Supplementary Information for:

Imidazolidines as hydride sources for the formation of late transition metal monohydrides

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Experimental section

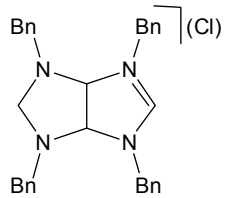
General procedures. All manipulations were carried out under nitrogen atmosphere. Deuterated solvents ($CDCl_3$, CD_2Cl_2, CD_3CN, C_6D_6) were used as received from commercial suppliers (VWR). NMR spectra were recorded on Varian Innova 300 and 500 MHz spectrometers at 298 K. Electrospray mass spectra (ESI-MS) were recorded on a Micromass Quatro LC instrument, and nitrogen was employed as drying and nebulising gas. High Resolution Mass Spectra (HR MS) were recorded on a Q-TOF Premier instrument. Elemental analyses were carried out in an EA 1108 CHNS-O Carlo Erba analyser. Neutral compounds 1,3-dimethylimidazolidine (**A**-Me),[1] 1,3-dibenzylimidazolidine (**A**-Bn),[2] 2,4,6,8-tetrabenzyl-2,4,6,8-tetraazabicyclo[3.3.0]octane (**B**),[3] 3-methyl-1,3-oxazolidine (**E**)[4] were prepared as described in the literature. 1,3,5-Trimethylhexahydro-1,3,5-triazine (**C**), N,N,N,N-tetramethylmethanediamine (**D**) and hexamethylenetetramine (**F**) were used as received from commercial suppliers (Aldrich). Metal complexes $[MCp^*Cl_2]_2$ (M = Rh[5], Ir[6]), $[RuCl_2(p\text{-cymene})]_2$,[7] **2a**,[8] $[IrCp^*Cl_2(PPh_3)]$ (**2b**),[5] $[RuCl_2(PPh_3)(p\text{-cymene})]$ (**4**)[9] and $[RuCl_2(PPh_3)_3]$ (**6**),[10] were synthesized according to literature methods.

Imidazolidines as reducing agents of metal chloride dimers. $[IrCp^*Cl_2]_2$ (1 equiv) and the amine under study (2 equiv) were placed together in an NMR tube and dissolved in CD_3CN (0.5 mL). A dark precipitate of $[IrCp^*(\mu\text{-H})Cl]_2$ immediately appeared. The reaction quantitatively afforded the di-μ-hydrido complex and the corresponding azolium salt after five minutes. The total conversion of the amine into its corresponding azolium salt was corroborated by ^1H NMR spectroscopy using anisole as internal standard. The black solid so formed was separated and redissolved in CD_2Cl_2 and its spectroscopic data compared to those reported in the literature for $[IrCp^*(\mu\text{-H})Cl]_2$,[11] showing complete agreement.

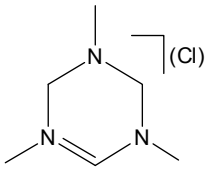
$[RuCl_2(p\text{-cymene})]_2$ or $[RhCp^*Cl_2]_2$ (1 equiv) and the amine under study (1 equiv) were placed together in an NMR tube and dissolved in $CDCl_3$ (0.5 mL). The evolution of the reaction was monitored by ^1H NMR spectroscopy, using anisole as internal standard. The reactions involving $[RhCp^*Cl_2]_2$ quantitatively afforded the mono-μ-hydrido complex and the corresponding azolium salts after five hours of reactions. Upon the same reactions conditions, 50% conversion was achieved when using $[RuCl_2(p\text{-cymene})]_2$. The mono-μ-hydrido complexes $[Ru_2(\mu\text{-Cl})(\mu\text{-}$

H)Cl_2(*p*-cymene)$_2$][12] and [$Rh_2Cp^*_2$(μ-Cl)(μ-H)Cl_2][13] were identified by comparison with previously reported spectroscopic data.

The spectroscopic data of the salts derived from 1,3-dimethylimidazolidine (**A**-Me)[14] and 1,3-dibenzylimidazolidine (**A**-Bn)[15] are in agreement with those reported in the literature. The spectroscopic data of the salts derived from 2,4,6,8-tetrabenzyl-2,4,6,8-tetraazabicyclo[3.3.0]octane (**B**) and 1,3,5-trimethylhexahydro-1,3,5-triazine (**C**) are not available in the literature and are given below.



^{1}H NMR (300 MHz, $CDCl_3$): δ 10.9 (s, 1H, NCHN), 6.99-7.36 (m, 20H, CH_{Ph}), 5.20 (d, $^2J_{H\text{-}H}$ = 14.7 Hz, 2H, CH_2Ph), 5.02 (s, 2H, CH_{ring}), 4.29 (d, $^2J_{H\text{-}H}$ = 14.7 Hz, 2H, CH_2Ph), 4.00-3.79 (m, 4H CH_2Ph; 2H, $CH_{2\ ring}$). ^{1}H NMR (500 MHz, CD_3CN): δ 8.85 (s, 1H, NCHN), 7.11-7.41 (m, 20H, CH_{Ph}), 5.25 (s, 2H, CH_{ring}), 4.76 (d, $^2J_{H\text{-}H}$ = 15 Hz, 2H, CH_2Ph), 4.38 (d, $^2J_{H\text{-}H}$ = 15 Hz, 2H, CH_2Ph), 4.01 (d, $^2J_{H\text{-}H}$ = 13 Hz, 2H, CH_2Ph), 3.91-3.96 (m, 2H CH_2Ph; 2H, $CH_{2\ ring}$). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 158.0 (NCHN), 137.4 ($C_{q\ Ph}$), 132.8 ($C_{q\ Ph}$), 129.1 (CH_{Ph}), 129.0 (CH_{Ph}), 128.8 (CH_{Ph}), 128.7 ($C_{q\ Ph}$), 128.6 (CH_{Ph}), 128.2 ($C_{q\ Ph}$), 2.7 (CH_{ring}), 72.3 ($CH_{2\ ring}$), 58.4 (CH_2Ph), 50.0 (CH_2Ph). Electrospray MS (20 V, *m/z*): 473.3 $[M]^+$.



^{1}H NMR (300 MHz, $CDCl_3$): δ 9.25 (s, 1H, NCHN), 4.28 (s, 4H, NCH_2N), 3.27 (s, 6H, NCH_3), 2.57 (s, 3H, NCH_3). ^{1}H NMR (300 MHz, CD_3CN): 8.65 (s, 1H, NCHN), 4.23 (s, 4H, NCH_2N), 3.15 (s, 6H, NCH_3), 2.57 (s, 3H, NCH_3). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 153.6 (NCHN), 67.0 (NCH_2N), 40.6 (NCH_3), 39.7 (NCH_3). Electrospray MS (20 V, *m/z*): 128.3 $[M]^+$.

