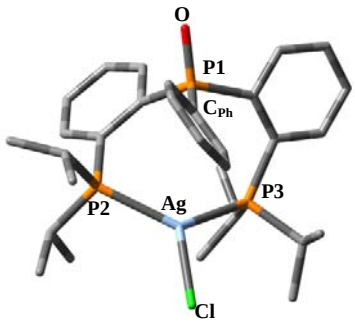

C	0.19156700	-1.51227600	2.02292600
C	1.05795100	-2.36305000	2.72754400
H	1.27588000	-3.34617500	2.32165000
C	1.58125500	-1.97013400	3.95619600
H	2.24761500	-2.63815100	4.49468700
C	1.23897000	-0.73259300	4.50180600
H	1.64954500	-0.42673000	5.45992200
C	0.35284500	0.10238700	3.82574300
H	0.07087500	1.06352400	4.24375600
C	-0.18032700	-0.29385400	2.59975800
H	-0.91718000	0.34034200	2.12052900
C	0.24673700	-2.04494700	-1.13473300
C	-0.38090300	-2.94948700	-2.01074400
H	-1.23112800	-3.52240500	-1.65420200
C	0.07359900	-3.16208400	-3.30672700
H	-0.45066700	-3.85688500	-3.95614200
C	1.21351500	-2.49939200	-3.74442800
H	1.60476600	-2.66813200	-4.74380400
C	1.86150200	-1.61723700	-2.88635700
H	2.75503800	-1.11719400	-3.24370900
C	1.39470100	-1.34967500	-1.58847600
C	3.30790000	0.92376500	-1.76344200
H	3.96830100	0.23358600	-2.30416900
C	4.17861100	1.91222500	-0.97478800
H	4.70854000	2.56376900	-1.67891500
H	4.93352000	1.41183800	-0.36458900
H	3.56927500	2.54811600	-0.32249800
C	2.44557900	1.69486100	-2.76538300
H	1.81742800	2.42309200	-2.24126000
H	1.79913700	1.04373000	-3.35963900
H	3.09009600	2.25041100	-3.45615800
C	3.41936600	-1.06886500	0.47395100
H	2.76831900	-1.87859000	0.82232200
C	4.56848800	-1.69888000	-0.31453000
H	5.28447800	-0.94736200	-0.66207400
H	4.21197200	-2.26360500	-1.18148300
H	5.11785500	-2.39545200	0.32922500
C	3.90051000	-0.30916100	1.71318400
H	4.39768400	-1.00545900	2.39775400
H	3.07032200	0.15722900	2.24879700
H	4.62011500	0.47489600	1.46493200
C	-2.32145400	-1.64224800	0.40180800
C	-3.18735100	-2.69987400	0.73235400
H	-2.73736300	-3.64447800	1.02438900
C	-4.56985500	-2.56734400	0.67348000
H	-5.20590300	-3.40614200	0.94127400
C	-5.12065300	-1.36315000	0.25478600
H	-6.19740500	-1.23921000	0.17903000
C	-4.27787700	-0.30660200	-0.07202500
H	-4.73109100	0.62052100	-0.40810700
C	-2.87791400	-0.40137800	0.00633600
C	-2.37690700	1.39838300	-2.25752400
H	-3.35968400	1.89122100	-2.24438900
C	-2.49136900	0.09483400	-3.04979100
H	-2.73464500	0.32625500	-4.09326800
H	-3.26987800	-0.56549000	-2.66144200
H	-1.54643600	-0.45755800	-3.04621600
C	-1.36056200	2.32880500	-2.92735300
H	-0.40438500	1.81393000	-3.05153000
H	-1.17016600	3.24336400	-2.36144400
H	-1.71795600	2.61524000	-3.92337400
C	-2.92193000	2.47432600	0.42576300
H	-3.97432900	2.32049100	0.15549900
C	-2.78024500	2.34708700	1.94393700
H	-1.75075100	2.56224900	2.25119200
H	-3.07145300	1.35652300	2.30849500
H	-3.42812300	3.08252400	2.43411600
C	-2.51070000	3.87638000	-0.03277500
H	-3.08485100	4.61639700	0.53665000
H	-2.72423200	4.04917700	-1.09117400
H	-1.44831500	4.06221400	0.16106700
O	-0.59822200	-3.74418000	0.75792300
P	-0.56501100	-2.25290600	0.53424600
P	2.23518000	-0.05164600	-0.57482900
P	-1.92296900	1.13279200	-0.44396800
Cl	1.00289200	3.56924100	1.29428200
Ag	0.46113800	1.43736600	0.22922200

