

Electronic Supplementary Information

Intramolecular C–H oxidative addition to iridium(I) triggered by trimethyl phosphite in *N,N'*-diphophanesilanediamine complexes

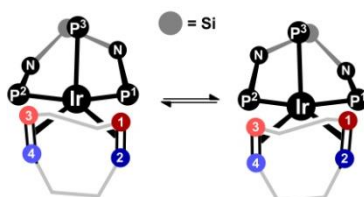
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▪ [Ir(SiNP){P(OMe) ₃ }(cod)] ⁺ (2 ⁺ , SPY-5-13)	7
▪ [Ir(SiNP){P(OMe) ₃ }(cod)] ⁺ (2 ⁺ , TBPY-5-13)	8
▪ [IrH(SiNP–H){P(OMe) ₃ } ₂] ⁺ (3 ⁺)	9
▪ [Ir(SiNP){P(OMe) ₃] ₂] ⁺ (4 ⁺)	10
▪ TS_4⁺_3⁺	11
▪ [Ir(SiNP)(CO)(cod)] ⁺	12
▪ IrCl(SiNP)(CO)	13
▪ IrHCl(SiNP–H)(CO)	14
▪ TS_CO	15
▪ IrHCl(SiNP–H){P(OMe) ₃ } (6 , OC-6-43)	16
▪ IrHCl(SiNP–H){P(OMe) ₃ } (6' , OC-6-34)	17
▪ IrCl(SiNP){P(OMe) ₃ } (7)	18
▪ TS_7_6'	19
▪ TS_7_6	20
▪ RhCl(SiNP){P(OMe) ₃ } (8)	21

1. Selected kinetic data for $[\text{Ir}(\text{SiNP})\{\text{P}(\text{OMe})_3\}(\text{cod})][\text{PF}_6]$ ($[\mathbf{2}][\text{PF}_6]$)



Scheme S1. Left-right exchange at the SiNP and cod ligands of $[\text{Ir}(\text{SiNP})\{\text{P}(\text{OMe})_3\}(\text{cod})]^+$ ($\mathbf{2}^+$) in CD_2Cl_2 .

Table S1. Kinetic constants obtained from the line shape analysis of the $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of $[\text{Ir}(\text{SiNP})\{\text{P}(\text{OMe})_3\}(\text{cod})][\text{PF}_6]$ ($[\mathbf{2}][\text{PF}_6]$) in CD_2Cl_2 .

T (K)	k (sec ⁻¹)
188	$3.00 \cdot 10^{-1}$
193	$7.50 \cdot 10^{-2}$
198	$1.60 \cdot 10^{-2}$
203	$4.20 \cdot 10^{-2}$
208	$8.50 \cdot 10^{-2}$
213	$1.90 \cdot 10^{-3}$
218	$6.50 \cdot 10^{-3}$
223	$2.60 \cdot 10^{-4}$
228	$9.50 \cdot 10^{-4}$

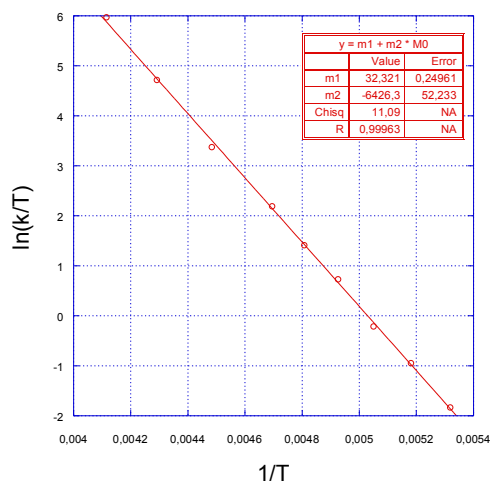
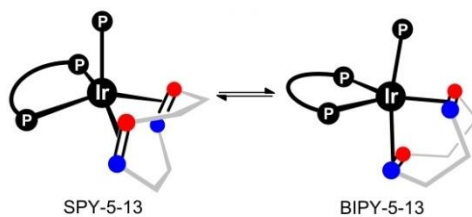


Fig. S1. Eyring plot for the left-right exchange at the SiNP and cod ligands of $[\text{Ir}(\text{SiNP})\{\text{P}(\text{OMe})_3\}(\text{cod})][\text{PF}_6]$ ($[\mathbf{2}][\text{PF}_6]$) in CD_2Cl_2 ; $\Delta H^\ddagger = 53.6 \pm 0.4 \text{ kJ} \cdot \text{mol}^{-1}$; $\Delta S^\ddagger = 71.2 \pm 2.0 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$.



Scheme S2. *Up-down* exchange at the cod ligand of $[\text{Ir}(\text{SiNP})\{\text{P}(\text{OMe})_3\}(\text{cod})]^+$ ($\mathbf{2}^+$) in CD_2Cl_2 .

Table S2. Kinetic constants obtained from ^1H - ^1H EXSY spectrum of $[\text{Ir}(\text{SiNP})\{\text{P}(\text{OMe})_3\}(\text{cod})][\text{PF}_6]$ ($\mathbf{[2]}[\text{PF}_6]$) in CD_2Cl_2 .

T (K)	k (sec ⁻¹)
203	3.60
208	6.45
213	13.3
223	37.7

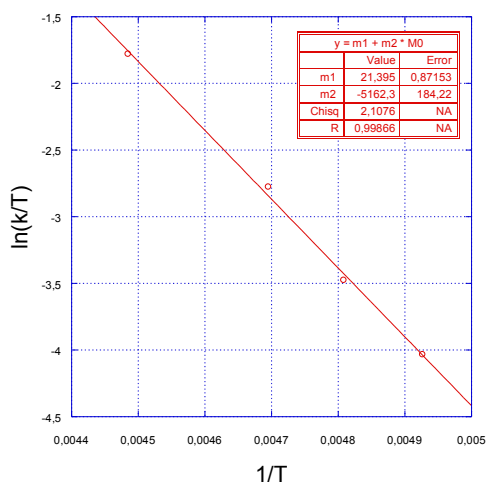


Fig. S2. Eyring plot for the *up-down* exchange at the cod ligand of $[\text{Ir}(\text{SiNP})\{\text{P}(\text{OMe})_3\}(\text{cod})][\text{PF}_6]$ ($\mathbf{[2]}[\text{PF}_6]$) in CD_2Cl_2 ; $\Delta H^\ddagger = 42.7 \pm 1.7 \text{ kJ}\cdot\text{mol}^{-1}$; $\Delta S^\ddagger = 19.6 \pm 7.1 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$.

2. Selected NMR data of $[\text{IrH}(\text{SiNP-H})\{\text{P}(\text{OMe})_3\}_2][\text{PF}_6]$ (**[3]** $[\text{PF}_6]$)

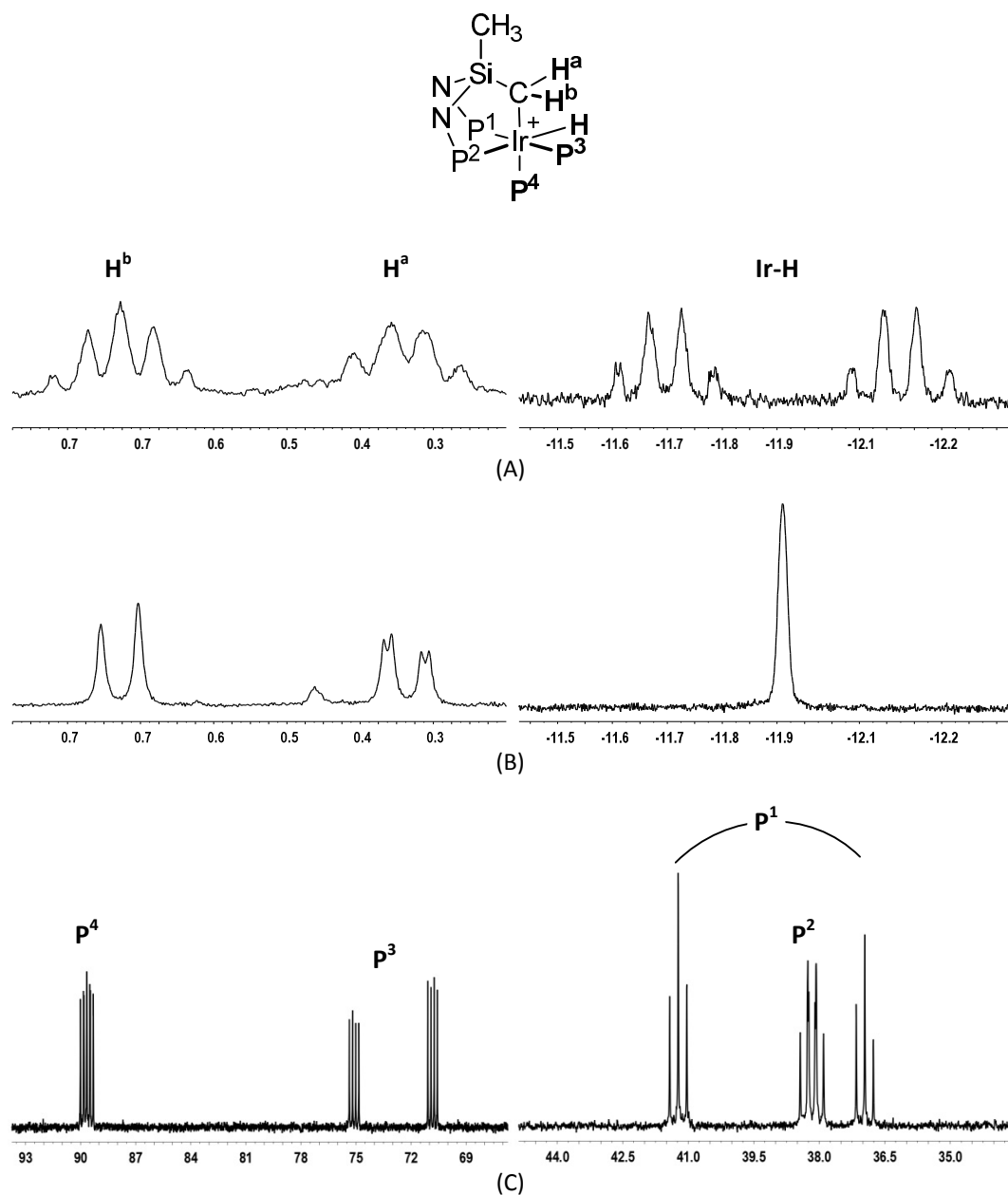
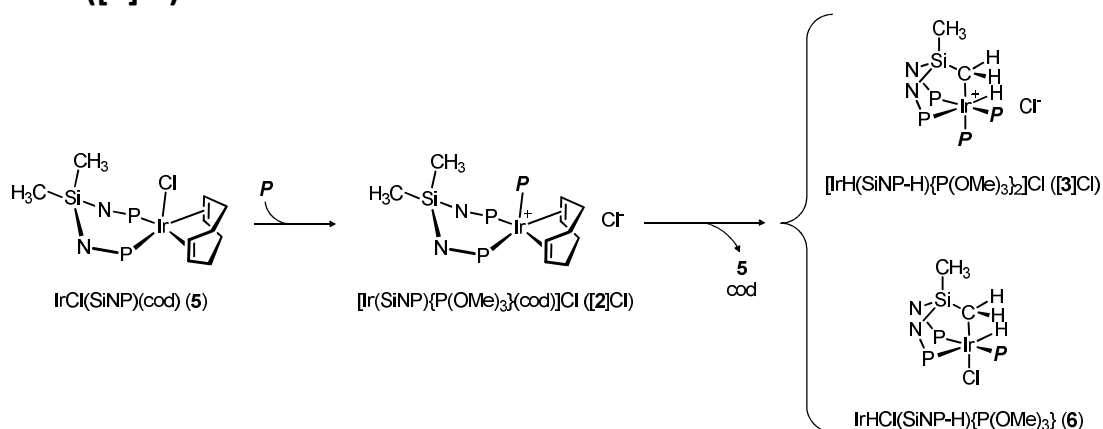


Fig. S3. Selected regions of the ^1H NMR (A), $^1\text{H}\{^{31}\text{P}\}$ (B) and $^{31}\text{P}\{^1\text{H}\}$ (C) spectra of $[\text{IrH}(\text{SiNP-H})\{\text{P}(\text{OMe})_3\}_2][\text{PF}_6]$ (**[3]** $[\text{PF}_6]$) (298 K, CD_2Cl_2) with the proposed assignment.