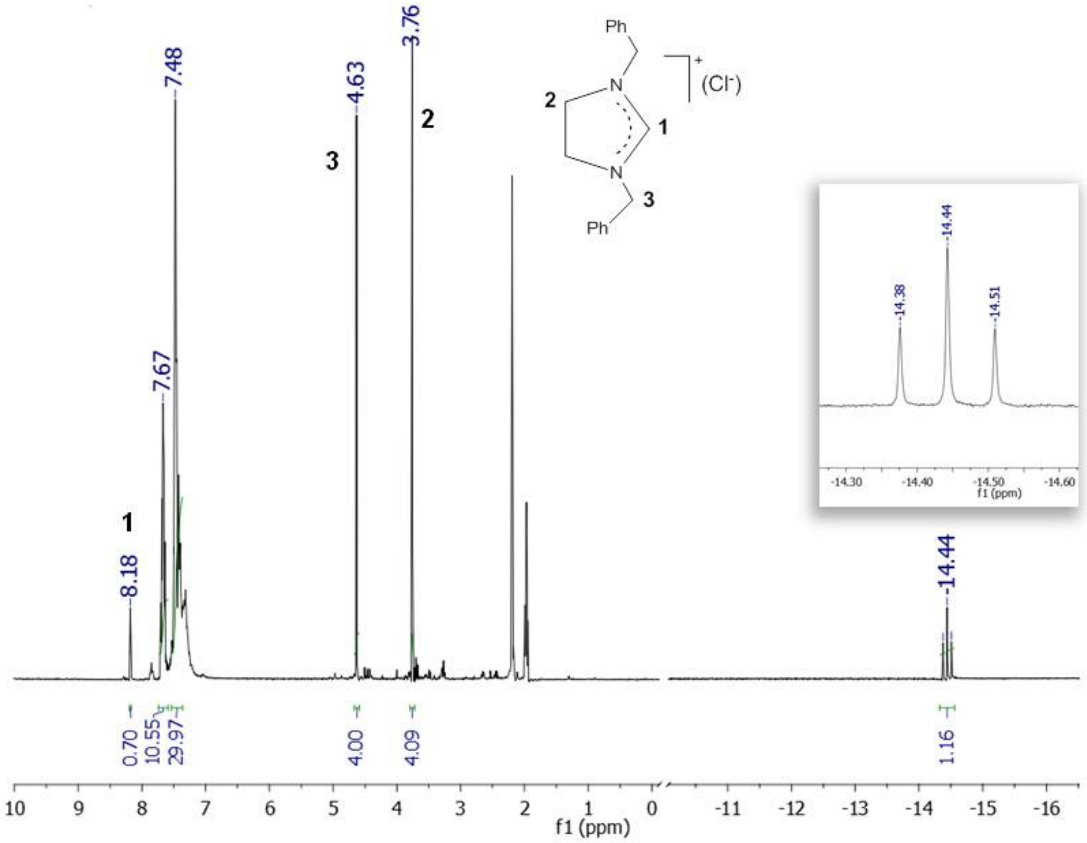
Synthesis of complex 1. A mixture of 1,3-dibenzylimidazolidine (**A**-Bn, 63 mg, 0.25 mmol) and [$IrCp^*Cl_2$]$_2$ (100 mg, 0.125 mmol) was refluxed in deoxygenated acetonitrile overnight. After this time, the volatiles were removed under vacuum. The crude solid was dissolved in CH_2Cl_2 and purified by column chromatography. Elution with CH_2Cl_2 afforded a yellow band that contained complex **1**. A pure sample of complex **1** was obtained by recrystallization from CH_2Cl_2. Yield: 29 mg (18 %). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.48-7.26 (m, 10H, CH_{Ph}), 5.59, 4.59 (AB, J_{AB} = 14.5 Hz, 4H, CH_2Ph), 3.48 (m, 4H, NCH_2CH_2N), 3.34 (m, 4H, NCH_2CH_2N), 1.66 (s, 15H, $C_5(CH_3)_5$). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 187.6 (Ir-

$C_{carbene}$), 136.7 ($C_{q\ Ph}$), 128.5, 128.3, 127.6 (CH_{Ph}), 89.4 ($C_5(CH_3)_5$), 55.7 (CH_2Ph), 48.7 (NCH_2CH_2N), 9.2 ($C_5(CH_3)_5$).

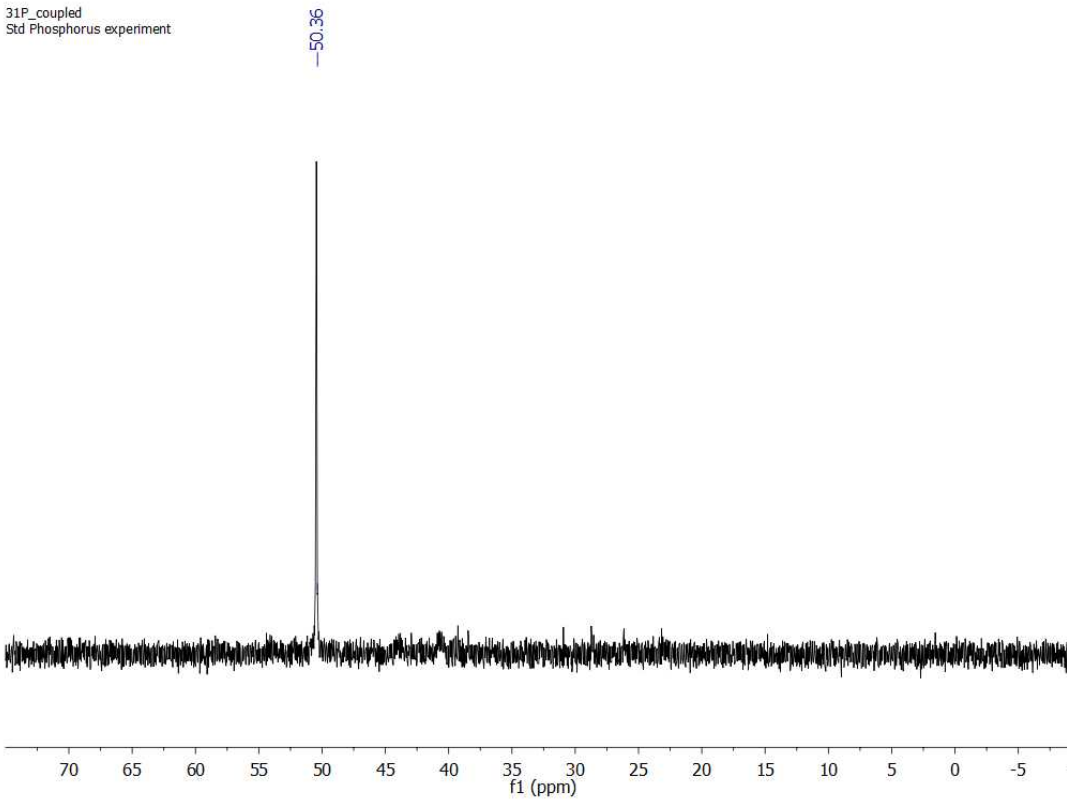
Study of the hydridic properties of imidazolidines. According to the literature,[16] cyclic aminals **A**-**C** (1 mmol) were reacted with acetic acid (1 mmol) in the presence of 5 mol% of $Pd(OAc)_2$ in CD_3CN (0.5 mL). The evolution of the reaction was monitored by ^1H NMR spectroscopy. In the reactions involving **A** and **B**, a black precipitate formed immediately with effervescent H_2 evolution. The NMR spectra of these experiments reveal the clean transformation of **A** and **B** to their corresponding salts after three hours at room temperature. Upon the same reaction conditions, no transformation of compound **C** was observed.

Imidazolidines as reducing agents of metal dichloride complexes. The dichloride complex (1 equiv), 1,3-dibenzylimidazolidine (**A**-Bn, 1 equiv) and AgOTf (1 equiv) were placed together in an NMR tube and dissolved in CD_3CN. The reaction mixture was heated at 45ºC under the exclusion of light. The clean formation of the mono-hydrido complexes, along with 1,3-dibenzylimidazolinium chloride, was monitored by means of ^1H NMR spectroscopy. The mono-hydrido complexes **3a**,[17] [IrCp*HCl(PPh_3)] (**3b**)[18-19] and [RuHCl(PPh_3)(*p*-cymene)] (**5**)[9] were identified by comparison with previously reported spectroscopic data. Mono-hydrido complex [RuHCl$(PPh_3)_2(CH_3CN)_2$] (**7**) was characterized directly from the reaction mixture.