- **5c***

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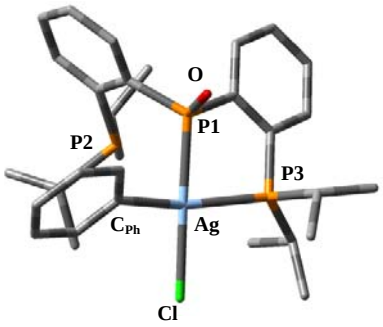
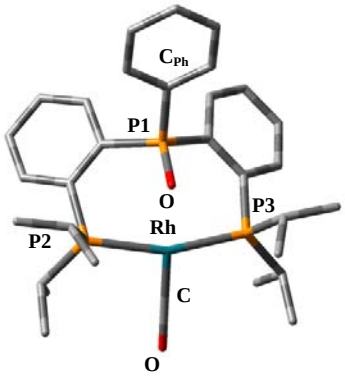


P	-2.58653900	0.00023400	0.02999100
P	1.50187300	1.34747700	1.16201400
P	0.13214400	0.06370900	-1.65034200
C	1.13430600	-2.52776900	-0.31315700
C	-2.09527300	1.58700700	-0.74398900
C	-2.64194200	1.08897500	2.57787300
H	-3.23096800	1.44653300	3.42972700
H	-2.08671700	1.93756900	2.16797700
H	-1.92119200	0.35396600	2.94740500
C	3.75329000	1.79042500	-0.57149200
H	4.22673300	2.29962600	0.26191600
C	2.58131400	0.53069000	-2.75020100
H	2.09648300	0.03895400	-3.58879900
C	1.37908000	-2.95375400	-1.61716500
H	0.80304700	-2.55408500	-2.44926600
C	1.88809400	-3.04157300	0.74415200
H	1.66248700	-2.76780700	1.76962300
C	-0.51154800	2.73929100	-2.17393900
H	0.41190400	2.73651400	-2.74575100
C	1.86668300	3.09789900	1.75483500
H	2.95424300	3.22682900	1.83231300
C	1.86452200	0.67113800	-1.55571900
C	-1.29931700	3.88642400	-2.13279000
H	-0.99000900	4.77500900	-2.67557100
C	-2.87466900	2.74966400	-0.70127200
H	-3.80086400	2.76957300	-0.13449300
C	-3.57401800	0.45046600	1.54364100
H	-4.31098100	1.19560900	1.21368100
C	2.38676200	-3.89257800	-1.86306200
H	2.56764100	-4.22569700	-2.88231500
C	3.15523500	-4.39201900	-0.81544300
H	3.94063500	-5.11753000	-1.01025500
C	3.87879500	1.02390500	-2.85575200
H	4.42767700	0.91318500	-3.78666400
C	2.45496700	1.28098900	-0.42976500
C	2.90330200	-3.96546800	0.48745400
H	3.48304600	-4.36525700	1.31610200
C	4.45998700	1.66656800	-1.76671500
H	5.46676900	2.06874600	-1.84131000
C	-0.88976500	1.59500100	-1.46369400
C	-2.47527600	3.89564900	-1.38536300
H	-3.08798700	4.79150700	-1.34057500
C	1.32614800	4.12039200	0.75313700
H	0.24168200	4.02469800	0.63488600
H	1.78193700	4.00687000	-0.23412600
H	1.53536800	5.13751200	1.10539800
C	-3.86349300	-2.27637300	-1.07575800
H	-4.41565500	-2.52532100	-0.16633200
H	-2.89776000	-2.78630800	-1.02377800
H	-4.41606700	-2.68836100	-1.92731200
C	-3.70123600	-0.76452600	-1.26773900
H	-3.10274100	-0.60962700	-2.17630400
C	-5.04108600	-0.04710000	-1.44301400
H	-5.57559300	-0.47875500	-2.29639000
H	-4.91434500	1.02091300	-1.64315700
H	-5.68416200	-0.16174700	-0.56461900
C	-4.32368800	-0.74688300	2.13562000
H	-3.63272500	-1.55578600	2.38792200
H	-5.08566900	-1.13697000	1.45629200
H	-4.83326100	-0.42874600	3.05207900
O	-0.13169100	-0.55685000	-3.00726800
C	1.25707200	3.33224700	3.14051100
H	1.42985000	4.36792400	3.45615500
H	1.68809400	2.68057800	3.90492900
H	0.17450700	3.16485300	3.13014200
C	2.53696600	0.22218500	2.27738200
H	2.73769400	-0.62932400	1.61454800
C	3.88032500	0.75863000	2.77254400
H	3.76488500	1.63989300	3.41238700
H	4.55534400	1.01489100	1.95233300
H	4.38180600	-0.00978500	3.37283000
C	1.67815800	-0.29301200	3.43933400
H	2.23661100	-1.04316300	4.01186400
H	0.75493100	-0.76362800	3.08811500
H	1.40563600	0.50658800	4.13631300
Ag	-0.52793300	-1.33004400	0.13270600
Cl	-1.24413400	-2.70551900	1.96031700