3. Selected NMR data for the evolution of $[\text{Ir}(\text{SiNP})\{\text{P}(\text{OMe})_3\}(\text{cod})]\text{Cl}$ ($[\mathbf{2}]\text{Cl}$) at 298 K



Scheme S3. Reaction of $\text{IrCl}(\text{SiNP})(\text{cod})$ (**5**) with $\text{P}(\text{OMe})_3$ (1:1) affording $[\mathbf{3}]\text{Cl}$ and **6** (298 K).

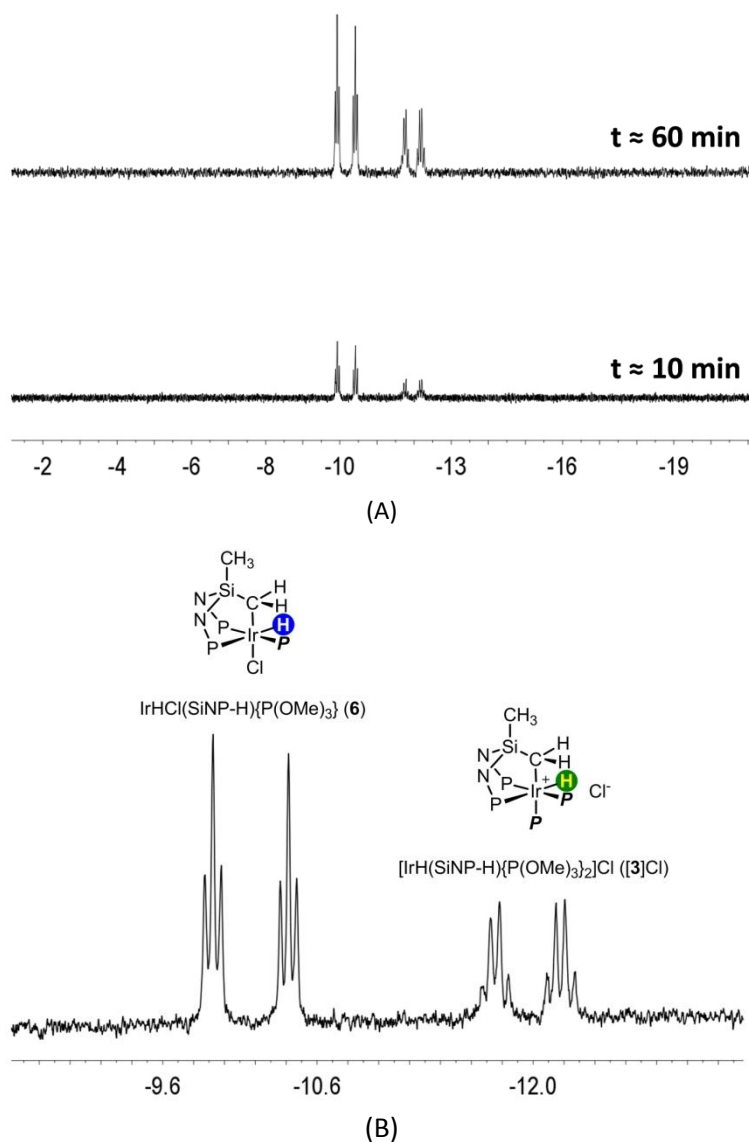


Figure S4. (A) Up-field region of the ^1H NMR spectra at different times after adding $\text{P}(\text{OMe})_3$ to $\text{IrCl}(\text{SiNP})(\text{cod})$ (**5**) (1:1, CDCl_3 , 298 K) and (B) the proposed assignment.

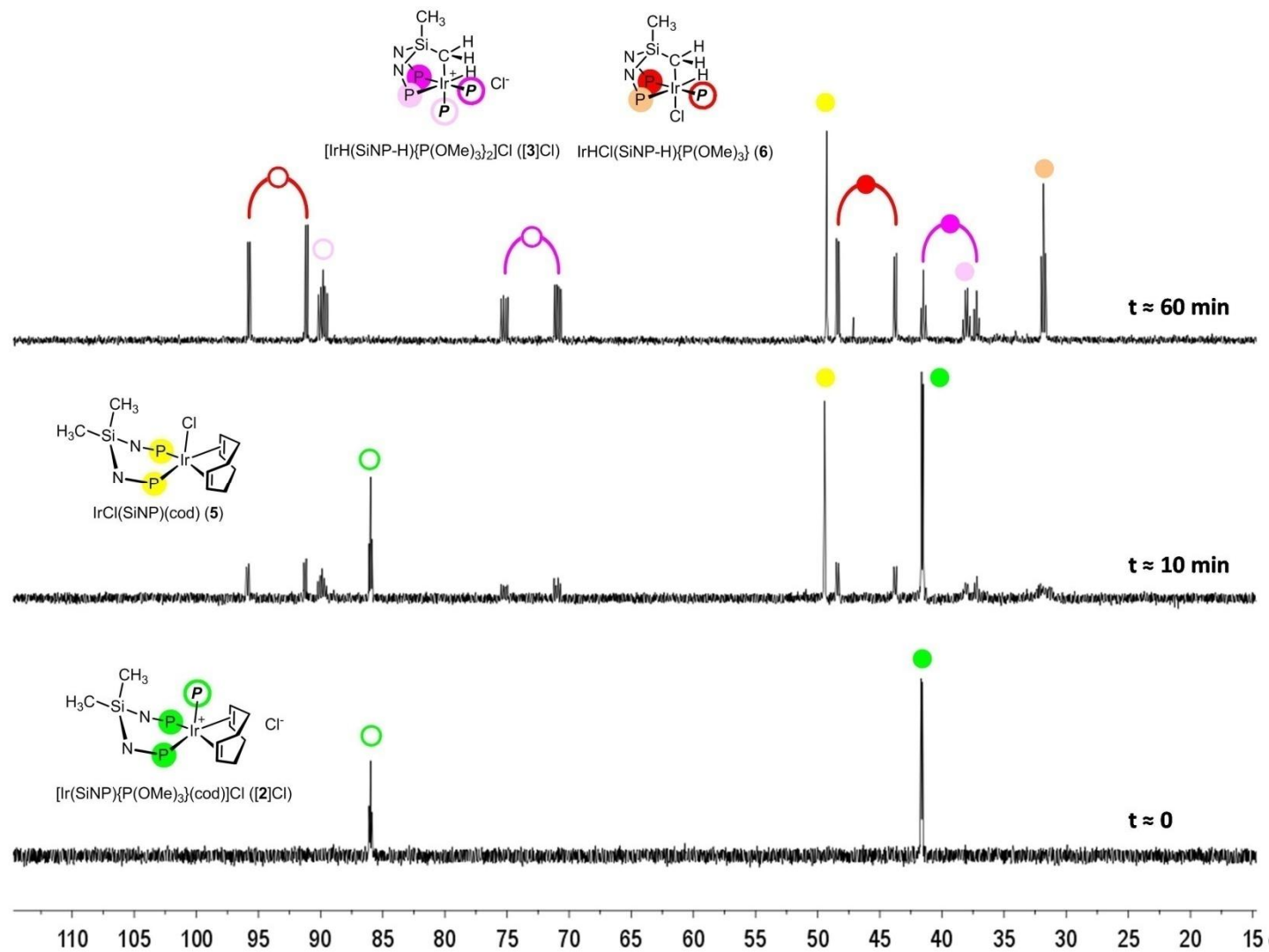


Figure S5. Full view of the $^{31}\text{P}\{^1\text{H}\}$ NMR spectra at different times after adding $\text{P}(\text{OMe})_3$ to $\text{IrCl}(\text{SiNP})(\text{cod})$ ($\mathbf{5}$) (1:1, CDCl_3 , 298 K).

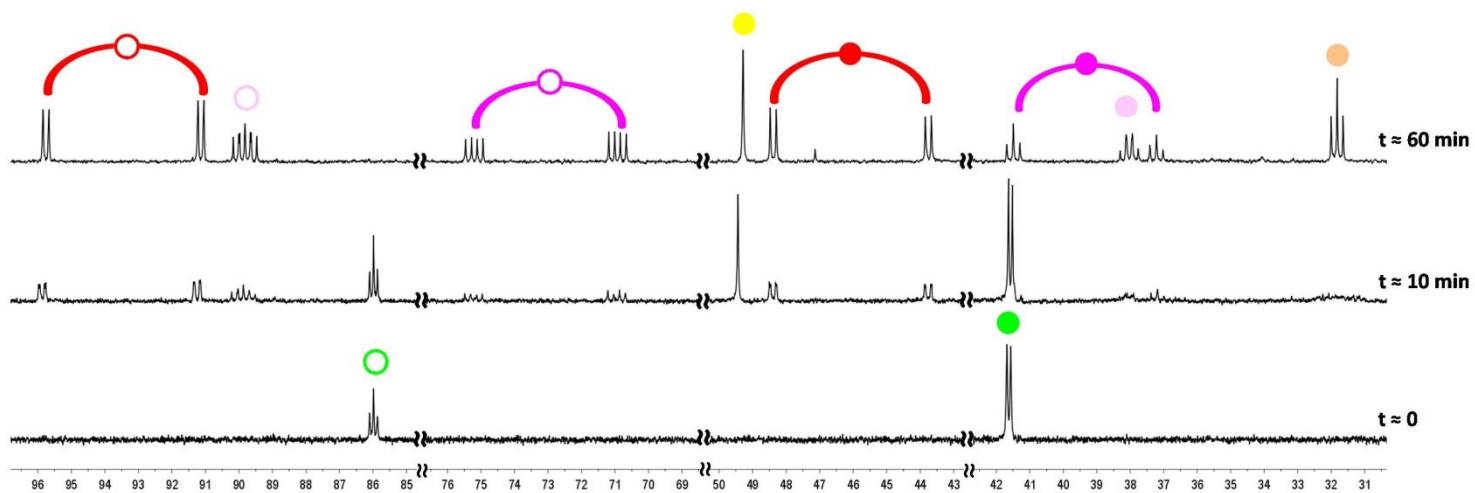
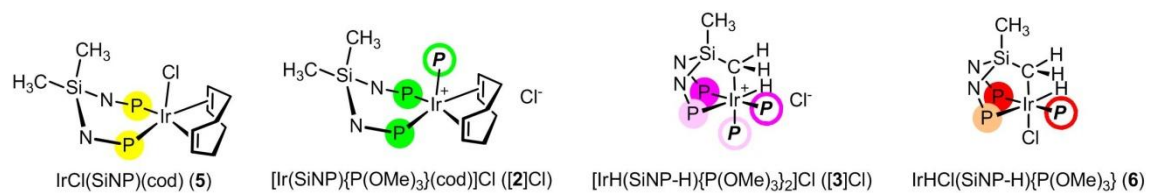
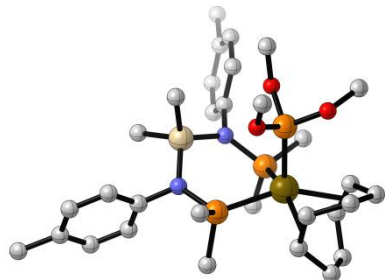


Figure S6. Selected regions of the $^{31}\text{P}\{^1\text{H}\}$ NMR spectra at different times after adding $\text{P}(\text{OMe})_3$ to $\text{IrCl}(\text{SiNP})(\text{cod})$ (**5**) (1:1, CDCl_3 , 298 K).