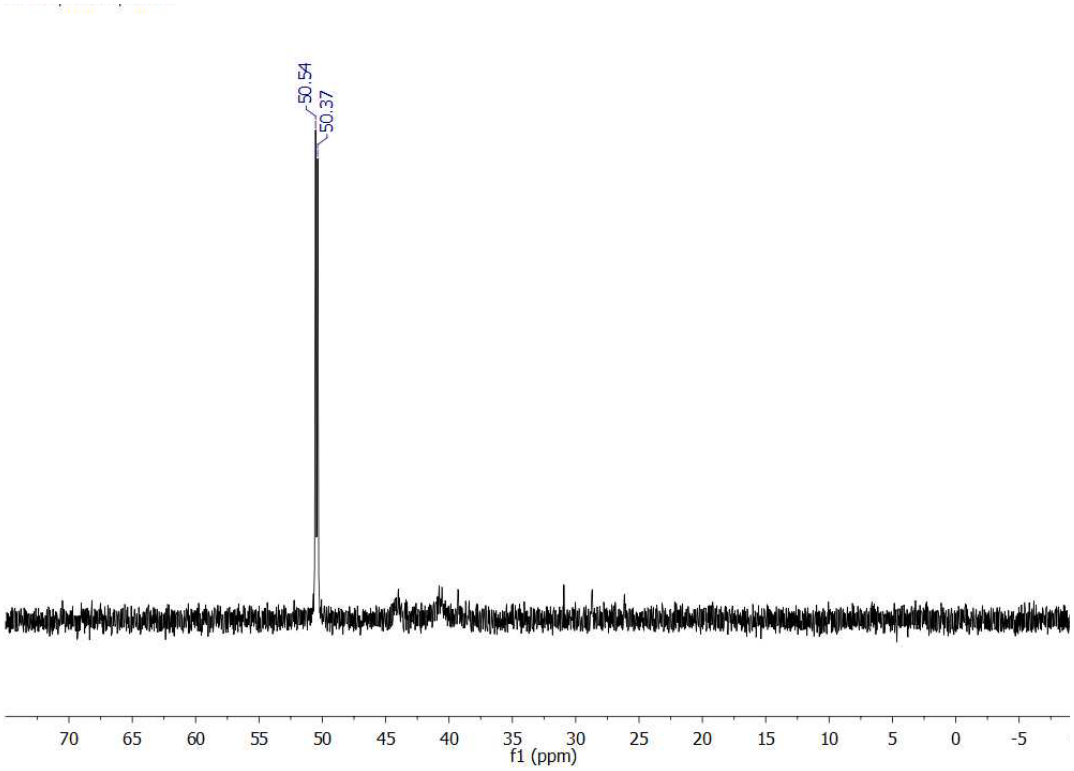
Characterization of [RuHCl$(PPh_3)_2(CH_3CN)_2$], 7. ^1H NMR (300 MHz, CD_3CN): δ 7.40-7.69 (m, 30H, CH_{Ph}), -14.44 (t, $^2J_{P\text{-}H}$ = 21 Hz, 1H, Ru-H). $^{31}P\{^1H\}$ NMR (122 MHz, CD_3CN): δ 50.45 (s, Ru*P*Ph_3). ^{31}P NMR (122 MHz, CD_3CN): δ 50.45 (d, $^2J_{P\text{-}H}$ = 21 Hz, Ru*P*Ph_3). Electrospray HR MS (25 V, *m/z*): 715.1876 $[Ru(PPh_3)_2(CD_3CN)_2H]^+$, 671.1401 $[Ru(PPh_3)_2(CD_3CN)H]^+$, 627.0923 $[Ru(PPh_3)_2H]^+$.



Supplementary Figure S1. ^{1}H NMR spectrum in CD_3CN of the reaction mixture of $[RuCl_2(PPh_3)_3]$ (**6**) with **A**-Bn which leads to $[RuHCl(PPh_3)_2(CH_3CN)_2]$ (**7**) and 1,3-dibenzylimidazolinium chloride



Supplementary Figure S2. $^{31}P\{^{1}H\}$ spectrum in CD_3CN of the reaction mixture of $[RuCl_2(PPh_3)_3]$ (**6**) with **A**-Bn which leads to $[RuHCl(PPh_3)_2(CH_3CN)_2]$ (**7**) and 1,3-dibenzylimidazolinium chloride



Supplementary Figure S3. ^{31}P NMR (decoupled in the aromatic region) spectrum in CD_3CN of the reaction mixture of $[RuCl_2(PPh_3)_3]$ (**6**) with **A**-Bn which leads to $[RuHCl(PPh_3)_2(CH_3CN)_2]$ (**7**) and 1,3-dibenzylimidazolinium chloride.

Computational details

All calculations of the iridium complexes and their reactions were carried out in Gaussian 09[20] using the PBE1PBE (also known as PBE0)[21] functional, tight optimizations, and the ultrafine integration grid (a pruned (99,590) grid). The basis sets[22] included 6-31+G(3pd) for the hydrides and both hydrogen atoms of the CH_2 group of the substrates involved in the reactions with Ir, Def2-QZVPP (with the corresponding ECP) for Ir,[23] 6-311+G(d) for Cl, and 6-31+G(d,p) for all other atoms. The hydride donor abilities of the substrates were calculated at the M06-2X/cc-pVQZ level. The default PCM method (solvent = acetonitrile) was used for all calculations of

this work with the UFF radii scaled by 1.1 (explicit hydrogens). The optimized geometries were verified to have the correct number of negative harmonic frequencies by frequency calculations which also provided the enthalpies and free energies reported here. The free energies were calculated under P = 468 atm (in acetonitrile) following the approach of Martin and co-workers.[24-25]

Supplementary Table S1. Calculated energies (Hartree) (in acetonitrile, P = 468 atm)

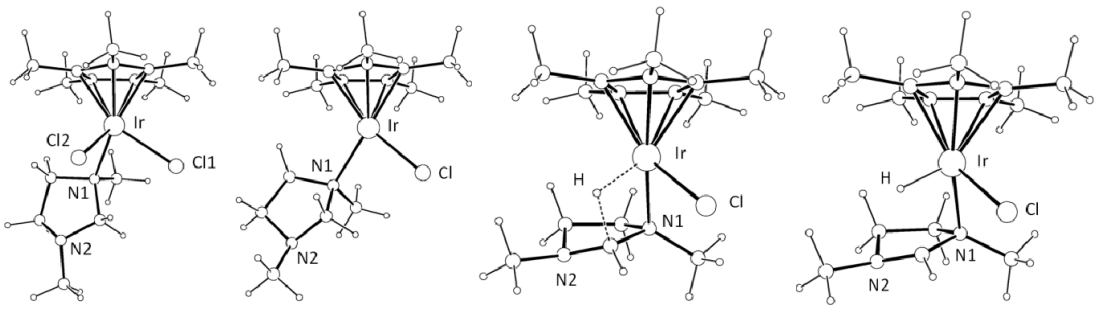
PBE1PBE data	E	H	G
$BImCH_2$	-459.162876	-458.954196	-458.993642
$BImCH^+$	-458.435862	-458.235962	-458.274989
$(Me_2N)_2CH_2$	-308.087501	-307.882850	-307.920468
$[(Me_2N)_2CH]^+$	-307.349053	-307.152393	-307.190543
$OxCH_2$	-287.478928	-287.337936	-287.368491
$[OxCH]^+$	-286.728100	-286.596261	-286.627014
$ImCH_2$	-306.888539	-306.705862	-306.740367
$[ImCH]^+$	-306.161465	-305.987365	-306.023167
H^-	-0.643943	-0.641582	-0.648137
Cl^-	-460.239347	-460.236987	-460.248565
MeCN	-132.606547	-132.556479	-132.578156
$[Cp^*IrCl_2]_2$	-2828.607404	-2828.116792	-2828.215407
$Cp^*_2Ir_2H_2Cl_2$	-1909.590690	-1909.090996	-1909.181812
$Cp^*IrCl_2(MeCN)$	-1546.920412	-1546.623622	-1546.692313
$Cp^*IrCl_2(ImCH_2)$	-1721.201291	-1720.770607	-1720.844492
$[Cp^*IrCl(ImCH_2)]^+$ (16e)	-1260.943795	-1260.515386	-1260.586218
$[Cp^*IrCl(ImCH_2)]^+$, ts	-1260.927397	-1260.503935	-1260.572569
$[Cp^*IrHCl(ImCH)]^+$	-1260.928689	-1260.503871	-1260.574802
$[Cp^*IrCl(OxCH_2)]^+$ (16e)	-1241.532239	-1241.145575	-1241.212425
$[Cp^*IrCl(OxCH_2)]^+$ ts	-1241.501621	-1241.120288	-1241.184794
$[Cp^*IrHCl(OxCH)]^+$	-1241.503697	-1241.120780	-1241.185885
$[Cp^*IrCl((Me_2N)_2CH_2)]^+$ (16e)	-1262.138853	-1261.688407	-1261.762120
$[Cp^*IrCl((Me_2N)_2CH_2)]^+$ (agostic)	-1262.118514	-1261.669071	-1261.744340
$[Cp^*IrCl((Me_2N)_2CH_2)]^+$ ts	-1262.106812	-1261.660697	-1261.733738
$[Cp^*IrHCl((Me_2N)_2CH)]^+$	-1262.109000	-1261.661144	-1261.734033
m06-2X data	E	H	G
$BImCH_2$	-459.66900347	-459.460177	-459.499306
$[BImCH]^+$	-458.94091260	-458.741069	-458.779951
$(Me_2N)_2CH_2$	-308.42328871	-308.218266	-308.255699

$[(Me_2N)_2CH]^+$	-307.68331491	-307.486404	-307.523632
$OxCH_2$	-287.79153368	-287.650230	-287.680623
$[OxCH]^+$	-287.03934983	-286.907551	-286.938117
$ImCH_2$	-307.22049903	-307.037574	-307.072232
$[ImCH]^+$	-306.49094981	-306.316896	-306.352530
H^-	-0.64200805	-0.639648	-0.646202