Compound 7*

- **7a***

  Sum of electronic and zero-point Energies= -2489.857273
  Sum of electronic and thermal Free Energies= -2489.929292



Rh	-0.00190700	-1.44543300	-0.33148700	C	3.84109000	1.50983300	2.65949400
P	-2.28960800	-1.07722700	-0.17893000	H	4.74698400	1.52929400	3.25774200
P	2.28677800	-1.08298300	-0.17910500	C	-1.51927700	1.42519100	1.08862800
P	0.00179100	1.54835100	0.07602100	C	-3.84013000	1.52198300	2.65589500
O	-0.00543900	-4.29632400	0.47587600	H	-4.74624300	1.54387200	3.25372700
C	0.00533800	3.21048300	-0.64222800	C	3.00491500	-2.83035600	1.91514500
C	-2.47559000	0.38237700	0.97071000	H	2.06020300	-3.37789300	1.88803100
C	-3.01196900	-2.82184200	1.91600200	H	2.89015100	-1.99627500	2.61185500
H	-3.77188300	-3.49540200	2.32559100	H	3.76316200	-3.50606500	2.32428400
H	-2.89504400	-1.98765300	2.61223000	C	-0.00402300	-3.17369200	0.18654900
H	-2.06862600	-3.37175200	1.88911400	C	-2.61516100	-1.24265900	-2.99256900
C	3.62898700	0.46378500	1.76475400	H	-3.07085400	-2.23611800	-3.00554900
H	4.39026000	-0.30406000	1.69503900	H	-1.52944100	-1.36643700	-3.03411800
C	1.75811000	2.47736300	1.98046100	H	-2.93273600	-0.72577100	-3.90439600
H	1.05381700	3.30028800	2.04246600	C	-3.03868100	-0.42008500	-1.77108400
C	-1.20545300	3.82222400	-0.99970400	H	-2.54473200	0.55605500	-1.85421200
H	-2.15224200	3.36013000	-0.73742000	C	-4.55101100	-0.20283000	-1.70447200
C	1.21879900	3.81970600	-0.99486000	H	-4.88707900	0.30892900	-2.61245800
H	2.16358400	3.35566200	-0.72885600	H	-4.84627700	0.41597200	-0.85164200
C	-1.75544300	2.48521200	1.97595700	H	-5.09725300	-1.14968100	-1.64858200
H	-1.05012600	3.30737500	2.03652000	C	-3.53203600	-3.57905800	-0.43751500
C	3.43089800	-2.38651500	0.51098600	H	-2.55272700	-4.02122400	-0.64048700
H	4.42872700	-1.93377100	0.56337700	H	-3.99732000	-3.32266200	-1.39148500
C	1.52098700	1.41957700	1.09074700	H	-4.15026500	-4.35294500	0.02901600
C	-2.89662500	2.53453600	2.76861600	O	0.00056000	0.51671000	-1.06985700
H	-3.04832000	3.36336900	3.45261800	C	3.52329000	-3.58769800	-0.43863500
C	-3.62917900	0.47396200	1.76319200	H	4.13991700	-4.36309100	0.02751400
H	-4.39160600	-0.29282300	1.69450700	H	3.98895800	-3.33200200	-1.39260200
C	-3.43689700	-2.37771400	0.51161700	H	2.54299100	-4.02768400	-0.64159300
H	-4.43364800	-1.92258100	0.56370200	C	3.03767300	-0.42682100	-1.77076800
C	-1.19893600	5.03282800	-1.68607000	H	2.54577300	0.55036400	-1.85373900
H	-2.13902000	5.50436500	-1.95519000	C	4.55041300	-0.21263300	-1.70358400
C	0.01058500	5.63771000	-2.02491700	H	5.09472100	-1.16056400	-1.64721900
H	0.01263200	6.58365000	-2.55810600	H	4.84658000	0.40579200	-0.85079100
C	2.89888200	2.52341400	2.77389600	H	4.88788700	0.29820800	-2.61156400
H	3.05131100	3.35055400	3.45978000	C	2.61290400	-1.24807500	-2.99272200
C	2.47560600	0.37536600	0.97160900	H	2.93071700	-0.73084700	-3.90426900
C	1.21747900	5.03034000	-1.68123700	H	1.52705000	-1.37074100	-3.03405000
H	2.15959800	5.49994700	-1.94659700	H	3.06761300	-2.24197200	-3.00655600

