Supplementary Information for

The Reactions of Terphenyl Substituted Digallene $Ar^{iPr4}GaGaAr^{iPr4}$ (Ar^{iPr4} = C_6H_3-2,6-(C_6H_3-2,6-$^iPr_2$)$_2$) with Transition Metal Carbonyls and Theoretical Investigation of the Mechanism of Addition

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Table S1. Selected X-ray Crystallographic Data for **1**–**5**.

Compound	**1**	**2**	**3**	**4**	**5**
Empirical formula	$C_{64}H_{74}Ga_2O_4Cr$	$C_{64}H_{74}Ga_2O_4Mo$	$C_{64}H_{74}Ga_2O_4W$	$C_{35}H_{37}GaMoO_5$	$C_{37}H_{37}Co_2GaO_7$
Formula weight , $gmol^{-1}$	1098.67	1142.61	1230.52	703.30	781.25
T (K) / l (Å)	90(2) / 0.71073	90(2) / 0.71073	90(2) / 1.54178	90(2) / 0.71073	87(2) / 0.71073
Crystal system	monoclinic	monoclinic	monoclinic	Monoclinic	triclinic
Space group / Z	$C2/c$ / 8	$C2/c$ / 8	$C2/c$ / 8	$P2_1/c$ / 8	$P\bar{1}$ / 2
a, Å	23.711(2)	23.888(4)	23.843(1)	22.150(6)	10.0661(7)
b, Å	23.470(3)	23.746(4)	23.6914(11)	16.423(4)	10.2335(7)
c, Å	21.496(2)	21.433(4)	21.3451(9)	19.316(5)	17.7113(13)
α, °	90	90	90	90	82.2490(10)
β, °	109.243(5)	108.830(2)	108.757(2)	106.648(4)	78.7020(10)
γ, °	90	90	90	90	82.3580(10)
V, $Å^3$	11294(2)	11506(4)	11416.9(9)	6732(3)	1762.1(2)
ρ, mg m^{-3}	1.292	1.319	1.432	1.388	1.472
Abs. coeff., mm^{-1}	1.182	1.190	5.096	1.211	1.736
F(000)	4608	4752	5008	2880	800.0
Crystal size, mm	0.27 x 0.25 x 0.22	0.37 x 0.35 x 0.35	0.18 x 0.09 x 0.07	0.36 x 0.20 x 0.10	0.27 x 0.18 x 0.16
θ range, °	2.47 to 29.999	1.244 to 27.500	3.06 to 68.24	1.568 to 27.495	1.18 to 27.53
Reflns collected	16464	51795	22960	59304	23339
Ind. reflns	14694	13208	10174	15435	8055
R(int)	0.0375	0.0188	0.0363	0.0347	0.0200
Obs. reflns [$I > 2\sigma(I)$]	58947	12117	8780	12833	7274
Completeness to 2θ	99.8%	100%	97.2%	100%	99.4%
Goodness-of-fit F^2	1.052	1.031	1.062	1.021	1.808
Final R [$I > 2\sigma(I)$]	$R1$ = 0.0228	$R1$ = 0.0199	$R1$ = 0.0344	*R1 = 0.0257*	$R1$ = 0.0404
	$wR2$ = 0.0617	$wR2$ = 0.0529	$wR2$ = 0.0881	*wR2 = 0.0581*	$wR2$ = 0.1220
R (all data)	$R1$ = 0.0269	$R1$ = 0.0225	$R1$ = 0.0409	*R1 = 0.0358*	$R1$ = 0.0448
	$wR2$ = 0.0636	$wR2$ = 0.0543	$wR2$ = 0.0919	*wR2 = 0.0628*	$wR2$ = 0.1261