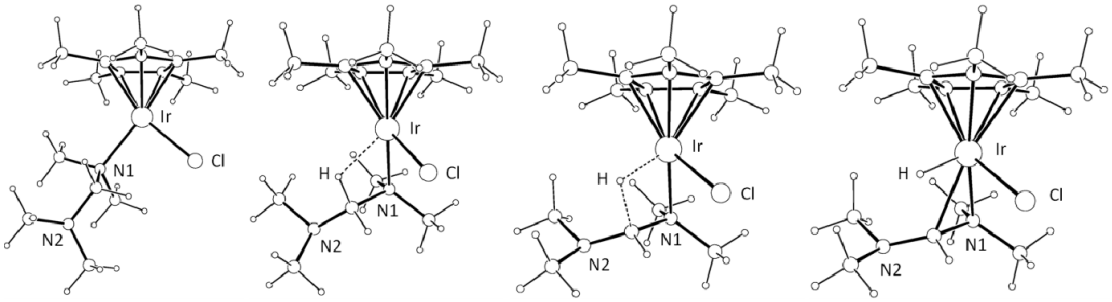
Supplementary Table S2. Enthalpies and energies (kcal/mol)[a] of reactions of $[Cp^*IrCl_2]_2$ with the substrates of Supplementary Table S1 affording the products presented in Supplementary Figures S4 – S6.

Compound	ΔH	ΔG
$Cp^*IrCl_2(MeCN)$	-5.5	-4.0
$Cp^*IrCl_2(ImCH_2)$	-4.0	2.2
$[Cp^*IrCl(ImCH_2)]^+$	7.5	8.3
ts-$[Cp^*IrCl(ImCH_2)]^+$	14.6	16.9
$[Cp^*IrHCl(ImCH)]^+$	14.7	15.5
$[Cp^*IrCl((Me_2N)_2CH_2)]^+$	9.9	11.0
ag-$[Cp^*IrCl((Me_2N)_2CH_2)]^+$	22.1	22.1
ts-$[Cp^*IrCl((Me_2N)_2CH_2)]^+$	27.3	28.8
$[Cp^*IrHCl((Me_2N)_2CH)]^+$	27.1	28.6
$[Cp^*IrCl(OxCH_2)]^+$	8.6	9.5
ts-$[Cp^*IrCl(OxCH_2)]^+$	24.5	26.9
$[Cp^*IrHCl(OxCH)]^+$	24.2	26.2

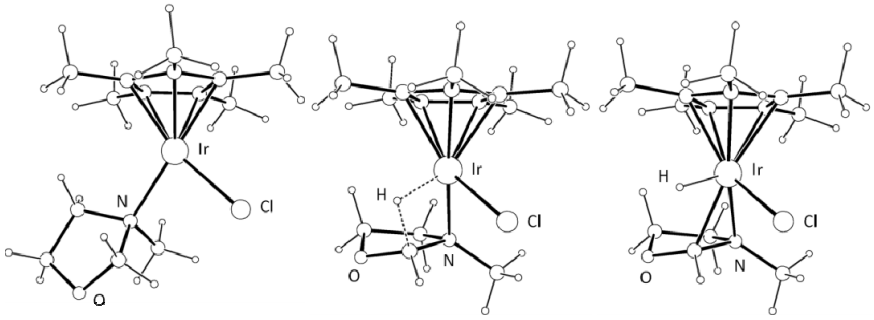
[a] all data in acetonitrile, relative to ½$[Cp^*IrCl_2]$ + substrate



Supplementary Figure S4. The calculated geometries of (left to right) $Cp^*IrCl_2(ImCH_2)$, $[Cp^*IrCl(ImCH_2)]^+$, the transition state *ts*-$[Cp^*IrCl(ImCH_2)]^+$, and $[Cp^*IrHCl(ImCH)]^+$ in acetonitrile.



Supplementary Figure S5. The calculated geometries of (left to right) $[Cp^*IrCl((Me_2N)_2CH_2)]^+$, the agostic complex *ag*-$[Cp^*IrCl((Me_2N)_2CH_2)]^+$, the transition state *ts*-$[Cp^*IrCl((Me_2N)_2CH_2)]^+$, and $[Cp^*IrHCl((Me_2N)_2CH)]^+$ in acetonitrile.



Supplementary Figure S6. The calculated geometries of (left to right) $[Cp^*IrCl(OxCH_2)]^+$, the transition state *ts*-$[Cp^*IrCl(OxCH_2)]^+$, and $[Cp^*IrHCl(OxCH)]^+$ in acetonitrile.

Optimized geometries of the Ir complexes at the PBE0 level

$[Cp^*IrCl_2]_2$

0 1

Ir	1.22280800	0.37773400	1.42299100
Cl	1.14722600	0.23226500	-1.05904000
Cl	1.69865700	-1.98996500	1.43285600
C	1.49309000	2.49392300	1.67403100
C	0.80217500	1.95177700	2.81031500
C	1.63641100	0.93764100	3.42280000
C	2.87836500	0.88795700	2.67339600
C	2.78166700	1.82503500	1.58966500
Cl	-1.14722600	-0.23226600	1.05904000
Ir	-1.22280800	-0.37773400	-1.42299100
C	1.03669000	3.61681500	0.80572400
C	-0.54201900	2.37318600	3.29524600
C	1.34054900	0.18270400	4.67484300
C	4.05597100	0.03922900	3.00772100
C	3.83864500	2.12096500	0.58088500
Cl	-1.69865700	1.98996500	-1.43285600
C	-1.49309000	-2.49392400	-1.67403100
C	-0.80217600	-1.95177700	-2.81031500
C	-1.63641200	-0.93764100	-3.42280000
C	-2.87836500	-0.88795700	-2.67339600
C	-2.78166600	-1.82503500	-1.58966500
H	1.38970700	4.56998700	1.21747100
H	-0.05218000	3.65270800	0.73579000
H	1.43037700	3.51873100	-0.20833600
H	-0.42013300	3.17715900	4.03092700
H	-1.07143800	1.54998900	3.77931400
H	-1.16382000	2.74756600	2.48006700
H	1.73081200	0.72762100	5.54279500
H	0.26568700	0.04952500	4.81634400
H	1.80544800	-0.80558200	4.65848600
H	4.66797000	0.55214700	3.75914600
H	3.74651400	-0.92445300	3.41663800
H	4.67969300	-0.14816900	2.13160200
H	4.42899800	2.98265600	0.91459200
H	4.51760600	1.27632600	0.44869900
H	3.40404200	2.36705900	-0.39054100
C	-1.03668900	-3.61681500	-0.80572500
C	0.54201900	-2.37318500	-3.29524700
C	-1.34055000	-0.18270400	-4.67484300
C	-4.05597100	-0.03922900	-3.00772000
C	-3.83864400	-2.12096500	-0.58088400
H	0.05218000	-3.65270700	-0.73579000
H	-1.43037600	-3.51873100	0.20833600
H	-1.38970700	-4.56998800	-1.21747100
H	1.07143800	-1.54998900	-3.77931500
H	1.16382000	-2.74756600	-2.48006800
H	0.42013300	-3.17715800	-4.03092800
H	-1.80544900	0.80558200	-4.65848600
H	-1.73081300	-0.72762000	-5.54279500
H	-0.26568800	-0.04952400	-4.81634400
H	-3.74651400	0.92445300	-3.41663800
H	-4.67969300	0.14816900	-2.13160100
H	-4.66797100	-0.55214700	-3.75914600
H	-3.40404200	-2.36705900	0.39054100
H	-4.42899800	-2.98265600	-0.91459200
H	-4.51760600	-1.27632600	-0.44869900