- **7b***

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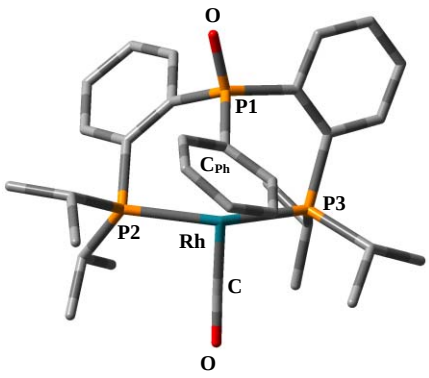
  Sum of electronic and thermal Free Energies= -2489.859805



Rh	-0.20622000	-0.89936600	0.23946900	C	-2.13280100	3.06203900	-2.84334400
P	2.04820700	-0.93568800	-0.40514000	H	-2.72601600	3.41384200	-3.68193500
P	-2.37932500	-0.17597800	-0.30215900	C	2.12840100	1.84583600	0.46595700
P	0.35692400	2.07523100	0.91925300	C	4.85588300	2.05990900	-0.16844200
O	-0.63788300	-3.63945300	-0.78775400	H	5.90699100	2.12824800	-0.43213800
C	-0.13129800	0.70139900	2.01729600	C	-2.34683400	-1.26154100	-2.94838200
C	2.80374100	0.72955100	-0.08206300	H	-1.58661900	-2.02412300	-2.76862200
C	1.73984100	0.00547800	-3.03307700	H	-1.84475300	-0.34614100	-3.26895300
H	1.96139000	-0.12829900	-4.09702600	H	-2.96445600	-1.61253300	-3.78183400
H	2.13643000	0.97678200	-2.72809100	C	-0.45878400	-2.53484700	-0.49402800
H	0.65198400	0.02793400	-2.91750800	C	2.40018300	-3.38430200	0.98155800
C	-2.53717500	1.93560700	-2.13708300	H	2.09261400	-4.02045500	0.14638800
H	-3.43835700	1.43107000	-2.46507000	H	1.50336400	-3.11336400	1.54402400
C	-0.25593700	3.27240000	-1.36900600	H	3.04045800	-3.99010400	1.63115800
H	0.61948800	3.83098700	-1.05077600	C	3.18329300	-2.15616400	0.50175400
C	-1.25857000	0.99913500	2.83920200	H	3.50045800	-1.58418800	1.38399100
H	-1.82996700	1.89821100	2.63170800	C	4.44558800	-2.60536100	-0.24538500
C	0.75222000	-0.31785400	2.45263600	H	5.00889100	-3.28503900	0.40251800
H	1.77519000	-0.34287100	2.10125300	H	5.12134600	-1.78833300	-0.50195400