4. Atomic coordinates of calculated molecular structures

[Ir(SiNP){P(OMe)₃}(cod)]⁺ (2⁺, SPY-5-13)

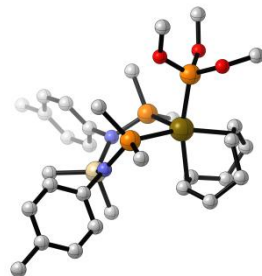


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H	0.46203100	4.26069600	-1.09062100
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C	-2.73188500	3.62198300	-0.37199100
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[Ir(SiNP){P(OMe)₃}(cod)]⁺ (2⁺, TBPY-5-13)

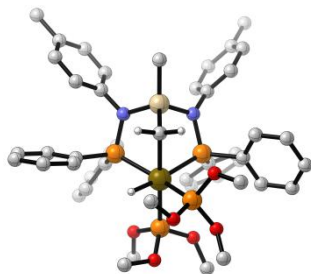


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H	-0.62717400	3.08118400	4.11363500
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H	-1.02824300	-4.10342800	-0.64037500
C	0.77143100	-3.31686300	-1.51889200
H	1.34726500	-3.93541700	-0.83210700
C	-1.10962500	-0.94299200	-2.57861800
H	-1.57248800	0.01846000	-2.39179400
C	0.25786500	-0.94011700	-2.84561400
H	0.75237800	0.02165900	-2.83989900
C	1.51044800	-3.15862800	-2.83487200
H	1.48824300	-4.10460000	-3.39746200
H	2.56054700	-2.95979400	-2.61097400
C	0.94710700	-2.00897600	-3.68357300
H	0.23018700	-2.38514500	-4.42087500
H	1.75244500	-1.53532000	-4.25108400
C	-1.58035100	-3.43731200	-2.65332200
H	-2.45323300	-4.06737000	-2.45452900
H	-1.05446900	-3.91796600	-3.48654200
C	-2.05478800	-2.02924800	-3.04499900
H	-3.03720000	-1.83590500	-2.60959800
H	-2.18005700	-1.93566400	-4.13432700
P	0.42469500	-2.65559100	1.34803000
O	2.02650800	-2.85761600	1.54467100
C	2.66130800	-3.29165800	2.76994100
H	3.65547200	-3.64157000	2.49075800
H	2.74667800	-2.44465800	3.45348100
H	2.11231400	-4.10819900	3.24447200
O	-0.18863400	-2.01640500	2.69428200
C	-0.36702900	-2.68984600	3.96276000
H	0.53103500	-2.57047300	4.57179000
H	-1.20690300	-2.19452500	4.44859600
H	-0.59057900	-3.74662200	3.81294000
O	-0.17127800	-4.16866700	1.48686100
C	0.51191300	-5.41399300	1.23976200
H	0.35671100	-6.05050400	2.11358500
H	0.07429900	-5.88590700	0.35766900
H	1.58100400	-5.26275100	1.08300700

[IrH(SiNP-H){P(OMe)₃}₂]⁺ (3⁺)

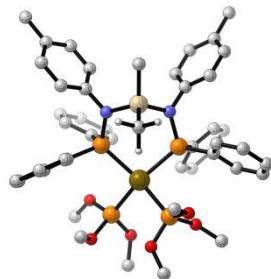


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C	2.32962000	1.77521800	-3.04198600
H	1.70038300	2.36550700	-3.71548900
H	2.88548300	1.04959700	-3.64334600
H	3.05344900	2.45016900	-2.57774700
C	-1.32785200	-2.54174900	4.02609400
H	-1.77696700	-1.66758100	4.50536000
H	-0.43128300	-2.83396800	4.57339700
H	-2.04290400	-3.36976400	4.01495700
C	-2.48544200	-4.26528900	0.93412700
H	-2.20463500	-4.20979500	-0.12034500
H	-3.31663100	-4.96138600	1.05606200
H	-1.63191700	-4.60944400	1.52613600
C	-4.15294400	-0.94366700	2.91939400
H	-4.97886300	-0.74325800	2.23355100
H	-4.20824000	-0.26291100	3.77126800
H	-4.21058900	-1.97786300	3.26068200
C	-4.33289100	0.12472900	-3.42610600
H	-4.74650300	-0.82601200	-3.77552300
H	-4.10824800	0.76096900	-4.28226200
H	-5.04416800	0.63308500	-2.77136500
C	-5.48683600	-1.60071100	-0.64695000
H	-5.79798800	-1.76049300	-1.68036900
H	-6.23749400	-1.00491900	-0.12548100
H	-5.35911300	-2.56360700	-0.14879800
C	-2.55803900	-3.11998700	-3.16014600
H	-2.44582500	-2.42241200	-3.99508500
H	-3.10128700	-4.00591000	-3.49172900
H	-1.57012200	-3.41034400	-2.79151700
C	0.92257600	3.41865600	-0.59988600
C	0.65410400	4.46064200	-1.49675900
H	0.00184300	4.28433700	-2.34426100

C	1.23150700	5.71816500	-1.32074800
H	1.01173200	6.50603000	-2.03665500
C	2.09197500	5.98257000	-0.24766400
C	2.35905900	4.93548800	0.64452800
H	3.02675600	5.10628900	1.48528600
C	1.78647300	3.67624800	0.47454900
H	1.99712900	2.88480900	1.18533600
C	2.69292900	7.35297600	-0.04652400
H	2.05089800	7.97640700	0.58805200
H	2.81831900	7.87908500	-0.99713900
H	3.67078800	7.29439200	0.44028100
C	-2.45129200	2.35516000	-0.54065700
C	-2.48411400	2.90186200	-1.82980400
H	-1.61161100	2.81979600	-2.46713600
C	-3.62965800	3.54691100	-2.29993200
H	-3.63194100	3.98495500	-3.29404100
C	-4.76495000	3.63558800	-1.49247500
H	-5.65302300	4.14627100	-1.85330400
C	-4.75221400	3.06708000	-0.21629800
H	-5.63252200	3.13089500	0.41684000
C	-3.60464200	2.43058500	0.25745000
H	-3.60315800	1.99929300	1.25304500
C	-0.82673200	2.12476600	1.79161000
C	-1.12673400	3.47389800	2.05640500
H	-1.46682300	4.12389600	1.25793200
C	-0.99326600	3.99113700	3.34379400
H	-1.22954500	5.03444400	3.53031300
C	-0.55546200	3.17208700	4.38712200
H	-0.45364600	3.57572700	5.39034800
C	-0.24973000	1.83491900	4.13469400
H	0.09863800	1.19201500	4.93755400
C	-0.38574000	1.31409600	2.84588500
H	-0.14357300	0.27389100	2.67126400
C	3.74782000	-0.13937600	-0.94342100
C	4.55617900	0.83392300	-0.34065000
H	4.10525300	1.58514700	0.29848900
C	5.92818400	0.87162700	-0.58565400
H	6.52974700	1.64343100	-0.11218200
C	6.54321000	-0.05955300	-1.43262000
C	5.72619700	-1.01627900	-2.04821900
H	6.16851600	-1.73688000	-2.73140300
C	4.35163200	-1.05507700	-1.81753400
H	3.74098100	-1.79269200	-2.32600200
C	8.03481400	-0.03792800	-1.66490600
H	8.42991500	0.98189300	-1.63922400
H	8.29614400	-0.47917700	-2.63092200
H	8.56277900	-0.60974100	-0.89164900
C	2.11072700	-2.97019000	-0.44136900
C	1.51936500	-3.64450500	-1.52164300
H	0.61864100	-3.24627000	-1.97170400

C	2.07811800	-4.81715500	-2.03100900
H	1.60139400	-5.32173900	-2.86639900
C	3.24374400	-5.34031600	-1.46897800
H	3.67624800	-6.25637300	-1.86010000
C	3.85304900	-4.67323200	-0.40634000
H	4.76732400	-5.06290900	0.03108000
C	3.29927300	-3.49523900	0.09671600
H	3.80371000	-2.98567900	0.90840200
C	2.08922400	-1.24847000	1.85987000
C	2.63141500	-0.05619300	2.35439000
H	2.67920700	0.81198400	1.71088900
C	3.11669000	0.02195000	3.66175700
H	3.54044900	0.95421700	4.02266600
C	3.06385700	-1.09458200	4.49473700
H	3.45159000	-1.04008500	5.50768100
C	2.51692300	-2.28872400	4.01580200
H	2.48294400	-3.16679700	4.65457600
C	2.02933400	-2.36490500	2.71194800
H	1.61234200	-3.29975500	2.35533700
N	0.38178100	2.09598300	-0.80848700
N	2.31464100	-0.12917700	-0.74778800
O	-0.89432700	-2.21436800	2.69343900
O	-2.95545300	-2.98780800	1.39798800
O	-2.91293200	-0.66265000	2.24270400
O	-3.08406600	-0.07857800	-2.73612300
O	-4.25776000	-0.84771300	-0.56283900
O	-3.33752300	-2.53798700	-2.10289800
Si	1.26440500	0.88818400	-1.78385100
P	-0.95469000	1.46362600	0.07488900
P	1.45258100	-1.32847400	0.12918500
P	-1.91917200	-1.71937400	1.52852600
P	-2.94110500	-1.08023400	-1.47162300
Ir	-0.90843300	-0.95582100	-0.40287000
H	-0.79044400	-2.47389600	-0.89034300

[Ir(SiNP){P(OMe)₃}₂]⁺ (4⁺)

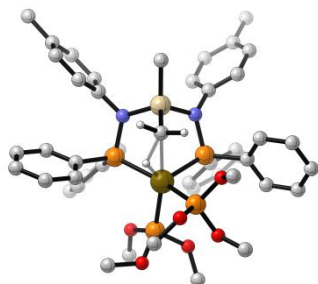


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H	0.19811300	1.40846900	-3.88706700
H	1.24045200	-0.01071900	-3.90556000
H	-0.23930000	-0.02199700	-2.92783500
C	3.00893500	2.30700800	-2.48898700
H	3.62420000	1.72061500	-3.17841200
H	2.59321700	3.15473300	-3.04319000
H	3.66215300	2.70339200	-1.70959500
N	0.63902000	2.22568400	-0.69925300
N	2.30035400	-0.14470700	-0.95227200
P	-0.86050700	1.64208000	-0.08330000
P	1.31902200	-1.22608100	-0.03083700
Ir	-1.05424000	-0.74119300	-0.07550600
C	1.18839700	3.50014300	-0.28420000
C	0.87038000	4.68654700	-0.95687800
C	2.07979500	3.55518900	0.79509800
C	1.43007500	5.89819300	-0.54957200
H	0.17688900	4.66106900	-1.79007900
C	2.64104000	4.76913100	1.18862200
H	2.31104600	2.64303000	1.33618500
C	2.32868600	5.96334600	0.52430800
H	1.16677800	6.80900100	-1.08136600
H	3.32787200	4.78984900	2.03083900
C	3.74330100	-0.29324600	-0.95363600
C	4.38732800	-1.11880800	-1.88420800
C	4.52815800	0.42976300	-0.04520400
C	5.77901600	-1.22042300	-1.89574500
H	3.79883500	-1.68441900	-2.59715200
C	5.91777400	0.32863200	-0.06932200
H	4.04247800	1.06937000	0.68395800
C	6.57098900	-0.49799300	-0.99357400
H	6.25638700	-1.86975900	-2.62529200
H	6.50444400	0.89956800	0.64579700

C	2.95849900	7.27276700	0.93465400
H	3.87509100	7.46434600	0.36323300
H	2.28428400	8.11551800	0.75642200
H	3.23036700	7.27253700	1.99402400
C	8.07780900	-0.58424000	-1.03530700
H	8.41453100	-1.57662900	-1.34908400
H	8.49377100	0.13946800	-1.74707900
H	8.51892700	-0.36839100	-0.05803600
C	-2.12254100	2.71418800	-0.92736200
C	-3.25014700	3.19955900	-0.24909600
C	-1.97236500	3.03199700	-2.28594000
C	-4.19741400	3.98342100	-0.91244700
H	-3.38885200	2.97585300	0.80212700
C	-2.91835800	3.81324900	-2.94940300
H	-1.09941800	2.68528900	-2.82505300
C	-4.03679000	4.29154800	-2.26329900
H	-5.05532200	4.36452900	-0.36581900
H	-2.77574700	4.05828400	-3.99813400
H	-4.77011500	4.90731800	-2.77539700
C	1.61812900	-2.86990200	-0.84053500
C	1.92048500	-4.04367200	-0.13528900
C	1.48682900	-2.94504600	-2.23798700
C	2.11240400	-5.25185000	-0.81203500
H	2.00902100	-4.01979400	0.94282000
C	1.67389800	-4.15079900	-2.91286900
H	1.24987700	-2.05146600	-2.80406100
C	1.99431000	-5.30989800	-2.20082900
H	2.36126900	-6.14650400	-0.24869800
H	1.57665000	-4.18409600	-3.99422300
H	2.15071900	-6.24808200	-2.72478400
C	2.16182600	-1.31106000	1.60439800
C	3.39857600	-1.95269600	1.78974700
C	1.58704400	-0.63010800	2.68709500
C	4.02943200	-1.92452700	3.03467000
H	3.87958600	-2.47104700	0.96841100
C	2.22407200	-0.59404500	3.92749800
H	0.63362200	-0.13236600	2.56247100
C	3.44533000	-1.24619200	4.10573100
H	4.98312900	-2.42800400	3.16225000
H	1.76098100	-0.06070200	4.75249600
H	3.94058200	-1.22455800	5.07209400
C	-1.06183300	2.19535800	1.67299400
C	-0.93201100	3.54397900	2.05369900
C	-1.46106300	1.25961800	2.64175700
C	-1.14995900	3.92890000	3.37639400
H	-0.67626400	4.30149300	1.32360100
C	-1.68651100	1.65051800	3.96340100
H	-1.61506000	0.22496900	2.34729900
C	-1.52142200	2.98446000	4.33578700
H	-1.03732900	4.97269000	3.65384300