$[Cp^*IrCl]_2(\mu\text{-}H)_2$

0 1

Ir	-0.77113300	-0.30593400	-1.09268000
C	-0.57895200	-2.33045100	-1.82246300
C	-0.73204900	-1.42594400	-2.95109300
H	0.93697800	-0.06560300	-0.66170300
Cl	-0.95674400	2.04729400	-1.61122200
C	-2.64418200	-1.25515500	-1.63169200
C	-2.01571000	-0.79777100	-2.83744400
C	-1.75595900	-2.22481600	-1.01022900
H	-0.90742000	0.06254400	0.64143500
C	0.53080200	-3.31176400	-1.65448100
C	0.22044400	-1.28634900	-4.09208200
Ir	0.80069600	0.30307300	1.07236600
C	-4.01994000	-0.90650800	-1.16859400
C	-2.60776500	0.15341300	-3.82026300
C	-2.09520700	-3.06896700	0.17104000
H	1.47325800	-2.92142200	-2.04629200
H	0.67871400	-3.56522200	-0.60411000
H	0.29018100	-4.22705000	-2.20975000
H	0.15088300	-0.29908300	-4.55426300
H	-0.00380400	-2.03418300	-4.86314400
H	1.25351500	-1.43850800	-3.77097100
C	2.67372000	1.25254800	1.61105200
C	1.78537800	2.22205700	0.98953300
Cl	0.98630100	-2.05009900	1.59102600
C	2.04541000	0.79535400	2.81694500
C	0.76170200	1.42341000	2.93061000
C	0.60844200	2.32772800	1.80185700
H	-4.10283000	-0.96642300	-0.08094000
H	-4.75082700	-1.60265100	-1.59897000
H	-4.30103200	0.10387600	-1.47420700
H	-1.83880700	0.73850200	-4.32815800
H	-3.29845500	0.84963400	-3.34111300
H	-3.16298700	-0.41354300	-4.57728400
H	-2.76046200	-2.54329700	0.86032300
H	-2.61180900	-3.97567600	-0.16778800
H	-1.19746600	-3.35919900	0.71889000
C	4.04946400	0.90393900	1.14788600
C	2.12454600	3.06609100	-0.19184000

C	2.63762000	-0.15566200	3.79983900
C	-0.19066500	1.28396500	4.07172100
C	-0.50138400	3.30896600	1.63391100
H	4.78032600	1.60024800	1.57803700
H	4.33069000	-0.10635000	1.45368800
H	4.13223600	0.96362900	0.06021100
H	2.64128900	3.97276100	0.14687800
H	2.78966400	2.54031200	-0.88117200
H	1.22677200	3.35638300	-0.73959600
H	3.19299600	0.41140700	4.55666200
H	1.86873800	-0.74063900	4.30798000
H	3.32820300	-0.85199200	3.32069100
H	0.03356600	2.03200700	4.84258700
H	-0.12094300	0.29681700	4.53412800
H	-1.22378300	1.43592700	3.75067100
H	-0.26086600	4.22419600	2.18931900
H	-1.44383500	2.91850200	2.02561400
H	-0.64925100	3.56254700	0.58356700

$Cp^*IrCl_2(MeCN)$

0 1

Ir	-2.11695300	-9.48306700	-12.12651800
C	-3.70682100	-8.90412200	-13.46661200
C	-4.23941100	-9.23748100	-12.15194300
C	-3.15374500	-11.12955900	-13.00987900
Cl	0.15422700	-9.85221500	-12.93645700
Cl	-1.46211800	-7.19375300	-11.58818400
N	-1.34874100	-9.94338600	-10.30706200
C	-3.91934700	-10.61912400	-11.89710600
C	-3.05102300	-10.05855300	-13.98930000
C	-3.87914900	-7.58987400	-14.14861900
C	-5.08010200	-8.34055000	-11.30705800
C	-2.68839300	-12.53341700	-13.20673400
C	-0.91500600	-10.20635200	-9.27142200
C	-4.32024300	-11.39770100	-10.69010600
C	-2.39911400	-10.18342900	-15.32347700
H	-4.87180500	-7.54757400	-14.61201200
H	-3.13230400	-7.44033500	-14.93059100
H	-3.79752400	-6.76425900	-13.43837900
H	-6.11922900	-8.36113900	-11.65670100
H	-4.72594200	-7.30821800	-11.35810200
H	-5.07046200	-8.65128500	-10.26008200
H	-3.43358700	-13.10048200	-13.77747700
H	-2.53725600	-13.04252500	-12.25230800
H	-1.74647300	-12.56221100	-13.75955600
C	-0.37377900	-10.53776800	-7.97103400
H	-5.28959100	-11.87450000	-10.87635700
H	-4.42391600	-10.75669700	-9.81217400
H	-3.59840300	-12.18388600	-10.45922600
H	-3.09780700	-10.65749100	-16.02286000
H	-1.49937400	-10.79962800	-15.26801800
H	-2.12019100	-9.20956600	-15.72981000
H	-1.13761300	-10.38586600	-7.20432300
H	-0.05447100	-11.58292600	-7.96041500
H	0.48470500	-9.89636600	-7.75708600

$Cp^*IrCl_2(ImCH_2)$

0 1

Ir	-2.15889800	-9.43251200	-12.06783600
Cl	-1.76217700	-7.12264000	-11.39342700
C	-3.01699900	-10.06621200	-13.93846300
C	-3.69689200	-8.90190600	-13.46548400
C	-4.29103100	-9.22538300	-12.17547800
C	-3.98493200	-10.59707700	-11.88719900
C	-3.15524000	-11.11884900	-12.95069700
N	-0.09951100	-8.69773000	-8.46253300
N	-1.17104200	-9.98214900	-10.15206600
Cl	0.09930300	-9.54195200	-12.97243500
C	-2.32101600	-10.20889400	-15.24833800
C	-3.85804700	-7.60736200	-14.18863400
C	-5.17252900	-8.31977900	-11.38350300
C	-4.55696500	-11.39138600	-10.76151900
C	-2.71946000	-12.53540200	-13.13408600
C	0.08904700	-9.23166300	-9.80510400
C	-1.11559500	-9.51109600	-7.82389700
C	1.13615500	-8.55546000	-7.72467300
C	-2.06976700	-9.72559500	-8.98104800
C	-0.84160900	-11.42714100	-10.20988900
H	-3.02270300	-10.62861400	-15.97934100
H	-1.46255900	-10.87856700	-15.17324700
H	-1.96959000	-9.24760100	-15.62763800
H	-4.81279600	-7.60268500	-14.72805800
H	-3.05817200	-7.45117300	-14.91559400
H	-3.85288400	-6.76485900	-13.49379200
H	-6.19129700	-8.34120700	-11.78889100
H	-4.81061800	-7.28979500	-11.42472700
H	-5.22133000	-8.61921600	-10.33410100
H	-5.47857800	-11.87071100	-11.11385700
H	-4.81946600	-10.76633200	-9.90625700
H	-3.89103600	-12.18817300	-10.42375400
H	-3.42520300	-13.06291200	-13.78735100
H	-2.68192800	-13.07663900	-12.18626800
H	-1.73022200	-12.59197700	-13.59536600
H	0.26076900	-8.43049100	-10.52074500
H	0.92815100	-9.94214700	-9.85501800
H	-0.72159200	-10.46819000	-7.43331900
H	-1.58483800	-8.97541500	-6.99250900
H	1.64157500	-9.52383000	-7.55014600
H	0.93357100	-8.09136400	-6.75492300
H	1.82495600	-7.90435600	-8.27190600
H	-2.75399300	-10.56339200	-8.84809100
H	-2.63367100	-8.81180500	-9.17800000
H	-0.15472600	-11.59773400	-11.04001800
H	-0.37360300	-11.76128900	-9.27702200
H	-1.75267500	-12.00102600	-10.37447000