C	2.84532000	3.02711300	0.71602400	H	4.20945300	-3.15681800	-1.15916100
H	2.31241300	3.85905400	1.16831300	C	1.89452100	-2.50076100	-2.78727800
C	-3.23935700	-1.05469600	-1.72291800	H	0.80530400	-2.55235400	-2.85297000
H	-4.05766400	-0.38243900	-2.00728900	H	2.23801900	-3.35361400	-2.19665600
C	-0.65356100	2.14285500	-0.62897300	H	2.28543100	-2.62615800	-3.80224900
C	4.19699900	3.13882700	0.40641500	O	0.17105900	3.38476100	1.62695800
H	4.72438500	4.06536700	0.61098000	C	-3.88016900	-2.37762700	-1.28357000
C	4.16282000	0.87530700	-0.40133800	H	-4.29805500	-2.87585700	-2.16445600
H	4.70186600	0.05056800	-0.85103200	H	-4.70015400	-2.23164300	-0.57884400
C	2.35528100	-1.14879900	-2.23862700	H	-3.16000300	-3.06531400	-0.83413200
H	3.44776300	-1.09203100	-2.33276400	C	-3.76460300	0.24900600	0.89405600
C	-1.55275600	0.23263700	3.94453900	H	-3.32545000	1.07178400	1.46478000
H	-2.39558200	0.49349700	4.57665400	C	-5.03474200	0.78358900	0.22609400
C	-0.74139500	-0.86867200	4.27624100	H	-5.56063900	0.01250600	-0.34475400
H	-0.98127100	-1.47297100	5.14617500	H	-4.83426500	1.63319400	-0.43257200
C	-0.96904600	3.72503500	-2.47016600	H	-5.72406100	1.13213900	1.00247600
H	-0.62894700	4.59995800	-3.01515700	C	-4.06167400	-0.89415100	1.87082500
C	-1.81820100	1.43699600	-1.03575000	H	-4.67260900	-0.51443000	2.69644800
C	0.40627600	-1.13018600	3.55143500	H	-3.14904400	-1.32154400	2.29348900
H	1.08702800	-1.91355800	3.86924500	H	-4.62573300	-1.70197300	1.39971000

- **7c***

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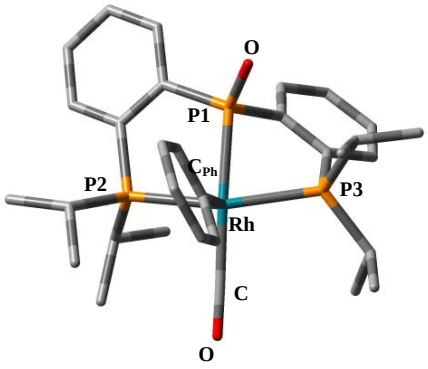