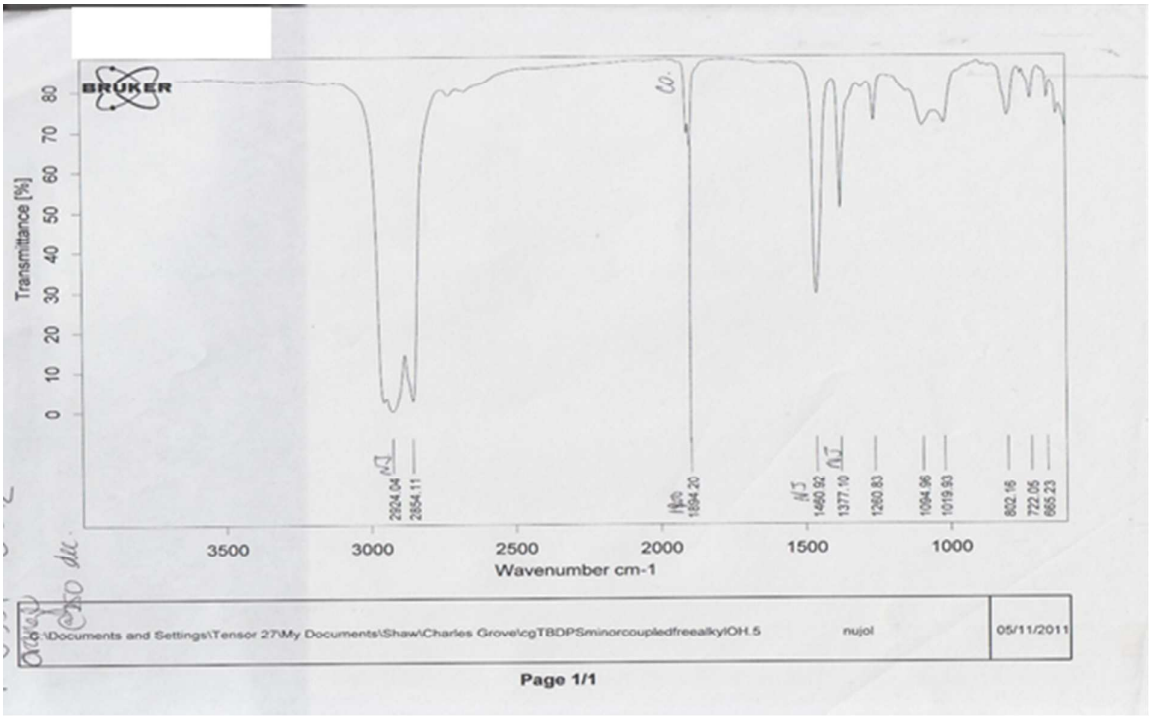


Figure S1: IR spectrum for *trans*-[Cr(GaAr$^{i\text{Pr}_4}$)$_2$(CO)$_4$] (**1**) Nujol Mull