H	-1.99931200	0.91136600	4.69501300
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P	-1.49018800	-2.73917900	0.95308100
P	-3.26907300	-0.60795300	-0.58737600
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O	-3.90586200	-2.10531300	-0.79814200
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O	-0.25474500	-3.16262200	1.92210000
O	-1.92353300	-4.14462100	0.25143500
C	-0.37041500	-4.21483900	2.89651300
H	0.61640900	-4.32617700	3.34741600
H	-1.09242400	-3.93774100	3.66924500
H	-0.66874400	-5.15272900	2.41940300
C	-3.77277000	-3.51174900	2.23027000
H	-4.50548500	-3.00421200	2.85952300
H	-4.22831600	-3.80579600	1.28364000
H	-3.40498200	-4.40356900	2.74578400
C	-1.69751200	-4.42729300	-1.13999800
H	-0.77302300	-4.99652400	-1.25449700
H	-2.54507100	-5.02327400	-1.48454500
H	-1.63795200	-3.50367500	-1.72011600
C	-5.27094700	-2.34501800	-1.18736500
H	-5.64822100	-1.55156500	-1.83751100
H	-5.28619500	-3.29386800	-1.72691500
H	-5.90361000	-2.42568400	-0.29870500
C	-5.52744800	0.67841200	0.26617400
H	-5.58620900	1.20603000	-0.68640000
H	-6.26051800	-0.13160900	0.30025400
H	-5.72212800	1.36977200	1.08674200
C	-3.33009200	-0.26880400	-3.24661700
H	-3.98907900	-1.05912600	-3.61961700
H	-3.39769400	0.60257000	-3.89869600
H	-2.29946400	-0.63404400	-3.23637300

TS_4⁺_3⁺

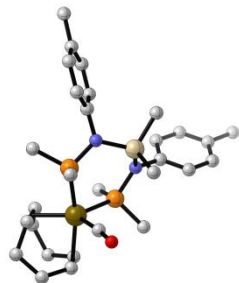


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C	-1.01806900	2.11484300	1.86167400
C	-0.65951800	1.28417800	2.93084400
H	-0.43795600	0.24021600	2.74947700
C	-0.58097700	1.79234000	4.23008600
H	-0.30065200	1.13509900	5.04796300
C	-0.86030300	3.13621600	4.47471600
H	-0.80352400	3.53047500	5.48522700
C	-1.21844000	3.97482100	3.41559700
H	-1.43763900	5.02242500	3.59915300
C	-1.30063400	3.46992500	2.11954300
H	-1.59077800	4.13052800	1.31001200
C	-2.70737200	2.20510100	-0.42410500
C	-2.85725100	2.66450000	-1.73986300
H	-2.01633500	2.61807700	-2.42268200
C	-4.07818200	3.17387200	-2.18406700
H	-4.16896300	3.54748500	-3.20027800
C	-5.17812200	3.20798100	-1.32491600
H	-6.12700600	3.61035900	-1.66736400
C	-5.04886600	2.72641600	-0.02014700
H	-5.89821800	2.75135900	0.65658700
C	-3.82388800	2.23001500	0.42820700
H	-3.73640000	1.87154500	1.44883400
C	2.30463600	-2.74112100	-0.51037300
C	1.57126200	-3.62218800	-1.31872000
H	0.52469900	-3.40404500	-1.50872900
C	2.16630500	-4.76326900	-1.86083800
H	1.58049200	-5.43418600	-2.48271600
C	3.50810100	-5.04238100	-1.59986400
H	3.97252900	-5.93132300	-2.01634800
C	4.25164900	-4.17316900	-0.79895000

H	5.29748800	-4.38097800	-0.59368300
C	3.65946600	-3.03067500	-0.26079000
H	4.25694900	-2.36897200	0.35571700
C	2.23047700	-1.05314500	1.82631000
C	2.57157900	-2.18746800	2.58018600
H	2.43937600	-3.17919200	2.16354300
C	3.09123700	-2.05396200	3.86815800
H	3.36618200	-2.94179700	4.43039500
C	3.26859000	-0.78637600	4.42819800
H	3.67994500	-0.68403300	5.42801200
C	2.91707300	0.34642600	3.69404500
H	3.04282300	1.33665300	4.12131900
C	2.40110600	0.21166400	2.40395200
H	2.12553700	1.09713400	1.84408100
C	0.54768200	3.55883400	-0.58956800
C	1.60592700	3.86229400	0.27830500
H	2.08873400	3.05983400	0.82563700
C	2.04469500	5.17526500	0.44067400
H	2.87234100	5.38001300	1.11500800
C	1.43669500	6.23400600	-0.24616900
C	0.38150100	5.92418700	-1.11418200
H	-0.10217300	6.72167200	-1.67259800
C	-0.05541600	4.61143300	-1.29115000
H	-0.86580800	4.40534100	-1.97882100
C	1.88847700	7.66030800	-0.04377400
H	1.74721400	8.25734100	-0.94935400
H	2.94490600	7.71042800	0.23493100
H	1.31690900	8.14541200	0.75720900
C	3.69384000	0.17533100	-1.00454900
C	4.25235400	-0.46502700	-2.12083500
H	3.61251200	-1.05203900	-2.77257300
C	5.61537000	-0.36485700	-2.39198000
H	6.02253200	-0.87111800	-3.26347100
C	6.46906900	0.37307100	-1.56052100
C	5.90535300	1.00581300	-0.44517200
H	6.54183800	1.58481700	0.21908100
C	4.54056500	0.91483100	-0.16986500
H	4.13147400	1.41871000	0.69724500
C	7.94023400	0.50494100	-1.87314400
H	8.53288000	0.64180100	-0.96413100
H	8.12907200	1.37185700	-2.51830100
H	8.31945200	-0.37723000	-2.39701500
C	0.01932000	-0.22817900	-2.46507400
H	0.64112300	-0.83580400	-3.13711400
H	-0.83950400	0.13571000	-3.02489200
C	2.10059200	2.10167700	-2.97311700
H	1.41393600	2.72902300	-3.55019600
H	2.64966500	1.46002100	-3.66727500
H	2.82361000	2.76141600	-2.48550300
Ir	-0.82750400	-0.95108100	-0.38598200

H	-0.28562600	-1.44980000	-1.90412400
P	-2.84251200	-1.30583500	-1.44607400
O	-3.14471800	-0.20896600	-2.59719200
O	-3.05999300	-2.62658300	-2.39301400
O	-4.13762500	-1.32359000	-0.46480500
C	-3.81190900	-0.44003900	-3.85435700
H	-3.89054900	0.53981200	-4.32701000
H	-3.22691200	-1.11670600	-4.48000800
H	-4.81118800	-0.85581600	-3.71043200
C	-2.90563800	-3.96742500	-1.91054000
H	-3.26931700	-4.62158500	-2.70474300
H	-1.85216000	-4.18139000	-1.71382800
H	-3.48842800	-4.13035400	-1.00019300
C	-5.48841700	-1.30256100	-0.96763200
H	-5.64471800	-2.09059100	-1.71017800
H	-6.13938700	-1.47705600	-0.11023400
H	-5.70990200	-0.32276100	-1.39801000
P	-1.56438400	-2.07905200	1.42703000
O	-2.82287900	-1.37754300	2.17036100
O	-2.17676400	-3.60902500	1.33016300
O	-0.43767700	-2.22847400	2.59496500
C	-3.97904500	-2.04791200	2.70188900
H	-4.56337400	-1.27654800	3.20589900
H	-4.56376800	-2.48750000	1.89233600
H	-3.70409200	-2.82703600	3.41677700
C	-1.29592200	-4.72068200	1.10987100
H	-0.71005600	-4.93501300	2.00866600
H	-1.92755300	-5.57997600	0.87863900
H	-0.61230600	-4.53178900	0.27728300
C	-0.77224900	-2.60969400	3.94115300
H	0.17133800	-2.64915900	4.48621800
H	-1.43151800	-1.86450200	4.39414900
H	-1.25385500	-3.59231500	3.96689300
Si	1.13936200	1.08412300	-1.72987600

[Ir(SiNP)(CO)(cod)]⁺

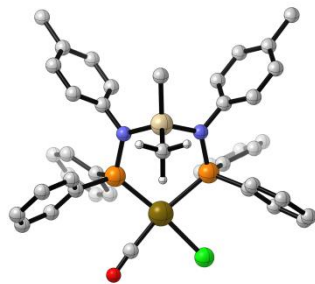


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H	0.36827500	1.41499100	-3.94611000
H	-0.06776100	-0.15079800	-3.25605300
C	-0.59980800	3.59469300	-1.94388400
H	0.29954100	4.00636700	-2.41315200
H	-1.42845000	3.70849600	-2.64942400
H	-0.82355400	4.18724400	-1.05579100
N	-1.66277700	1.18284600	-0.55599200
N	1.21498200	1.56098600	-0.72209200
P	-1.71436100	-0.39208600	0.15750400
P	1.89599600	0.01945900	-0.37570800
Ir	0.35094700	-1.76192500	0.01027700
C	-2.88345000	1.96923900	-0.61969100
C	-3.72737000	1.88828400	-1.73718900
C	-3.21730200	2.86244100	0.40644100
C	-4.86933500	2.68355300	-1.82440600
H	-3.49273500	1.19137600	-2.53520500
C	-4.36845000	3.64613500	0.31608100
H	-2.57567500	2.94675500	1.27521100
C	-5.21327000	3.57663500	-0.79994100
H	-5.50643800	2.60204200	-2.70132500
H	-4.60770600	4.32969100	1.12671600
C	1.86971000	2.77556200	-0.26137700
C	3.11259000	3.18827600	-0.75579800
C	1.23897300	3.57845100	0.69981800
C	3.70025900	4.36964800	-0.29944300
H	3.63531800	2.58883400	-1.49081900
C	1.82427200	4.76423600	1.13794400
H	0.28112000	3.27237800	1.10686500
C	3.06845400	5.18519900	0.64714500
H	4.66898000	4.66196600	-0.69618000

H	1.30866600	5.36572400	1.88214900
C	-6.43763500	4.45385100	-0.90861800
H	-6.20915300	5.38313000	-1.44514600
H	-7.24091100	3.95316600	-1.45712500
H	-6.81795500	4.73283800	0.07811400
C	3.69138300	6.48070700	1.10892800
H	4.77400800	6.48072100	0.95522100
H	3.28154300	7.33421500	0.55479100
H	3.49567300	6.66174800	2.17024600
C	-3.21635500	-1.17192000	-0.59793300
C	-4.52110700	-0.83770700	-0.19218200
C	-3.06106900	-2.04280000	-1.68895500
C	-5.63029000	-1.38439100	-0.83911900
H	-4.67982500	-0.14507600	0.62570300
C	-4.17027100	-2.58299100	-2.34159800
H	-2.06857800	-2.29773700	-2.03960600
C	-5.45890800	-2.26024000	-1.91263700
H	-6.62865700	-1.11761100	-0.50587400
H	-4.02454900	-3.25545600	-3.18145900
H	-6.32351100	-2.68418700	-2.41439300
C	2.97497600	-0.42708000	-1.81250500
C	3.64188700	-1.66588700	-1.83568200
C	3.11838900	0.43513600	-2.90734300
C	4.45462400	-2.01278100	-2.91390700
H	3.52101200	-2.36749000	-1.01764100
C	3.92217200	0.07942400	-3.99404900
H	2.59217000	1.38107200	-2.92413800
C	4.59702300	-1.14055000	-3.99716400
H	4.97031600	-2.96819600	-2.91058200
H	4.01471200	0.75874900	-4.83583400
H	5.22384600	-1.41593200	-4.83974300
C	3.08116400	0.37088200	0.99416700
C	4.45421000	0.10910500	0.87159700
C	2.60380900	0.93539200	2.19073000
C	5.32577900	0.39382300	1.92604900
H	4.85575200	-0.30700200	-0.04408300
C	3.47705300	1.22527400	3.23727200
H	1.55036500	1.16269100	2.30534700
C	4.84122400	0.95095000	3.10901100
H	6.38498000	0.18418700	1.81351800
H	3.09073300	1.66552100	4.15124100
H	5.52079400	1.17471500	3.92563800
C	-2.18552900	-0.08613900	1.91671300
C	-3.09975500	-0.88428700	2.62221100
C	-1.48596600	0.90871700	2.61952500
C	-3.32200200	-0.67468000	3.98661000
H	-3.64739800	-1.67330900	2.12001100
C	-1.70631300	1.11794100	3.97992800
H	-0.76575500	1.52551800	2.09319000
C	-2.62963000	0.32596100	4.66888600