$[Cp^*IrCl(ImCH_2)]^+$

1 1

Ir	-1.18706100	-9.16701200	-12.31295900

C	-2.14350100	-7.71355700	-13.54783100
C	-3.07611200	-8.14137900	-12.50860900
C	-2.46044300	-9.99328800	-13.76685500
Cl	1.11118700	-9.35395200	-12.68292600
N	-0.81662600	-9.88890100	-10.27554100
C	-1.79595400	-8.84395100	-14.34713700
C	-1.68446400	-6.31179400	-13.74417000
C	-3.29219800	-9.54286300	-12.66323200
C	-3.75199500	-7.22053900	-11.55159900
C	-2.38678200	-11.38922500	-14.27616500
C	0.20611800	-9.07874500	-9.55048500
C	-2.00936400	-9.76877900	-9.36309500
C	-0.36689600	-11.30960000	-10.31301200
C	-0.91896300	-8.85609100	-15.55203500
H	-2.43399600	-5.77149500	-14.33532500
H	-0.73469100	-6.26778200	-14.27950400
H	-1.57375500	-5.79035500	-12.79071900
C	-4.25866600	-10.40029500	-11.91968300
H	-4.50594500	-6.63540600	-12.09132400
H	-3.04750700	-6.51706400	-11.10059400
H	-4.26470700	-7.76036400	-10.75350500
H	-3.19065300	-11.54600900	-15.00616000
H	-2.51607800	-12.11771700	-13.47303000
H	-1.43566500	-11.58462100	-14.77480000
N	-0.01506900	-9.40906500	-8.16498000
H	0.01228200	-8.01301900	-9.77046700
H	1.21111000	-9.33464400	-9.88734900
C	-1.45809700	-9.31134500	-8.00164600
H	-2.52149200	-10.73077000	-9.32228000
H	-2.69178800	-9.02454700	-9.76689600
H	0.53959300	-11.37793500	-10.91522800
H	-0.16708000	-11.65866300	-9.29639400
H	-1.14894500	-11.91920700	-10.76811600
H	-1.53588700	-8.76322400	-16.45293500
H	-0.35148600	-9.78622800	-15.62430000
H	-0.20819600	-8.02790900	-15.53918600
H	-5.16954700	-10.50497300	-12.52083500
H	-4.54341400	-9.96761700	-10.95973200
H	-3.86392400	-11.40373600	-11.74504600
C	0.75006100	-8.60005800	-7.23896400
H	-1.80026700	-9.93579100	-7.17135900
H	-1.77332000	-8.27209300	-7.80162700
H	0.54484000	-8.92537400	-6.21534000
H	0.50477100	-7.52519700	-7.31604300
H	1.81957200	-8.72719300	-7.42915500

ts-[Cp*IrCl(ImCH$_2$)]$^+$

1 1

Ir	-1.13493000	-9.50414000	-11.92790700
C	-1.94670600	-7.72059700	-12.84859600
C	-2.99400100	-8.35579500	-12.08857000
C	-2.32654700	-9.84337900	-13.75174100
Cl	0.65135600	-10.97223700	-12.63104400
N	-1.07698700	-10.49373600	-9.97866400
C	-1.49413400	-8.64721700	-13.85052000
C	-1.46717600	-6.31915400	-12.67020400
C	-3.23488400	-9.66244800	-12.67773100
C	-3.89197500	-7.67910600	-11.10594900
C	-2.23766600	-11.01705500	-14.66575100
C	0.05181500	-9.65102600	-9.85988500
C	-2.05029900	-10.00445400	-8.95695000
C	-0.87221400	-11.95432300	-9.91019600
C	-0.48969300	-8.38510500	-14.92252300
H	-2.09231400	-5.64780800	-13.27079100
H	-0.43369100	-6.20343200	-13.00187900
H	-1.53100900	-5.99716500	-11.62889800
C	-4.29383600	-10.61819800	-12.24092300
H	-4.77388800	-7.29976100	-11.63653500
H	-3.40747900	-6.82617700	-10.62699200
H	-4.25396000	-8.35616400	-10.32899500
H	-2.75378000	-10.78596400	-15.60504700
H	-2.70375200	-11.90409100	-14.23240600
H	-1.19816600	-11.25704100	-14.90080000
N	-0.10188100	-8.77500800	-8.84164900
H	0.09905200	-8.68435600	-11.22497700
H	1.03058900	-10.05381600	-10.10120400
C	-1.52853000	-8.62363300	-8.58845700
H	-1.99755700	-10.68259800	-8.09958300
H	-3.06347700	-10.01342900	-9.35508500
H	-0.14168800	-12.25639500	-10.65763400
H	-0.53238300	-12.22824200	-8.90614300
H	-1.82988000	-12.43283500	-10.12090700
H	-0.99672600	-8.03707100	-15.83017500
H	0.06775000	-9.29097000	-15.17049100
H	0.22702400	-7.61867400	-14.61976900
H	-5.24349700	-10.35408900	-12.72127000
H	-4.45665000	-10.58505400	-11.16092600
H	-4.05048100	-11.64578400	-12.51714500
C	0.76564400	-7.62115800	-8.74141100
H	-1.71473200	-8.36476200	-7.54458700
H	-1.94340800	-7.83848100	-9.23402000
H	0.64316000	-7.16716900	-7.75690800
H	0.51717000	-6.87930000	-9.51502700
H	1.80541900	-7.93097300	-8.86131100

[Cp*IrHCl(ImCH)]$^+$

1 1

Ir	-1.51951300	-9.77439900	-11.88552600
C	-2.71614300	-8.27070100	-12.85948000
C	-3.54523700	-8.93352300	-11.88803200
C	-2.92639200	-10.52441100	-13.46969500
Cl	0.34267100	-11.10775400	-12.67577300
N	-1.18083100	-10.62197500	-9.86485800
C	-2.26728100	-9.26092000	-13.80601400
C	-2.43972500	-6.80527400	-12.91952500
C	-3.69929600	-10.32237800	-12.30741000
C	-4.38988200	-8.25210100	-10.86170400
C	-2.79555200	-11.77733200	-14.26570300

C	-0.11717600	-9.72757700	-9.89998300
C	-2.07519300	-10.12970800	-8.77491100
C	-0.90111800	-12.07025100	-9.78083400
C	-1.46922000	-9.01860000	-15.04402700
H	-3.24131800	-6.31151500	-13.48156500
H	-1.49487200	-6.59573100	-13.42436000
H	-2.40126200	-6.35960600	-11.92341800
C	-4.57912700	-11.32367100	-11.63666000
H	-5.36804100	-8.02295600	-11.30239900
H	-3.95177400	-7.30866200	-10.53030100
H	-4.57522900	-8.87722400	-9.98544100
H	-3.38493000	-11.68999600	-15.18601300
H	-3.15573300	-12.64794000	-13.71431700
H	-1.75497000	-11.95624300	-14.54933900
N	-0.24584600	-8.74392300	-9.01172600
H	-0.38492300	-8.66229100	-11.68226300
H	0.83889400	-10.02106800	-10.31572800
C	-1.63717400	-8.68539200	-8.57765700
H	-1.86350200	-10.72999800	-7.88419900
H	-3.12150200	-10.25205700	-9.04597500
H	-0.21511800	-12.35325300	-10.57671000
H	-0.47106300	-12.29937300	-8.80093500
H	-1.84609300	-12.60054300	-9.90462500
H	-2.14111100	-8.86676700	-15.89709400
H	-0.82217100	-9.86980200	-15.26768300
H	-0.84002600	-8.13139100	-14.94581100
H	-5.60014600	-11.22931500	-12.02569600
H	-4.63332800	-11.16745100	-10.55655600
H	-4.24464400	-12.34707100	-11.81737300
C	0.55397800	-7.54088400	-9.08413800
H	-1.71112000	-8.35339000	-7.54099200
H	-2.19007800	-7.99216300	-9.22397400
H	0.52663500	-7.03641700	-8.11727400
H	0.16029600	-6.86788600	-9.85833000
H	1.58632500	-7.80081300	-9.32250000

[Cp*IrCl($(Me_2N)_2CH_2$)]$^+$

1 1

Ir	-1.35309800	-9.38488200	-12.28386100
C	-2.19517300	-7.79606300	-13.38912000
C	-3.25741400	-8.38962900	-12.59221100
C	-2.39195100	-10.00521900	-14.03349400
Cl	0.96044300	-9.65179900	-12.46514800
N	-1.19148100	-9.80630700	-10.14695000
C	-1.70410900	-8.78322000	-14.32072200
C	-1.75877600	-6.37629100	-13.30583100
C	-3.36443900	-9.75996500	-12.97256900
C	-4.13353200	-7.63332700	-11.65366700
C	-2.20200400	-11.30968100	-14.72332800
C	-0.29745300	-8.78194700	-9.47916200
C	-2.51242600	-9.78692000	-9.48192500
C	-0.62149600	-11.16479100	-9.95685700
C	-0.67479200	-8.56512300	-15.37648100
H	-2.41779500	-5.76268100	-13.93263400
H	-0.73583600	-6.24758700	-13.66381000
H	-1.82202900	-5.99811200	-12.28295800
C	-4.35138600	-10.76297500	-12.48279500
H	-4.84674300	-7.04238700	-12.24042700
H	-3.56435700	-6.93612700	-11.03357900
H	-4.70786600	-8.29323800	-11.00216500
H	-2.93719000	-11.39382700	-15.53313600
H	-2.35904200	-12.14900600	-14.04220000
H	-1.20576300	-11.39466900	-15.16043500
N	-0.13133500	-9.01565000	-8.07371100
H	-0.76179800	-7.80928800	-9.67425400
H	0.65557600	-8.82262200	-10.01088200
C	-0.69989600	-7.99068900	-7.21401400
H	-3.16087000	-10.53110900	-9.94476100
H	-2.95830200	-8.79685400	-9.57613900
H	0.37598000	-11.21182800	-10.39343100
H	-0.57521900	-11.38932200	-8.88634600
H	-1.26773700	-11.89337200	-10.45155400
H	-1.16164500	-8.22560300	-16.29755600
H	-0.12796200	-9.48334800	-15.59873000
H	0.05097700	-7.80656700	-15.07660200
H	-5.12673400	-10.90539800	-13.24466700
H	-4.84311300	-10.43745900	-11.56481300
H	-3.88367900	-11.73427900	-12.30108500
C	1.22168400	-9.37095200	-7.67720400
H	-0.69172000	-8.33986100	-6.17694900
H	-0.13990300	-7.04036700	-7.25908300
H	1.21708600	-9.71763100	-6.63921800
H	1.92321800	-8.52198100	-7.75159200
H	1.59945300	-10.18536200	-8.30035900
H	-1.73812300	-7.79168200	-7.49120500
H	-2.39028900	-10.02993800	-8.42143600