Rh	-0.14214700	-0.46119500	0.42604800	C	4.36024900	2.72494600	-1.35601000
P	-2.44709100	0.11084500	0.08745400	H	5.36493400	3.13665800	-1.34347500
P	2.22635900	-0.21380000	0.64720200	C	-0.90534700	2.37492300	-0.35420800
P	0.04443900	1.10601300	-1.29958100	C	-2.63248900	4.19182700	0.88202000
O	-0.39388700	-2.27264700	2.93893700	H	-3.30789800	4.89947000	1.35329600
C	-0.08168700	-2.07685200	-0.81785500	C	1.80530800	1.57433800	2.72892600
C	-2.12015700	1.92124900	0.21214600	H	0.79230200	1.20631200	2.93210400
C	-3.16919300	0.13878700	2.84095100	H	1.74101400	2.35190800	1.96246400
H	-3.99230300	0.04795300	3.55730500	H	2.16786700	2.04397200	3.64894800
H	-2.80209300	1.16650600	2.88762500	C	-0.31610100	-1.60055700	2.01495000
H	-2.37352800	-0.52408200	3.18870200	C	-3.35190200	-1.51176500	-2.10736500
C	4.01547800	1.72740900	-0.44738100	H	-3.96462000	-2.18949700	-1.50702500
H	4.76519100	1.38304600	0.25694700	H	-2.35028300	-1.93248400	-2.19727500
C	2.13686500	2.66345200	-2.28547000	H	-3.78969900	-1.48130400	-3.11036400
H	1.40221500	3.00285700	-3.01028900	C	-3.32164200	-0.08377300	-1.55821900
C	0.54247400	-2.01436200	-2.06476200	H	-2.65526700	0.49542800	-2.21063400
H	0.95754700	-1.09263100	-2.45570500	C	-4.70940000	0.56170400	-1.54117100
C	-0.67527200	-3.27433300	-0.40688700	H	-5.09465100	0.58937500	-2.56558500
H	-1.20185300	-3.35400800	0.53772400	H	-4.69200700	1.59288700	-1.17588900
C	-0.56492100	3.72954000	-0.27654900	H	-5.42588200	-0.01119100	-0.94331500
H	0.36936900	4.07802500	-0.70643300	C	-4.11521500	-1.72856900	1.43266500
C	2.74404300	0.43011800	2.32843200	H	-3.27496700	-2.40758000	1.60772200
H	3.74262700	0.85315900	2.16004600	H	-4.59189500	-2.01152400	0.49262300
C	1.77493900	1.68900200	-1.34713700	H	-4.84122900	-1.89545400	2.23478300
C	-1.42374100	4.63308700	0.34333500	O	-0.49949400	0.92956800	-2.69880200
H	-1.15576100	5.68385200	0.40024500	C	2.85480300	-0.61542300	3.43872600
C	-2.97990700	2.84425000	0.81999800	H	3.13136700	-0.11158100	4.37089600
H	-3.92448300	2.52379900	1.24783200	H	3.62365800	-1.36321600	3.23598200
C	-3.67056400	-0.26279600	1.45095700	H	1.91122200	-1.13491500	3.62260400
H	-4.54217800	0.35719300	1.20227300	C	3.28383700	-1.68016300	0.15495300
C	0.59045200	-3.15292100	-2.87607000	H	3.03763300	-1.78157400	-0.90972400
H	1.07454000	-3.08198200	-3.84613700	C	4.79324100	-1.45306200	0.28433300
C	0.01719500	-4.35092100	-2.46144600	H	5.09488500	-1.22210300	1.31093200
H	0.05682700	-5.22878900	-3.09874700	H	5.15442400	-0.66247800	-0.37531800
C	3.42939700	3.17902300	-2.29015200	H	5.31107600	-2.37362700	-0.00388000
H	3.70973800	3.93714400	-3.01515900	C	2.84951900	-2.97506100	0.85140900
C	2.72496800	1.17726900	-0.45232100	H	3.40439500	-3.80928000	0.41062800
C	-0.62080000	-4.40525300	-1.22602000	H	1.78782800	-3.18313200	0.70960600
H	-1.08827300	-5.32501500	-0.88569500	H	3.06967900	-2.97023400	1.92130000

- **Ligand**
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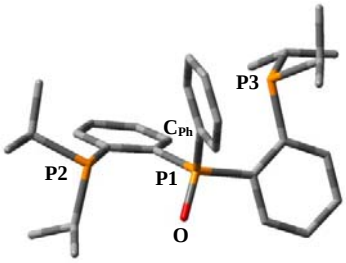
  Sum of electronic and thermal Free Energies= -2266.069826