H	-4.03947300	-1.29789000	4.51187700
H	-1.15860200	1.89792700	4.50020100
H	-2.80481200	0.48736600	5.72810900
C	0.45516500	-2.19432700	-1.84519200
O	0.53315800	-2.56330200	-2.94253800
C	-1.08171500	-3.46132600	0.89956800
H	-2.07936300	-3.19257500	0.56941900
C	-0.26553800	-4.04607500	-0.06487900
H	-0.71698700	-4.20649400	-1.04062200
C	1.86528000	-2.70378900	1.26668000
H	2.84529800	-2.25172700	1.13849000
C	0.95527100	-1.95062700	2.10089100
H	1.36001900	-1.02834500	2.50432000
C	1.91168500	-4.23743500	1.25246600
C	-0.90239200	-3.67116400	2.39611600
C	-0.02423500	-2.59877200	3.06364700
H	2.93709300	-4.56205400	1.05144300
H	1.67110000	-4.61415500	2.25293600
H	-1.89358100	-3.67994100	2.85817400
H	-0.48303300	-4.66951600	2.55455800
H	0.52154200	-3.03043300	3.91590600
H	-0.66360800	-1.81732100	3.47951700
C	0.98345300	-4.85789800	0.19671300
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IrCl(SiNP)(CO)

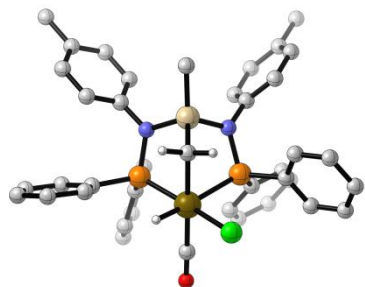


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H	1.02362100	-0.05268600	-3.80472700
H	-0.04049700	-1.14474200	-2.89160300
C	0.29694100	2.84931500	-2.55514400
H	1.19021900	2.90286700	-3.18536300
H	-0.57399800	3.05326600	-3.18583100
H	0.36454600	3.63653700	-1.80154600
N	-1.32491000	1.06834100	-0.82076800
N	1.59129600	0.83742700	-0.80614800
P	-1.86022400	-0.40113600	-0.09799000
P	1.74347400	-0.58844100	0.14647600
Ir	-0.25702700	-2.01043300	0.13621200
Cl	-2.01636500	2.31746500	-0.58616600
C	-3.05544200	2.74156200	-1.42428000
C	-1.63355000	3.14174400	0.48013500
C	-3.69841200	3.95855800	-1.19120000
H	-3.36489300	2.11385800	-2.25268200
C	-2.27622800	4.35919900	0.70164300
H	-0.84003100	2.81354200	1.14412900
C	-3.32047500	4.79114100	-0.12854500
H	-4.50604500	4.26599000	-1.85079300
H	-1.96423100	4.98048900	1.53731700
C	2.63158900	1.84312600	-0.78251900
C	3.72613300	1.77864100	-1.65349300
C	2.54063300	2.92946100	0.10020300
C	4.70551200	2.77457100	-1.63408700
H	3.81201700	0.94819700	-2.34481300
C	3.51853900	3.92190500	0.10848500
H	1.69939400	2.98852000	0.78303300
C	4.62081000	3.86364300	-0.75771000
H	5.54740000	2.70286500	-2.31804300
H	3.42566500	4.75387000	0.80223000

C	-3.99797400	6.12177700	0.09903000
H	-3.49222900	6.92163100	-0.45619200
H	-5.03905000	6.10268500	-0.23614300
H	-3.98334100	6.40180500	1.15635500
C	5.66625100	4.95383900	-0.75725400
H	6.58247400	4.62896700	-1.25779100
H	5.30459500	5.84821300	-1.27942900
H	5.92361300	5.25977500	0.26185500
C	-3.35342700	-0.92048800	-1.07340500
C	-4.39334400	-1.63544600	-0.45646000
C	-3.42832600	-0.68471400	-2.45365000
C	-5.47899400	-2.09785200	-1.20247900
H	-4.36398700	-1.83126500	0.61036200
C	-4.51621600	-1.14299700	-3.19921800
H	-2.63979800	-0.13345900	-2.95030800
C	-5.54472900	-1.85208600	-2.57553200
H	-6.27510200	-2.64592000	-0.70716300
H	-4.55851400	-0.94307000	-4.26590100
H	-6.39163700	-2.20864800	-3.15426700
C	3.18615100	-1.50168100	-0.56277700
C	4.15371900	-2.12592100	0.23871900
C	3.26065700	-1.66498000	-1.95544500
C	5.18643000	-2.86632000	-0.34148800
H	4.10612000	-2.04447200	1.31786000
C	4.28979800	-2.40796500	-2.53446900
H	2.51333100	-1.21008700	-2.59462900
C	5.26004900	-3.00743500	-1.72777000
H	5.93055000	-3.33563800	0.29531200
H	4.33209500	-2.51695200	-3.61419300
H	6.06367700	-3.58378100	-2.17657900
C	2.32780800	-0.02805200	1.80050300
C	3.62543400	0.47186400	2.01460900
C	1.42883100	-0.05178400	2.87661500
C	4.00899600	0.92348100	3.27739800
H	4.34012600	0.50804000	1.20037700
C	1.81281000	0.40312000	4.13967100
H	0.42403300	-0.42411200	2.72317200
C	3.10514400	0.88882900	4.34260100
H	5.01496600	1.30375300	3.42775200
H	1.10256600	0.37400000	4.96054300
H	3.40832000	1.23932100	5.32483300
C	-2.65407200	0.01304300	1.52729900
C	-3.74397500	0.89734400	1.62958700
C	-2.22533000	-0.65560200	2.68426800
C	-4.35170700	1.13382200	2.86245500
H	-4.13019400	1.39732000	0.74939000
C	-2.83720900	-0.42187000	3.91846400
H	-1.42670800	-1.38667200	2.60366900
C	-3.89632000	0.48104600	4.01135000
H	-5.18808900	1.82391900	2.92302300

H	-2.48993900	-0.95273500	4.79986100
H	-4.37500600	0.66551500	4.96867000
Cl	1.22803600	-3.84566300	0.80022100
C	-1.53144200	-3.33208500	-0.12444400
O	-2.25287100	-4.21767500	-0.33170000

IrHCl(SiNP-H)(CO)

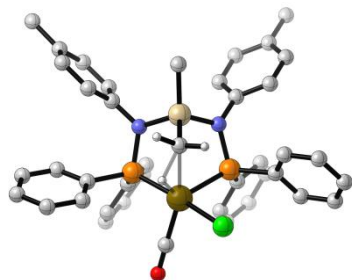


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C	0.35521600	2.29089600	-2.92685400
H	-0.48115800	2.30434500	-3.63286500
H	1.28232700	2.18751500	-3.49924600
H	0.38034700	3.25367300	-2.40968600
C	-1.92232700	2.34975700	-0.58445400
C	-2.86716900	2.87280900	-1.47753100
H	-3.17900300	2.28294700	-2.33195100
C	-3.40049200	4.14778400	-1.28078200
H	-4.12722000	4.53281600	-1.99182000
C	-3.01249500	4.94159400	-0.19317800
C	-2.06481200	4.41329800	0.69493100
H	-1.73910400	5.00592800	1.54625600
C	-1.53015500	3.13928800	0.50717500
H	-0.80996800	2.74231700	1.21485300
C	-3.61113500	6.31036300	0.02972000
H	-4.47366100	6.25874600	0.70587600
H	-3.95922200	6.75207400	-0.90838000
H	-2.88682100	6.99432500	0.48229400
C	-3.49400700	-0.80112800	-0.82386100
C	-3.71398500	-0.50659800	-2.17724600
H	-2.95661700	0.02363600	-2.74374000
C	-4.90024000	-0.88908800	-2.80578300
H	-5.05738400	-0.64416300	-3.85220100
C	-5.87893700	-1.58425500	-2.09252900
H	-6.80256800	-1.88131600	-2.58051200
C	-5.66241200	-1.89869900	-0.74904100
H	-6.41619500	-2.44292100	-0.18757000
C	-4.47823900	-1.51226600	-0.11898500
H	-4.32899500	-1.76183200	0.92654500
C	-2.39757800	0.03499500	1.68296500
C	-3.51892900	0.85417800	1.91657000

H	-4.09056900	1.24687400	1.08283700
C	-3.91420800	1.16044000	3.21753100
H	-4.78092200	1.79407500	3.38069200
C	-3.20211100	0.64922000	4.30656900
H	-3.51527100	0.88369800	5.31977400
C	-2.09235500	-0.16664700	4.08756400
H	-1.53383500	-0.56978600	4.92655700
C	-1.69159300	-0.46969100	2.78358900
H	-0.82621200	-1.10191900	2.63005300
C	2.63670100	1.80221700	-0.73615000
C	2.42664700	3.06718000	-0.16811600
H	1.49132300	3.27889400	0.33977000
C	3.39015300	4.06982800	-0.27906000
H	3.19524300	5.04263900	0.16524200
C	4.59821300	3.84707600	-0.95286300
C	4.79312100	2.58808700	-1.53691100
H	5.70812900	2.39089000	-2.08999100
C	3.82987200	1.58369700	-1.44160800
H	3.99800400	0.62947500	-1.92707500
C	5.65696300	4.92065800	-1.03838100
H	6.23292600	4.84058200	-1.96513700
H	6.36843500	4.84117800	-0.20681900
H	5.21668100	5.92108400	-0.99403100
C	3.41892300	-1.38565200	-0.20052000
C	4.52447500	-1.06168200	0.60362800
H	4.39635700	-0.45235300	1.49070700
C	5.80205600	-1.51729800	0.27249800
H	6.64336500	-1.26244900	0.90996700
C	5.99629600	-2.29315600	-0.87081800
H	6.98996400	-2.64862100	-1.12689400
C	4.90590200	-2.61174900	-1.68446300
H	5.04743400	-3.21448000	-2.57650300
C	3.62751700	-2.16324400	-1.35175500
H	2.78995600	-2.42199700	-1.98937300
C	1.84912300	-0.34327800	1.97229400
C	1.55777800	0.92085200	2.49824900
H	1.30582400	1.73442000	1.83176700
C	1.59637700	1.14090700	3.87750700
H	1.37380100	2.12874300	4.26946500
C	1.91617900	0.09688000	4.74543300
H	1.94482600	0.26752400	5.81740800
C	2.20245700	-1.17130900	4.23016400
H	2.45480700	-1.98853300	4.89901100
C	2.17258000	-1.39075300	2.85361800
H	2.41351800	-2.37738900	2.46967400
N	-1.32824100	1.05612900	-0.79785700
N	1.60649000	0.79387200	-0.67307200
Si	0.16517400	0.84015000	-1.75619400
P	-1.87891500	-0.38504600	-0.03421300
P	1.74616300	-0.69018000	0.16897300

Ir	-0.05343300	-2.01024400	-0.48720000
H	1.05307200	-2.98234500	-1.09184000
Cl	-1.63989400	-3.58869100	-1.57670000
C	-0.15233800	-3.10451400	1.06635300
O	-0.20963700	-3.82767400	1.96716800

TS_CO

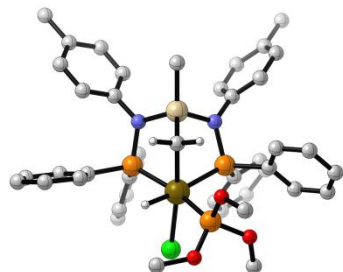


F	-1.90390600	-0.44797800	-0.01207400
P	1.72660600	-0.62108200	0.19012600
Si	0.09514200	0.93707300	-1.68208700
N	-1.42166200	1.04531500	-0.76032000
N	1.54461000	0.89017300	-0.62055400
C	-2.31983500	-0.11594100	1.75424300
C	-1.74707000	-0.93726900	2.73565500
H	-1.04110000	-1.70582900	2.43878900
C	-2.08090500	-0.77765100	4.08243900
H	-1.63091500	-1.42705700	4.82737000
C	-2.98248900	0.21456900	4.46536700
H	-3.24143800	0.34218100	5.51290300
C	-3.56143700	1.03889600	3.49633800
H	-4.27217000	1.80713100	3.78790800
C	-3.24332500	0.86994700	2.14941000
H	-3.72674300	1.49527000	1.40780500
C	-3.55529300	-0.85647500	-0.72410400
C	-3.75884700	-0.74227400	-2.10893000
H	-2.97100900	-0.34305000	-2.73905100
C	-4.96593000	-1.12948400	-2.68679800
H	-5.10681800	-1.02731500	-3.75907000
C	-5.98432800	-1.66155100	-1.89244800
H	-6.92361600	-1.96911600	-2.34309700
C	-5.78338500	-1.80640500	-0.52041300
H	-6.56545900	-2.22848200	0.10431100
C	-4.57748100	-1.40890000	0.06082100
H	-4.43798900	-1.53122900	1.12920400
C	3.42455100	-1.23759200	-0.19795600
C	3.59747300	-2.36638300	-1.01248800
H	2.72187900	-2.89849200	-1.37097400
C	4.87935900	-2.81497100	-1.33837800
H	4.99607600	-3.69520200	-1.96387600
C	6.00180300	-2.14353700	-0.85385800
H	6.99864700	-2.49571000	-1.10415800