ag-[Cp*IrCl($(Me_2N)_2CH_2$)]$^+$

1 1

Ir	-1.34536100	-9.50575500	-12.03460800
C	-2.09674600	-7.68976200	-12.93961800
C	-3.18712200	-8.35814500	-12.25936100
C	-2.31830200	-9.80045300	-13.88139000
Cl	0.65995500	-10.67005300	-12.59138900
N	-1.31241800	-10.47125100	-10.08872300
C	-1.57234400	-8.55867900	-13.95135100
C	-1.62925600	-6.30455500	-12.65525300
C	-3.32457200	-9.66326100	-12.84853400
C	-4.12119100	-7.72488400	-11.28391100
C	-2.14170800	-10.96423600	-14.79327000
C	-0.21269300	-9.51849700	-9.77960300
C	-2.53347000	-10.29516200	-9.28237200
C	-0.86832400	-11.87584600	-9.94384600
C	-0.50173400	-8.23629500	-14.93726800
H	-2.18237900	-5.60718000	-13.29596000
H	-0.56562100	-6.18512300	-12.87023500
H	-1.80879500	-6.02150200	-11.61647600
C	-4.35912900	-10.67713400	-12.50388300

H	-4.88835100	-7.16884200	-11.83583600
H	-3.61002100	-7.01658200	-10.62795600
H	-4.63884600	-8.46313600	-10.66844100
H	-2.69870200	-10.77769800	-15.71920500
H	-2.52049800	-11.88682900	-14.34949800
H	-1.09118200	-11.11077800	-15.05034700
N	-0.18220300	-8.85414300	-8.52259300
H	-0.20849100	-8.72404400	-10.63065800
H	0.72144400	-10.05657700	-9.93570100
C	-0.98759600	-7.64326800	-8.41784200
H	-2.28667800	-10.33705400	-8.21639900
H	-3.21973800	-11.10751700	-9.52430200
H	0.04520000	-12.03831400	-10.51245400
H	-0.70018800	-12.10000000	-8.88418400
H	-1.65179200	-12.52792500	-10.33380300
H	-0.95529000	-7.86444200	-15.86325200
H	0.09309300	-9.11936900	-15.17914900
H	0.17308100	-7.46615700	-14.55808100
H	-5.25354900	-10.49149700	-13.11065100
H	-4.65434200	-10.61877800	-11.45470200
H	-4.01580000	-11.69220800	-12.71264000
C	1.18794600	-8.60833700	-8.07756200
H	-0.86743600	-7.22806600	-7.41483300
H	-0.67460100	-6.87920500	-9.14934200
H	1.16220600	-8.24517900	-7.04719800
H	1.70638000	-7.85772500	-8.69550800
H	1.75995700	-9.53867000	-8.09680900
H	-2.04674700	-7.85037700	-8.56206800
H	-3.01448100	-9.34825000	-9.51334700

ts-[Cp*IrCl($(Me_2N)_2CH_2$)]$^+$

1 1

Ir	-1.24824500	-9.52625100	-11.87346800
C	-1.98737300	-7.69937500	-12.76649600
C	-3.09720500	-8.37900800	-12.14781500
C	-2.26441600	-9.76592900	-13.82193600
Cl	0.57447500	-10.98402900	-12.49620100
N	-1.37249700	-10.56465400	-9.94266000
C	-1.43270800	-8.56738300	-13.77045000
C	-1.54792700	-6.30276400	-12.48053400
C	-3.27560100	-9.64720900	-12.83509700
C	-4.07315400	-7.76288200	-11.19998700
C	-2.08487600	-10.88352500	-14.79069400
C	-0.26969400	-9.70210600	-9.71549100
C	-2.62852900	-10.35062300	-9.20407600
C	-1.01615500	-12.00341300	-9.86536600
C	-0.33227700	-8.23895600	-14.72338900
H	-2.07725100	-5.61971200	-13.15551200
H	-0.47636200	-6.17389900	-12.64434300
H	-1.77879300	-6.00361100	-11.45644500
C	-4.37110600	-10.62571300	-12.57479200
H	-4.80131700	-7.17315100	-11.76988000
H	-3.59128000	-7.08854300	-10.48859300
H	-4.63563100	-8.51336900	-10.64081300
H	-2.51900900	-10.59837200	-15.75630000
H	-2.57989200	-11.79589400	-14.45263200
H	-1.02678300	-11.10501500	-14.94736800
N	-0.13389200	-8.78371700	-8.71763500
H	-0.07016900	-8.74396400	-11.05900600
H	0.66181800	-10.21772000	-9.93065600
C	-1.15782300	-7.79080900	-8.41228800
H	-2.46768700	-10.52959100	-8.13570000
H	-3.35442600	-11.07392100	-9.57648300
H	-0.08231000	-12.18675000	-10.39164900
H	-0.92759100	-12.29257100	-8.81297600
H	-1.81340400	-12.57476600	-10.34255300
H	-0.75153700	-7.82513800	-15.64808700
H	0.24600900	-9.12895500	-14.98062800
H	0.35270800	-7.50012900	-14.30183000
H	-5.23563800	-10.37748700	-13.20206400
H	-4.70548900	-10.59919700	-11.53575000
H	-4.06745100	-11.64731800	-12.81217300
C	1.21903600	-8.23100900	-8.64562400
H	-0.73466300	-7.07857000	-7.70412100
H	-1.44851800	-7.24504700	-9.32041700
H	1.36651800	-7.78986900	-7.65872700
H	1.37159700	-7.45478000	-9.40950800
H	1.95787300	-9.02159200	-8.78621600
H	-2.03721100	-8.23125700	-7.94824700
H	-3.01257700	-9.34919800	-9.36873400

[Cp*IrHCl($(Me_2N)_2CH$)]$^+$

1 1

Ir	-1.55538000	-9.79880000	-11.77556700
C	-2.74684000	-8.26076800	-12.71902700
C	-3.60841200	-8.97090900	-11.81413000
C	-2.92244300	-10.48264700	-13.44163800
Cl	0.28671900	-11.13684200	-12.57553500
N	-1.29506000	-10.66259000	-9.75821000
C	-2.25583400	-9.20634500	-13.69368900
C	-2.49717200	-6.78962300	-12.71781900
C	-3.74136000	-10.33812000	-12.30267800
C	-4.49558300	-8.33473900	-10.79439500
C	-2.76446100	-11.69714800	-14.28933100
C	-0.31884100	-9.66507300	-9.82758900
C	-2.45511300	-10.52528500	-8.86240300
C	-0.76337400	-12.04328900	-9.65537200
C	-1.42150100	-8.90226300	-14.89369300
H	-3.27733700	-6.29700200	-13.31034700
H	-1.53067500	-6.54448000	-13.16164100
H	-2.52762500	-6.37069500	-11.71004900
C	-4.64291500	-11.37803000	-11.72575100
H	-5.40165800	-7.97119100	-11.29460100
H	-4.02472300	-7.47689500	-10.31032900
H	-4.81752200	-9.03653700	-10.02262600
H	-3.32892800	-11.56661400	-15.22011600
H	-3.13890200	-12.59190900	-13.78849600
H	-1.71611100	-11.86090400	-14.55197500