P	-0.21679600	-0.16318000	1.06083200
C	1.49088400	-0.74684500	1.53077800
C	2.73302800	-0.60989000	0.85881800
C	3.89054400	-1.03304000	1.53215800
C	3.84697300	-1.61644800	2.79535300
C	2.62286300	-1.77420200	3.43403200
C	1.46327500	-1.32642000	2.80978300
P	2.86550200	0.14867700	-0.83694100
C	4.07536500	1.55146500	-0.48906000
C	3.47893000	2.54799400	0.50718000
C	-0.84895800	-1.22925700	-0.28876500
C	-0.04622700	-2.27244800	-0.76022300
C	-0.51164200	-3.16455200	-1.72260700
C	-1.80106400	-3.01683400	-2.21962600
C	-2.62108200	-2.00147500	-1.73073400
C	-2.18439500	-1.09982800	-0.75049400
P	-3.30131300	0.20089800	-0.01746800
C	-4.61131800	0.40677700	-1.35385300
C	-5.72275800	1.32412000	-0.83091400
C	-4.11486700	-0.84719800	1.33339200
C	-5.11199400	-1.90195500	0.86104100
C	3.94091300	-1.02398600	-1.87159700
C	5.38160400	-1.33491900	-1.45900100
C	3.18559200	-2.31758500	-2.18216500
C	-3.97141100	1.01798600	-2.60484700
C	4.45045900	2.25528600	-1.79681000
H	-2.18094700	-3.70102100	-2.97387000
H	0.12996100	-3.96627800	-2.07664700
H	-3.63237900	-1.92260200	-2.11620500
H	0.95524900	-2.39230700	-0.36306800
H	-4.67320800	-2.57195500	0.11517100
H	3.72604400	-2.90190700	-2.93637100
H	3.09606700	-2.94502900	-1.28779000
H	-5.43558100	-2.52075500	1.70718600
H	2.18054600	-2.11893900	-2.56359300
H	-5.06528300	-0.55882100	-1.61468100
H	-6.01345200	-1.45431500	0.42734600
H	-3.19174100	0.37858400	-3.02861700
H	2.56694600	-2.22398200	4.42138500
H	0.50294800	-1.39418700	3.31247300
H	-4.72946100	1.18245800	-3.38023400
H	5.90760000	-1.81112900	-2.29569400
H	4.76786500	-1.93549000	3.27641900
H	5.41774500	-2.03749000	-0.62120400
H	3.98478900	-0.44870300	-2.80830100
H	-3.51627200	1.98689800	-2.37156900
H	-6.44744900	1.53236500	-1.62726300
H	-6.27056500	0.87930500	0.00409400
H	4.85698800	-0.89002000	1.06261400
H	5.95240700	-0.44233200	-1.18568300
H	-5.31532900	2.28326000	-0.49197400
H	4.98558800	1.12799200	-0.04352500
H	4.97281100	1.59691400	-2.49779600
H	3.23129500	2.07457900	1.46111600
H	3.55962800	2.64668300	-2.30048100
H	5.11307500	3.10409800	-1.59073500
H	2.56806500	3.00848900	0.11351700
H	4.20032300	3.34891100	0.70879400
O	-1.08525300	-0.25492200	2.29275900
C	-0.12705600	1.56093300	0.46975600
C	-0.19999000	2.54989100	1.45699600
C	-0.08056400	1.93075900	-0.87779000
C	-0.20193000	3.89664600	1.10080200
H	-0.28701300	2.25495600	2.49859000
C	-0.09871800	3.27769100	-1.23147900
H	-0.03393700	1.16788700	-1.64715100
C	-0.15287400	4.26170500	-0.24370800
H	-0.25672000	4.65971900	1.87219700
H	-0.07304500	3.55995300	-2.28045300
H	-0.16589600	5.31181700	-0.52326100
C	-4.68520200	0.05247100	2.43444500
H	-5.53716300	0.65008300	2.09266300
H	-5.03365200	-0.56022100	3.27486500
H	-3.91574600	0.73211000	2.80922500
H	-3.24025100	-1.34716800	1.76491900