C	5.84106700	-1.02071900	-0.03817400
H	6.71089200	-0.49538600	0.34563900
C	4.56328500	-0.57031000	0.28982300
H	4.45559600	0.29860400	0.93037200
C	1.84536500	-0.26908000	1.99467400
C	2.56680900	-1.12797900	2.83988400
H	3.11357400	-1.96891700	2.42605200
C	2.59681900	-0.90350800	4.21672000
H	3.16079800	-1.57542000	4.85713600
C	1.91254500	0.18200500	4.76707500
H	1.94421500	0.36011600	5.83815400
C	1.18112700	1.03203600	3.93632600
H	0.63100400	1.86816900	4.35770300
C	1.13945800	0.80073100	2.56131600
H	0.54293000	1.44473800	1.92535100
C	-2.09172900	2.30531300	-0.58100300
C	-1.51236800	3.30094500	0.21850900
H	-0.56402500	3.10112600	0.70675800
C	-2.13322200	4.53860100	0.38574500
H	-1.65558000	5.29351900	1.00573600
C	-3.36180200	4.82198900	-0.22246400
C	-3.93597600	3.82389900	-1.02198300
H	-4.88290200	4.01816800	-1.52041200
C	-3.31372000	2.59046100	-1.20998100
H	-3.77571700	1.84223400	-1.84232500
C	-4.05513800	6.14738300	-0.01241500
H	-4.83619100	6.07140500	0.75458900
H	-4.53909700	6.49624200	-0.93026500
H	-3.35223900	6.91965800	0.31331200
C	2.58970500	1.87690300	-0.70502300
C	3.50871100	1.84264300	-1.76478100
H	3.44444800	1.04074100	-2.49376100
C	4.50363100	2.81110900	-1.87866200
H	5.20354300	2.75899800	-2.70908800
C	4.62244300	3.84432900	-0.93927100
C	3.70853500	3.86873600	0.12137500
H	3.77793800	4.65514500	0.86912300
C	2.70522000	2.90587900	0.23860200
H	2.01342100	2.94630800	1.07160300
C	5.68393000	4.90948400	-1.08138900
H	6.58268000	4.51703200	-1.56664600
H	5.97474500	5.31825000	-0.10908400
H	5.32525000	5.74752300	-1.69226400
C	0.12819900	-0.72146700	-2.54345900
H	0.99263600	-0.73572900	-3.22047100
H	-0.75665900	-1.00525500	-3.11276900
C	0.22165400	2.46076200	-2.77368400
H	0.33529400	3.38169500	-2.19538400
H	-0.68642900	2.55433600	-3.37799200
H	1.07678300	2.38036500	-3.45087000

Ir	-0.00536700	-1.93608800	-0.54975000
H	0.72126900	-1.92660300	-2.04070500
Cl	-1.54398100	-3.48976400	-1.66273100
C	0.41781300	-3.32019700	0.62979900
O	0.66487100	-4.17330900	1.38192800

IrHCl(SiNP-H){P(OMe)₃} (6, OC-6-43)

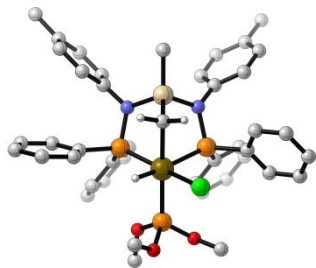


C	-0.20948700	-0.79403800	-2.13597200
H	0.41975300	-1.52314800	-2.65862600
H	-1.11570500	-0.66646200	-2.73186700
C	1.35718600	1.84473300	-3.18183400
H	0.53081200	2.14587200	-3.83404400
H	2.07238500	1.27424700	-3.78305600
H	1.85924000	2.75109400	-2.83375300
C	-4.19799700	-2.69296300	-2.93827100
H	-4.40329400	-3.72682900	-2.64668800
H	-4.07045500	-2.63587300	-4.02106900
H	-5.02306500	-2.04973100	-2.62356100
C	-4.46295000	-2.14705300	1.17925600
H	-4.60589300	-3.21815900	1.34562000
H	-5.40528600	-1.61598500	1.32494100
H	-3.70616200	-1.77502600	1.87382600
C	-1.80136500	-4.96557500	-0.39344500
H	-1.22867700	-5.03249700	-1.32411200
H	-2.28584600	-5.92550500	-0.20004500
H	-1.14361300	-4.70247500	0.43721400
C	-0.40401100	3.17592300	-0.80995500
C	-1.20331000	3.92540800	-1.68472800
H	-1.88291100	3.41044700	-2.35435500
C	-1.13096100	5.31873400	-1.69789600
H	-1.75974500	5.87557600	-2.38878400
C	-0.26075800	6.01275900	-0.84767300
C	0.53927000	5.25920500	0.02148100
H	1.22535600	5.76834700	0.69450000
C	0.46700000	3.86729600	0.04603600
H	1.07247000	3.30122500	0.74584300
C	-0.20649600	7.52247600	-0.84671900
H	-0.89813800	7.94511100	-0.10679400
H	-0.48419000	7.93418500	-1.82167700
H	0.79476700	7.88768000	-0.59808600
C	-3.18588800	1.18644700	-0.39992000

C	-3.43071800	1.19109900	-1.78235900
H	-2.61015400	1.03184000	-2.47376500
C	-4.71655200	1.39765600	-2.28099600
H	-4.88247800	1.40704400	-3.35489600
C	-5.78624500	1.59326600	-1.40444500
H	-6.78807000	1.75674400	-1.79169300
C	-5.55857800	1.57772700	-0.02855500
H	-6.38332200	1.72926600	0.66255400
C	-4.26989800	1.37453200	0.46998100
H	-4.11154500	1.36735400	1.54281800
C	-1.49333700	1.60428900	1.87393600
C	-1.92591400	2.93227900	2.05722000
H	-2.27019400	3.51599200	1.21077500
C	-1.92939300	3.50522400	3.32746900
H	-2.26127600	4.53212500	3.45353800
C	-1.51396000	2.75963500	4.43468800
H	-1.52279800	3.20713100	5.42510000
C	-1.09966900	1.43971600	4.26524500
H	-0.78374200	0.84921200	5.11989100
C	-1.08591800	0.86243400	2.99214600
H	-0.78520700	-0.17248100	2.87202300
C	3.44111300	0.65244900	-1.06681000
C	3.84780800	1.96513300	-0.78290300
H	3.14306300	2.65379700	-0.32815800
C	5.12926100	2.40672100	-1.10894800
H	5.40965400	3.43292900	-0.88307500
C	6.05797400	1.55638000	-1.72093200
C	5.64288000	0.25268800	-2.01953800
H	6.33068100	-0.42646000	-2.51794800
C	4.35812400	-0.19274500	-1.71085700
H	4.05851100	-1.19786500	-1.98172400
C	7.45952900	2.02329100	-2.03573500
H	7.49077500	3.10119700	-2.22204100
H	7.86191100	1.51587200	-2.91798300
H	8.14456900	1.81770100	-1.20326000
C	2.81121300	-2.41408800	0.05207500
C	4.01567600	-2.50588600	0.76732700
H	4.24359200	-1.78481400	1.54366300
C	4.93413200	-3.52022400	0.49033000
H	5.85764600	-3.57677200	1.05954900
C	4.67047200	-4.45240200	-0.51296800
H	5.38532300	-5.24180500	-0.72778800
C	3.48033100	-4.36589600	-1.23866700
H	3.26457000	-5.08770600	-2.02147900
C	2.55813100	-3.35818800	-0.95632200
H	1.63196600	-3.30466400	-1.51755700
C	2.08301100	-0.45214100	2.01261100
C	2.46035000	0.86946200	2.28042500
H	2.52099400	1.58291500	1.46950300
C	2.77116400	1.27045400	3.58130100

H	3.06921900	2.29776900	3.77071900
C	2.69926900	0.35571600	4.63155800
H	2.94306300	0.66636000	5.64376800
C	2.31037800	-0.96189500	4.37655100
H	2.24335200	-1.67874600	5.18993700
C	2.00284200	-1.36654300	3.07802600
H	1.68584800	-2.38660500	2.89461700
N	-0.44063200	1.74144500	-0.80980000
N	2.09515900	0.23040700	-0.78580800
O	-2.96315400	-2.23371600	-2.36247400
O	-4.07985100	-1.90522900	-0.18565100
O	-2.86536500	-4.00921600	-0.50862500
Si	0.70059500	0.77254000	-1.78387800
P	-1.47758500	0.79901700	0.21361000
P	1.62848000	-1.00909500	0.31757900
P	-2.65215500	-2.41225100	-0.77779600
Ir	-0.66215200	-1.48222800	-0.15101700
H	-0.08261000	-2.90291600	-0.58139700
Cl	-1.04269700	-2.53966000	2.11685800

IrHCl(SiNP-H){P(OMe)₃} (6', OC-6-34)

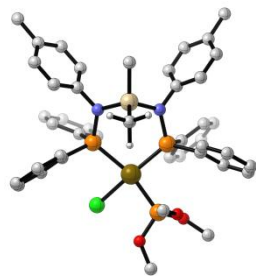


C	0.16670700	-0.07003300	-2.53237900
H	1.05861900	-0.38503200	-3.08340900
H	-0.68876200	-0.12604000	-3.20917600
C	0.82085900	3.13313900	-2.52074100
H	-0.03394500	3.44030800	-3.13214300
H	1.68299400	3.00440000	-3.18152100
H	1.04634500	3.94677300	-1.82562700
C	0.08948000	-4.19505600	2.92721100
H	-0.89644800	-4.11535200	3.39148600
H	0.86761700	-4.00711200	3.66944300
H	0.21233100	-5.19506100	2.50172400
C	0.15944500	-5.09090100	-1.10587700
H	-0.19101700	-4.58038500	-2.00505300
H	0.00817500	-6.16863600	-1.20245200
H	1.22447200	-4.89009800	-0.95008300
C	-3.32220000	-3.74089500	0.65649700
H	-3.56710900	-3.11487000	-0.20365100
H	-4.12572900	-3.70406700	1.39550200
H	-3.17051400	-4.77122100	0.32466600
C	-1.56678500	3.08591800	-0.39948200
C	-2.65285200	3.66384500	-1.07476200
H	-3.16085400	3.09715400	-1.84602300
C	-3.08032800	4.95353300	-0.76057100
H	-3.92361600	5.37748500	-1.30108400
C	-2.43750400	5.71880600	0.22186300
C	-1.34480200	5.14331300	0.88155400
H	-0.81903100	5.71366000	1.64378000
C	-0.92054100	3.84889700	0.58376400
H	-0.07636400	3.41897900	1.11280700
C	-2.92089900	7.10722200	0.56932800
H	-3.74075400	7.07354900	1.29818000
H	-3.29670900	7.63336800	-0.31386000
H	-2.12120100	7.71165600	1.00772200
C	-3.48159700	0.22053800	-0.93805300