N	-0.16675400	-8.56095300	-9.05178400
H	-0.41611600	-8.69494700	-11.69291100
H	0.62828200	-10.06439300	-10.17511300
C	-1.27070200	-7.72395500	-8.60262200
H	-2.12493100	-10.60075200	-7.82110900
H	-3.13644500	-11.34853400	-9.07686700
H	0.11271900	-12.15624100	-10.28925700
H	-0.50822500	-12.24145800	-8.60967700
H	-1.53958600	-12.73371400	-9.98797200
H	-2.06854600	-8.71666700	-15.75903400
H	-0.76088300	-9.73795400	-15.13535500
H	-0.80357700	-8.01587300	-14.73559500
H	-5.60997500	-11.34659600	-12.24200700
H	-4.83928300	-11.20842700	-10.66539100
H	-4.23411500	-12.38379700	-11.84404400
C	1.02029000	-7.78821900	-9.40775800
H	-0.84779700	-6.84876100	-8.10936800
H	-1.87241800	-7.38375000	-9.45626000
H	1.28892100	-7.14430700	-8.56912600
H	0.82988300	-7.16350900	-10.29344100
H	1.85773200	-8.45580100	-9.61678600
H	-1.90417900	-8.23333900	-7.87950300
H	-2.96856400	-9.58505200	-9.03077700

[Cp*IrCl(OxCH$_2$)]$^+$

1 1

Ir	-1.19525500	-9.13315600	-12.32053000
C	-2.15240000	-7.70947300	-13.59064500
C	-3.08682900	-8.11884500	-12.54609500
C	-2.45959200	-9.99673600	-13.75910600
Cl	1.10668200	-9.32059200	-12.66262200
N	-0.83277800	-9.83839700	-10.27431300
C	-1.79484500	-8.85736600	-14.36095700
C	-1.69834000	-6.31098700	-13.81795000
C	-3.29829300	-9.52388400	-12.67090300
C	-3.76813900	-7.18392800	-11.60736500
C	-2.37540600	-11.40309900	-14.23658300
C	0.16877300	-9.01809500	-9.53190600
C	-2.00753600	-9.69075100	-9.36491700
C	-0.38340400	-11.25941400	-10.28455000
C	-0.91185200	-8.89383800	-15.56088800
H	-2.44713000	-5.78926100	-14.42649200
H	-0.74583500	-6.27544600	-14.34898800
H	-1.59571700	-5.76568500	-12.87709800
C	-4.26682800	-10.36412800	-11.91076600
H	-4.54649500	-6.63566400	-12.15129600
H	-3.07348200	-6.44895800	-11.19306000
H	-4.25119400	-7.71090000	-10.78267500
H	-3.16043700	-11.57437200	-14.98356800
H	-2.52589300	-12.11454600	-13.42208300
H	-1.41202300	-11.60934000	-14.70661100
H	-0.06081600	-7.96027700	-9.71469600
H	1.18297400	-9.24993500	-9.85183500
C	-1.39273800	-9.54905700	-7.96006000
H	-2.66921400	-10.55089400	-9.46484200
H	-2.54671100	-8.78512400	-9.64154200
H	0.53139700	-11.33493400	-10.87254000
H	-0.19491800	-11.60380600	-9.26378200
H	-1.15882400	-11.87553300	-10.74067200
H	-1.52544200	-8.82745700	-16.46637000
H	-0.33833500	-9.82189300	-15.60751500
H	-0.20671300	-8.06083400	-15.56543600
H	-5.16973300	-10.49502900	-12.51873000
H	-4.56588000	-9.89969000	-10.97004000
H	-3.86920500	-11.35932400	-11.69853800
H	-1.51377200	-10.44210200	-7.34250800
H	-1.81452000	-8.68751300	-7.43169700
O	0.00644800	-9.36128900	-8.18590000

ts-[Cp*IrCl(OxCH$_2$)]$^+$

1 1

Ir	-1.13557600	-9.43041500	-12.08422500
C	-2.05646400	-7.73128600	-13.09160200
C	-3.04838900	-8.33964400	-12.24486600
C	-2.41727100	-9.91997700	-13.83550800
Cl	0.62062200	-10.92152400	-12.79069000
N	-0.96518100	-10.24276900	-10.08094300
C	-1.61626400	-8.71703100	-14.04511500
C	-1.61316700	-6.30877300	-13.03420300
C	-3.27788000	-9.68946600	-12.73488600
C	-3.93122800	-7.62426500	-11.27727100
C	-2.34239100	-11.14590100	-14.67783000
C	0.08803100	-9.30534600	-10.25225200
C	-1.84860300	-9.66660600	-9.03360400
C	-0.66059400	-11.67126100	-9.87057100
C	-0.66724900	-8.50507900	-15.17660600
H	-2.28481500	-5.70445900	-13.65514600
H	-0.59900300	-6.18782600	-13.41886200
H	-1.64618700	-5.91176300	-12.01787200
C	-4.28941300	-10.63494900	-12.18209300
H	-4.85405200	-7.33728400	-11.79581100
H	-3.47335300	-6.70823100	-10.89995700
H	-4.22322200	-8.24849100	-10.42987500
H	-2.90053100	-10.97687900	-15.60610100
H	-2.77600500	-12.01142600	-14.17382500
H	-1.30944200	-11.38255900	-14.94231700
H	0.11206800	-8.48775200	-11.70130900
H	1.09169100	-9.69244700	-10.40110600
C	-1.36738500	-8.22557700	-8.93115800
H	-1.66402700	-10.21753600	-8.10635300
H	-2.89950800	-9.76669500	-9.30374800
H	0.01967500	-12.01762300	-10.64528100
H	-0.21445800	-11.80267200	-8.88009300
H	-1.59808100	-12.22580000	-9.93179700
H	-1.22482300	-8.23480000	-16.08077000
H	-0.09606500	-9.41177600	-15.38668500
H	0.03914600	-7.70119900	-14.95985200
H	-5.26320400	-10.42725600	-12.64144100

H	-4.40899400	-10.52026900	-11.10232400
H	-4.03252100	-11.67466800	-12.39153500
H	-1.37693900	-7.83405800	-7.91501200
H	-1.91038900	-7.55034000	-9.59542400
O	0.00119000	-8.29787500	-9.36275200

$[Cp^*IrHCl(OxCH)]^+$

1 1

Ir	-1.49352100	-9.85797800	-11.84105500
C	-2.67836800	-8.28236900	-12.78256400
C	-3.53525200	-8.95814900	-11.85292500
C	-2.93586800	-10.50588600	-13.48679900
Cl	0.24515900	-11.30583100	-12.64245200
N	-1.21878800	-10.66366100	-9.85153900
C	-2.23511200	-9.25662700	-13.75943100
C	-2.38454500	-6.82049900	-12.80174000
C	-3.70601100	-10.33080700	-12.31852300
C	-4.40504000	-8.29996600	-10.83393600
C	-2.83673100	-11.72825900	-14.33028700
C	-0.25248400	-9.66806700	-10.12190900
C	-2.07288500	-10.11306700	-8.76777700
C	-0.84174500	-12.07580800	-9.65471900
C	-1.42263300	-8.98923600	-14.98241500
H	-3.18345100	-6.30822600	-13.35070900
H	-1.43941000	-6.60614800	-13.30335200
H	-2.34298900	-6.39945300	-11.79547600
C	-4.59848600	-11.33858400	-11.67745300
H	-5.38760700	-8.12235200	-11.28807000
H	-4.01382100	-7.33147100	-10.51839200
H	-4.57249200	-8.91953800	-9.95044200
H	-3.42691700	-11.58304800	-15.24258300
H	-3.22031000	-12.61009200	-13.81461200
H	-1.80266400	-11.92179000	-14.62592000
H	-0.35742600	-8.78649600	-12.02953100
H	0.76463300	-9.97815400	-10.33701700
C	-1.67685700	-8.64128700	-8.72839200
H	-1.79691600	-10.62981600	-7.84367100
H	-3.12999300	-10.28623600	-8.96596000
H	-0.16913200	-12.38895500	-10.44976900
H	-0.35577300	-12.17997300	-8.67999700
H	-1.75131600	-12.67752800	-9.68400500
H	-2.08905800	-8.80186300	-15.83213800
H	-0.78914800	-9.84417800	-15.22856000
H	-0.78103800	-8.11545500	-14.85367600
H	-5.62073100	-11.20266700	-12.05032300
H	-4.63373300	-11.22322200	-10.59181800
H	-4.28938800	-12.36022000	-11.90431700
H	-1.64209700	-8.23038100	-7.72015300
H	-2.31190500	-8.01878100	-9.36085300
O	-0.34424600	-8.63357000	-9.25702400

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