C	-3.61689700	0.53704100	-2.29831100
H	-2.75463600	0.88193400	-2.85806600
C	-4.84700100	0.41156000	-2.94157300
H	-4.93203400	0.66686400	-3.99402400
C	-5.96112200	-0.05461200	-2.24053800
H	-6.91934100	-0.15562700	-2.74236200
C	-5.83378100	-0.39751900	-0.89484500
H	-6.69316400	-0.76634900	-0.34161700
C	-4.60298900	-0.26241700	-0.24796800
H	-4.52299300	-0.52803500	0.80064900
C	-2.26672600	0.60690300	1.62274000
C	-3.18113800	1.61609400	1.98322100
H	-3.63965700	2.23410000	1.21990800
C	-3.52015200	1.82388100	3.31889900
H	-4.22518200	2.60873900	3.57812300
C	-2.96187100	1.02203300	4.31813900
H	-3.23278100	1.18041800	5.35855200
C	-2.06226100	0.01535300	3.97279700
H	-1.62367400	-0.61512700	4.74056400
C	-1.71500600	-0.18947200	2.63468000
H	-1.01356600	-0.97441600	2.38418500
C	2.97642900	1.91851600	-0.50149900
C	3.20740800	2.84246400	0.52594500
H	2.49161800	2.93108000	1.33430600
C	4.34800300	3.64713300	0.52034000
H	4.50102300	4.35485700	1.33176000
C	5.29330500	3.56409800	-0.50833300
C	5.05966900	2.63777400	-1.53400600
H	5.77730300	2.54512400	-2.34586900
C	3.92517500	1.82998500	-1.53345600
H	3.76860500	1.11240400	-2.33272900
C	6.50953400	4.45986400	-0.52971300
H	6.33841900	5.34789300	-1.15133700
H	7.38166300	3.94205400	-0.94142800
H	6.76700400	4.81031400	0.47417600
C	3.31861700	-1.27625200	-0.50563400
C	4.51352700	-0.93995900	0.15704500
H	4.49093600	-0.28832800	1.02281300
C	5.74117000	-1.43375600	-0.28404900
H	6.64912100	-1.16362900	0.24766200
C	5.80312100	-2.26367400	-1.40413700
H	6.75918400	-2.64998700	-1.74642500
C	4.62911900	-2.58947400	-2.08355900
H	4.66455300	-3.22921000	-2.96088000
C	3.39956300	-2.09881200	-1.63937200
H	2.49342800	-2.35774700	-2.17471800
C	1.94055100	-0.39338700	1.85666700
C	1.43207800	0.70966700	2.55393100
H	0.90982900	1.48781700	2.01001200
C	1.57917000	0.81359900	3.93863500

H	1.17763300	1.67884200	4.45794000
C	2.23211400	-0.19264800	4.64957900
H	2.35449700	-0.11098500	5.72601100
C	2.72580200	-1.30851000	3.96893900
H	3.23471500	-2.09869200	4.51425100
C	2.57715200	-1.41082300	2.58615300
H	2.96584200	-2.28317500	2.07357600
N	-1.09229400	1.77087100	-0.72312100
N	1.78244400	1.11777500	-0.54109000
O	0.25199500	-3.18926300	1.91377200
O	-0.61740900	-4.68723700	0.03201000
O	-2.14464300	-3.25582900	1.32772600
Si	0.41849400	1.51715200	-1.64710000
P	-1.81201400	0.30590900	-0.14530300
P	1.70581000	-0.51404600	0.02446600
P	-0.69252000	-3.14737600	0.58430200
Ir	-0.22097400	-1.42871700	-0.87731200
H	0.74129300	-2.43547500	-1.63369400
Cl	-1.92476600	-2.47535900	-2.33147800

IrCl(SiNP){P(OMe)₃} (7)

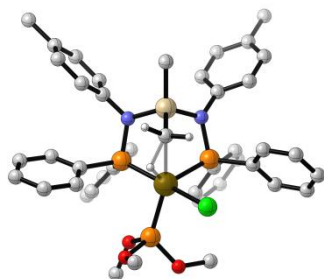


Si	1.02803600	1.28306600	-1.79272800
C	0.44779700	0.27085400	-3.27580400
H	-0.18699600	0.87258100	-3.93576000
H	1.31916300	-0.03586000	-3.86614900
H	-0.10199800	-0.62564800	-2.97869400
C	1.92236900	2.78832700	-2.48075100
H	2.75376500	2.46453100	-3.11495100
H	1.23528500	3.37693800	-3.09719900
H	2.32637100	3.44534600	-1.70819300
N	-0.32850000	1.85176300	-0.79280700
N	2.18441200	0.34721300	-0.82236500
P	-1.43725200	0.72839700	-0.05029900
P	1.65879500	-0.99693600	0.14069400
Ir	-0.67704900	-1.36898300	0.25818800
C	-0.43429200	3.27605600	-0.59356300
C	-1.24769500	4.07170600	-1.41075300
C	0.30935000	3.90032600	0.41833100
C	-1.31649800	5.45206100	-1.21255800
H	-1.83577000	3.60329500	-2.19223200
C	0.24293600	5.27957300	0.60309800
H	0.92527400	3.28675500	1.06848500
C	-0.57107500	6.08252100	-0.20843900
H	-1.95859700	6.04932300	-1.85572900
H	0.82741900	5.73955800	1.39645900
C	3.56672200	0.76388300	-0.82144300
C	4.50036200	0.20896300	-1.70583100
C	3.99899000	1.76789300	0.05759700
C	5.82548000	0.64957500	-1.70744800
H	4.19016000	-0.57643900	-2.38534800
C	5.32066900	2.20634600	0.04543700
H	3.28827000	2.19290800	0.75890900
C	6.26014300	1.65703100	-0.83848100
H	6.53196400	0.20047100	-2.40154600
H	5.62928200	2.98475900	0.73938000

C	-0.61929700	7.58077800	-0.02132300
H	0.21519200	8.07258100	-0.53710200
H	-1.54456800	8.00525900	-0.42182400
H	-0.55095000	7.85540600	1.03609900
C	7.68633100	2.15441600	-0.86476300
H	8.35868000	1.41904200	-1.31613500
H	7.77441800	3.07962700	-1.44828900
H	8.05285600	2.37381000	0.14324000
C	-3.02440500	1.06291400	-0.97815800
C	-4.26121800	1.18622500	-0.32872000
C	-3.00485400	1.13122700	-2.37989500
C	-5.43737800	1.38148800	-1.05793200
H	-4.31218900	1.13378800	0.75231600
C	-4.17654800	1.32833800	-3.11019900
H	-2.06321300	1.03532600	-2.90649100
C	-5.40092000	1.45481800	-2.44986600
H	-6.38272900	1.48486900	-0.53179400
H	-4.13266400	1.38637100	-4.19465900
H	-6.31513300	1.61203600	-3.01536300
C	2.48545200	-2.46123400	-0.64152100
C	3.04805300	-3.50183500	0.11274100
C	2.46307100	-2.58535000	-2.03860700
C	3.60107300	-4.61714700	-0.51873400
H	3.03981500	-3.45311400	1.19400800
C	3.01130900	-3.70239300	-2.66954500
H	2.01271500	-1.80516200	-2.63994500
C	3.58798300	-4.72132400	-1.90968600
H	4.03435400	-5.41064400	0.08353800
H	2.98440900	-3.77598400	-3.75338800
H	4.01657000	-5.59236800	-2.39756100
C	2.55654100	-0.76681500	1.73825000
C	3.93705200	-0.98683900	1.87773500
C	1.83610100	-0.29156500	2.84280700
C	4.57415800	-0.74309800	3.09478100
H	4.51960500	-1.34984400	1.03855800
C	2.47508100	-0.04109100	4.05770400
H	0.76959700	-0.12743400	2.74975700
C	3.84549800	-0.26959400	4.18736200
H	5.64183100	-0.92186300	3.18652400
H	1.89784600	0.32318300	4.90280000
H	4.34350200	-0.08253600	5.13485200
C	-1.87609700	1.45446000	1.61414600
C	-2.39036300	2.75194000	1.79080300
C	-1.76165800	0.62767400	2.74348800
C	-2.73491900	3.21590600	3.06098900
H	-2.54089500	3.40419300	0.93947800
C	-2.11121200	1.09053300	4.01407600
H	-1.41979600	-0.39584500	2.60650100
C	-2.59017300	2.39014300	4.17773100
H	-3.12358000	4.22425100	3.17414600

H	-2.01706800	0.42809300	4.86997200
H	-2.86271400	2.75390800	5.16481900
P	-2.72667100	-2.30554500	0.01322400
O	-3.88570800	-1.83037600	1.05993200
O	-2.65556500	-3.92976800	0.08670500
O	-3.57693000	-2.07650800	-1.38043200
C	-3.78318300	-4.79706400	-0.03887100
H	-4.49228200	-4.43926100	-0.79304400
H	-3.39738500	-5.77348100	-0.34019500
H	-4.29172800	-4.90061500	0.92559200
C	-5.30406100	-1.93652100	0.86088400
H	-5.58946400	-1.55389800	-0.12051000
H	-5.64211500	-2.97138400	0.96906300
H	-5.76639900	-1.33094800	1.64330800
C	-2.96270700	-2.41520800	-2.62837800
H	-2.94849700	-3.50133400	-2.77331600
H	-3.56281900	-1.94698200	-3.41065300
H	-1.93669000	-2.03668100	-2.67476600
Cl	0.03502900	-3.34905300	1.45487400

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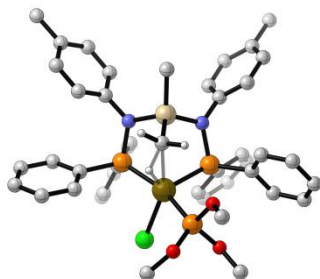


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Si	-0.18354900	1.48235100	-1.66996400
N	-1.69803900	1.28501200	-0.75219900
N	1.25963700	1.57660400	-0.61443700
C	-2.30765600	-0.05623400	1.74535100
C	-1.54686500	-0.75364900	2.69420000
H	-0.70326900	-1.34937700	2.35978700
C	-1.85492100	-0.67374600	4.05471600
H	-1.25391400	-1.22177100	4.77443500
C	-2.91924000	0.11765500	4.48473600
H	-3.15946900	0.18282300	5.54252400
C	-3.68007300	0.82525100	3.54960200
H	-4.51292600	1.44095300	3.87799200
C	-3.38436000	0.73394100	2.18983000
H	-4.00293800	1.26560200	1.47590300
C	-3.51101700	-0.91823200	-0.70132400
C	-3.76587000	-0.82836400	-2.07989300
H	-3.05126900	-0.33124400	-2.72691400
C	-4.92853200	-1.36488600	-2.62898200
H	-5.10901900	-1.27766700	-3.69666400
C	-5.84845100	-2.02828900	-1.81355600
H	-6.75251600	-2.45172800	-2.24195000
C	-5.59300900	-2.15231700	-0.44850700
H	-6.29867000	-2.67190100	0.19391900
C	-4.43319400	-1.60319900	0.10407300
H	-4.25644500	-1.70417500	1.16937300
C	3.44344100	-0.24427000	-0.35418100
C	3.77303900	-1.23668800	-1.28809100
H	2.98284900	-1.86483900	-1.68458300
C	5.09830700	-1.42994100	-1.68402900
H	5.33562200	-2.20901100	-2.40296500
C	6.11276300	-0.63477800	-1.15114900
H	7.14448400	-0.78810700	-1.45561700

C	5.79752000	0.35731200	-0.21990800
H	6.58124800	0.98183400	0.19953700
C	4.47481700	0.55282100	0.17547700
H	4.24854400	1.32694000	0.90032100
C	1.80112700	0.41560500	1.91188000
C	2.73988000	-0.23149000	2.73117800
H	3.41955900	-0.95807200	2.30313700
C	2.81113100	0.05631600	4.09442900
H	3.55152900	-0.44606400	4.71089000
C	1.94280800	0.99033000	4.66357300
H	2.00411000	1.21809100	5.72413000
C	0.99399600	1.62593100	3.86273300
H	0.30249700	2.34216600	4.29673300
C	0.92169200	1.33498600	2.49969200
H	0.16885600	1.81941500	1.88882600
C	-2.56717600	2.40532900	-0.51768400
C	-2.15842500	3.45078200	0.32361800
H	-1.18737300	3.39190600	0.80497700
C	-2.97458800	4.56092000	0.53823800
H	-2.62608900	5.35946300	1.18904800
C	-4.23475400	4.66239400	-0.06330800
C	-4.63919100	3.61584000	-0.90329400
H	-5.60639600	3.67139400	-1.39769800
C	-3.82224400	2.51034500	-1.13749000
H	-4.15573400	1.72264100	-1.80212200
C	-5.13569800	5.84676900	0.19634800
H	-5.69891100	6.12569500	-0.69995900
H	-4.56404700	6.72102300	0.52155800
H	-5.86922100	5.62559400	0.98208100
C	2.14574900	2.70965500	-0.64512400
C	3.05753800	2.86563700	-1.70131800
H	3.10970500	2.09906200	-2.46828400
C	3.88947300	3.98067200	-1.77011400
H	4.58230700	4.07699200	-2.60271900
C	3.85001700	4.97785900	-0.78572600
C	2.93896900	4.81952400	0.26504300
H	2.87845800	5.58107800	1.03897200
C	2.09899300	3.70712500	0.33760700
H	1.40299500	3.61089700	1.16211800
C	4.77650400	6.16939800	-0.84646200
H	5.75615700	5.93402100	-0.41146600
H	4.37088500	7.02084600	-0.29210000
H	4.95079300	6.48947100	-1.87852800
C	0.13232200	-0.05301700	-2.67993800
H	0.99780500	0.14486500	-3.32688600
H	-0.68605600	-0.42797400	-3.29350900
C	-0.31117500	3.09187500	-2.63559300
H	-1.23205400	3.09280100	-3.22785300
H	0.53534600	3.19408700	-3.32085000
H	-0.32851300	3.97377200	-1.98956700

Ir	0.13529000	-1.42271700	-0.77100100
H	0.86324400	-1.16610300	-2.25472400
P	0.89882300	-3.21537700	0.31836100
O	2.10258600	-4.16232400	-0.30801200
O	1.61329900	-2.90703900	1.75541100
O	-0.10888300	-4.47906000	0.67316700
C	1.91604700	-4.79836200	-1.57904400
H	2.87911000	-5.23689300	-1.85073600
H	1.15829200	-5.58388800	-1.50788800
H	1.60515900	-4.07270800	-2.33741300
C	2.22270800	-3.94564500	2.53893600
H	3.12324700	-4.32098100	2.04649500
H	2.48116500	-3.49250900	3.49856500
H	1.52505300	-4.77299400	2.69618300
C	-1.47623700	-4.27200900	1.05201000
H	-2.02528000	-3.76778800	0.25401200
H	-1.89748900	-5.26726100	1.21276200
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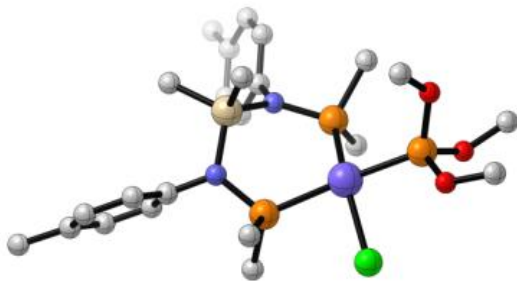


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N	-0.55072300	1.76546200	-0.81105800
N	2.07831400	0.33359500	-0.76071800
C	-1.53337400	1.57143200	1.91613200
C	-1.10226100	0.79725000	3.00361800
H	-0.77522500	-0.22445900	2.83599300
C	-1.11439300	1.32721400	4.29699100
H	-0.77820000	0.71471000	5.12824300
C	-1.55415200	2.63202100	4.51565100
H	-1.56287100	3.04398000	5.52143400
C	-1.99611700	3.40807700	3.43968800
H	-2.34913000	4.42216000	3.60704100
C	-1.99373000	2.88089400	2.14929200
H	-2.36134600	3.48352000	1.32590700
C	-3.26492500	1.12138400	-0.30893000
C	-3.55852300	1.22228400	-1.67879800
H	-2.75095900	1.18193200	-2.40219100
C	-4.87137000	1.37169200	-2.12434800
H	-5.07187900	1.46223200	-3.18880300
C	-5.92477000	1.40323000	-1.20775200
H	-6.94820600	1.52219300	-1.55268100
C	-5.65045900	1.27820600	0.15545400
H	-6.46143000	1.29793200	0.87866800
C	-4.33506500	1.13731600	0.60102800
H	-4.14146400	1.04176800	1.66397000
C	2.82958700	-2.31422300	0.09920700
C	2.40040800	-3.45433900	-0.59415100
H	1.36045800	-3.51111000	-0.90652600
C	3.28439200	-4.50422800	-0.85018700
H	2.93619500	-5.38436600	-1.38387600
C	4.60611000	-4.43055400	-0.40793500
H	5.29289400	-5.25024900	-0.60088400
C	5.04113500	-3.30380800	0.29352200

H	6.06721200	-3.24259200	0.64533200
C	4.15990500	-2.25271100	0.54687400
H	4.50952800	-1.38522700	1.09673200
C	2.16489600	-0.32359700	2.03385400
C	2.30787500	-1.24518900	3.08549200
H	2.14111900	-2.30053200	2.90521900
C	2.65004200	-0.80672500	4.36460900
H	2.75443100	-1.53050300	5.16799300
C	2.85983600	0.55178900	4.61261300
H	3.13317700	0.88911200	5.60863800
C	2.71509200	1.47328600	3.57558900
H	2.87194600	2.53241800	3.75941100
C	2.36289000	1.03727300	2.29742500
H	2.24435300	1.75678500	1.49781100
C	-0.56237400	3.20370900	-0.82146200
C	0.31144900	3.92569000	0.00553600
H	0.96280800	3.38194700	0.68104100
C	0.33488400	5.31932200	-0.01773300
H	1.02556400	5.85087200	0.63285200
C	-0.51905400	6.04554400	-0.85760400
C	-1.39093000	5.32167900	-1.68108900
H	-2.06067700	5.85630100	-2.35082200
C	-1.41358800	3.92698900	-1.66944700
H	-2.09604800	3.39280900	-2.31963600
C	-0.51953100	7.55613700	-0.85541000
H	-0.78824200	7.95861000	-1.83695300
H	0.46136200	7.95702600	-0.58236100
H	-1.24462200	7.95265200	-0.13327200
C	3.41961500	0.71357700	-1.11730800
C	4.21121100	-0.11295500	-1.92995800
H	3.81476600	-1.06717400	-2.25943900
C	5.49157800	0.28032300	-2.31591600
H	6.08161200	-0.38081300	-2.94629600
C	6.02661800	1.51245000	-1.91819400
C	5.22504100	2.34370200	-1.12652900
H	5.60344000	3.31487000	-0.81630100
C	3.94656100	1.95313800	-0.72895600
H	3.34141100	2.62584000	-0.13119600
C	7.42552100	1.92121600	-2.31529800
H	7.70410100	1.50306000	-3.28751500
H	8.16539200	1.56685100	-1.58627800
H	7.52404700	3.00944900	-2.37378100
C	-0.05814300	-0.72898000	-2.42316800
H	0.67756600	-1.13266800	-3.13507200
H	-1.01819300	-0.63092800	-2.92783900
C	1.30846700	1.98833100	-3.09615200
H	0.47873500	2.30507600	-3.73662100
H	2.03758500	1.45910300	-3.71755400
H	1.79209000	2.88927900	-2.70966200
Ir	-0.59690600	-1.38774800	-0.09892600

H	-0.08026800	-1.75913200	-1.77898800
P	-2.50971300	-2.46140500	-0.69593200
O	-3.09284500	-1.96137400	-2.14053800
O	-2.53946400	-4.07335100	-1.02259400
O	-3.72068300	-2.29349500	0.38248900
C	-3.89582600	-2.73897100	-3.03711200
H	-4.00027100	-2.14355400	-3.94680600
H	-3.41536900	-3.69208200	-3.26889400
H	-4.89059400	-2.92876400	-2.62223000
C	-1.93093100	-5.04253100	-0.15220400
H	-2.05615700	-6.00969800	-0.64505400
H	-0.87264900	-4.82028300	-0.00488000
H	-2.42196400	-5.05390300	0.82446100
C	-5.01181900	-2.89667900	0.24421600
H	-4.94135500	-3.90057500	-0.18592500
H	-5.43925200	-2.96327300	1.24692900
H	-5.65584500	-2.26682100	-0.37848700
Si	0.66978300	0.86421900	-1.72886700
Cl	-0.55388800	-2.79603800	1.93942900

RhCl(SiNP){P(OMe)₃} (8)



Si	0.98149100	1.17712200	-1.79656600
C	0.37245400	0.13110000	-3.24469500
H	-0.28056400	0.71396800	-3.90342100
H	1.23166700	-0.18540300	-3.84736400
H	-0.16641900	-0.76307700	-2.92079900
C	1.86378300	2.66999600	-2.52377600
H	2.68899600	2.33648000	-3.16091300
H	1.16837100	3.24619600	-3.14260900
H	2.27523500	3.34082000	-1.76712900
N	-0.37738600	1.76548300	-0.80618000
N	2.14625700	0.25484000	-0.82584400
P	-1.49760800	0.65437400	-0.06620500
P	1.61622000	-1.08670600	0.14970000
C	-0.46091600	3.18879600	-0.58824600
C	-1.26383100	4.00653900	-1.39402500
C	0.29082600	3.78873100	0.43224700
C	-1.31355300	5.38475300	-1.17722500
H	-1.85831000	3.55721300	-2.18169600
C	0.24320800	5.16630100	0.63564700
H	0.89808100	3.15846700	1.07443600
C	-0.55930500	5.99129500	-0.16490300
H	-1.94740800	5.99942800	-1.81208600
H	0.83367000	5.60725700	1.43532900
C	3.52568100	0.68022600	-0.82751600
C	4.46362400	0.12361500	-1.70654100
C	3.95229600	1.69290100	0.04439600
C	5.78627200	0.57134800	-1.71051900
H	4.15871200	-0.66894700	-2.38002600
C	5.27165800	2.13837200	0.02995200
H	3.23933500	2.11933400	0.74253100
C	6.21483500	1.58788400	-0.84915600
H	6.49571900	0.12064100	-2.40058100
H	5.57546500	2.92345600	0.71850500
C	-0.58693400	7.48745300	0.04194100

H	0.24830300	7.97546600	-0.47620300
H	-1.51082600	7.92849300	-0.34365400
H	-0.50446100	7.74742400	1.10198900
C	7.63823800	2.09303200	-0.87839800
H	8.31538300	1.35698800	-1.32146300
H	7.72220200	3.01289600	-1.47097400
H	8.00207000	2.32440300	0.12789500
C	-3.09022300	1.00089500	-0.97457500
C	-4.32469200	1.07200400	-0.31177300
C	-3.08320100	1.11304500	-2.37350600
C	-5.51070400	1.25923300	-1.02584400
H	-4.36524000	0.98500900	0.76766000
C	-4.26594800	1.30240900	-3.08849300
H	-2.14284800	1.06090400	-2.90926300
C	-5.48741300	1.37612300	-2.41546800
H	-6.45410900	1.32231100	-0.49001600
H	-4.23239500	1.39588800	-4.17080100
H	-6.41000800	1.52650400	-2.96898800
C	2.43231800	-2.56063400	-0.62477400
C	2.94827400	-3.61737000	0.14147300
C	2.44200700	-2.68262200	-2.02234100
C	3.48706600	-4.74573100	-0.47857200
H	2.91319700	-3.56901700	1.22218500
C	2.97607800	-3.81307600	-2.64183400
H	2.02855700	-1.88971400	-2.63378200
C	3.50605400	-4.84797900	-1.86986200
H	3.88415900	-5.55113200	0.13278100
H	2.97537700	-3.88384300	-3.72624600
H	3.92368000	-5.72939400	-2.34854300
C	2.52892400	-0.84912200	1.73672900
C	3.90601900	-1.09177100	1.86898000
C	1.82599500	-0.34287400	2.83872000
C	4.55766300	-0.83863100	3.07646200
H	4.47405100	-1.47990200	1.03101700
C	2.47938600	-0.08268300	4.04374400
H	0.76132100	-0.16318400	2.75398100
C	3.84675800	-0.33313400	4.16626000
H	5.62265800	-1.03524600	3.16287900
H	1.91565900	0.30494800	4.88762500
H	4.35574900	-0.13882500	5.10643200
C	-1.91622500	1.35259000	1.60988400
C	-2.43183000	2.64693400	1.80485700
C	-1.78028200	0.51433400	2.72846800
C	-2.76084700	3.09686100	3.08385600
H	-2.59281000	3.30609700	0.96044600
C	-2.11550300	0.96388300	4.00787700
H	-1.43168900	-0.50579600	2.58345300
C	-2.59838300	2.25961200	4.18983200
H	-3.15103500	4.10264500	3.21300300
H	-2.00589900	0.29407300	4.85602800

H	-2.85933600	2.61225900	5.18402500
P	-2.79240200	-2.42726500	0.05026300
O	-3.93484200	-1.97710700	1.12752000
O	-2.70418000	-4.05276300	0.08972400
O	-3.67642800	-2.18054300	-1.32535000
C	-3.82651800	-4.93008100	-0.02567900
H	-4.55608200	-4.56573800	-0.75687900
H	-3.43838500	-5.89707600	-0.35303400
H	-4.31067900	-5.05515300	0.94859000
C	-5.35651000	-2.09203300	0.95851400
H	-5.66635600	-1.69549400	-0.01012600
H	-5.68378400	-3.13144600	1.05585800
H	-5.80629700	-1.50398000	1.76135700
C	-3.07964200	-2.49271200	-2.58773200
H	-3.05861000	-3.57588200	-2.75315300
H	-3.69348800	-2.01531000	-3.35361100
H	-2.05674600	-2.10574200	-2.64686400
Rh	-0.73332800	-1.46341300	0.27528400
Cl	-0.02931500	-3.38236800	1.58015800