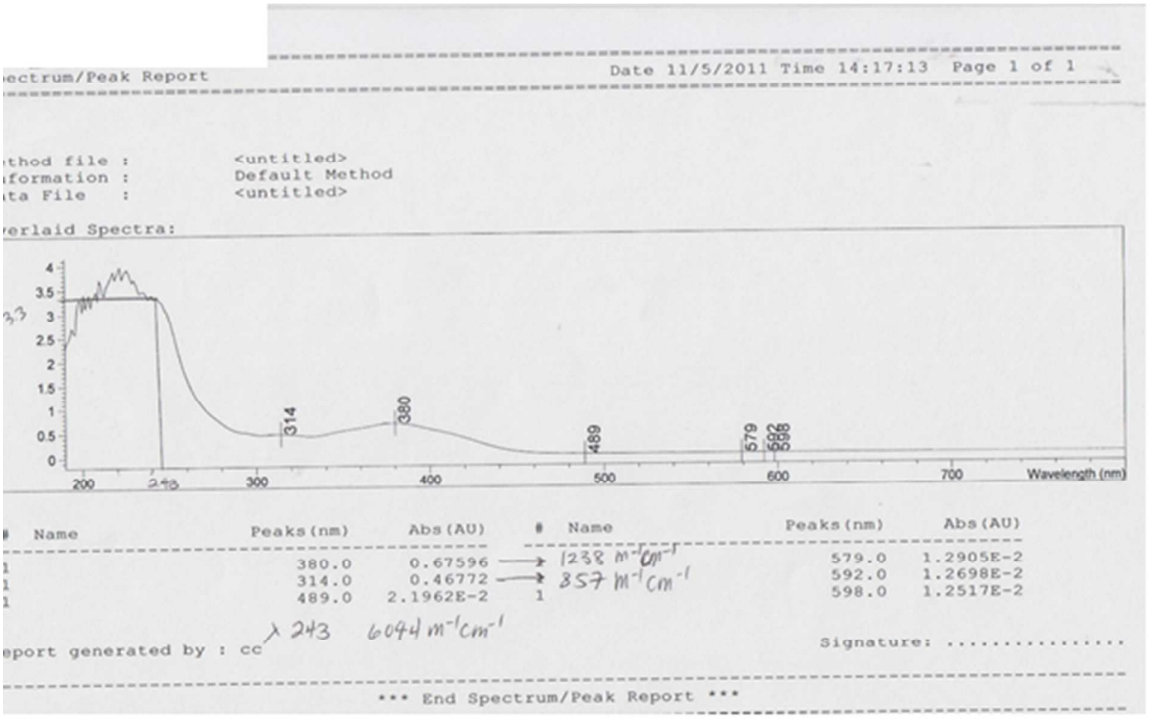


Figure S2: UV-Vis spectrum for *trans*-[Cr(GaAr$^{i\text{Pr}4}$)$_2$(CO)$_4$] (**1**) in hexanes at 25ºC

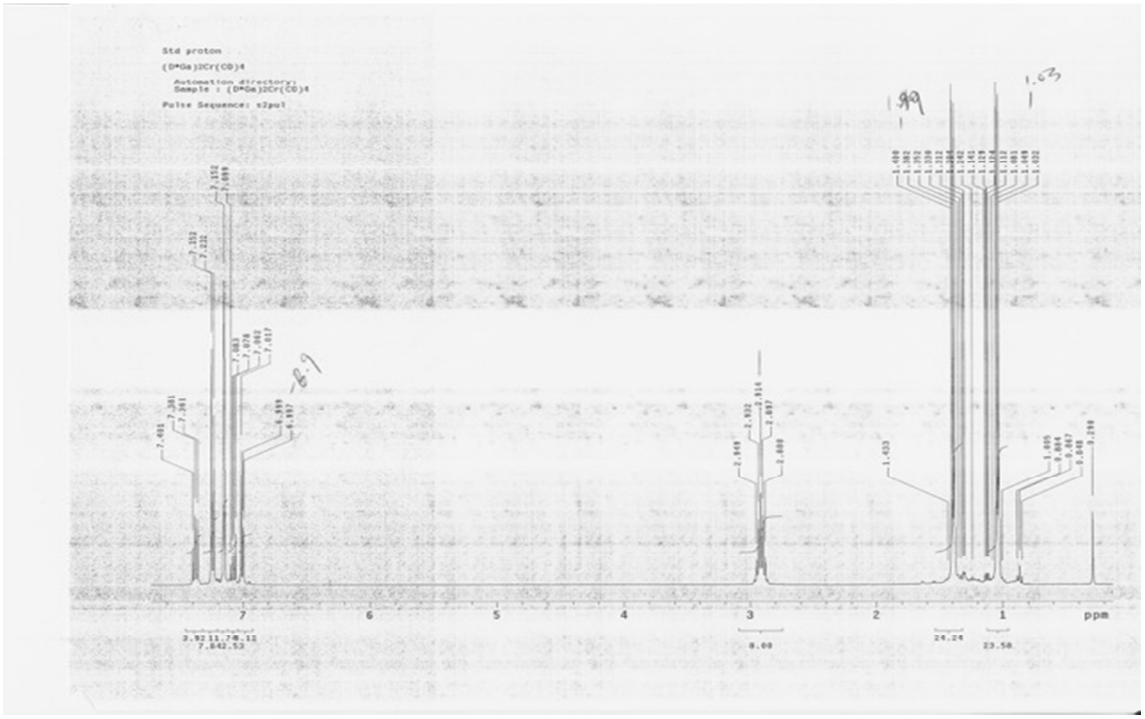


Figure S3: ^{1}H NMR spectrum for *trans*-[Cr(GaAr^{iPr4})$_2$(CO)$_4$] (**1**) in C_6D_6 at 25ºC

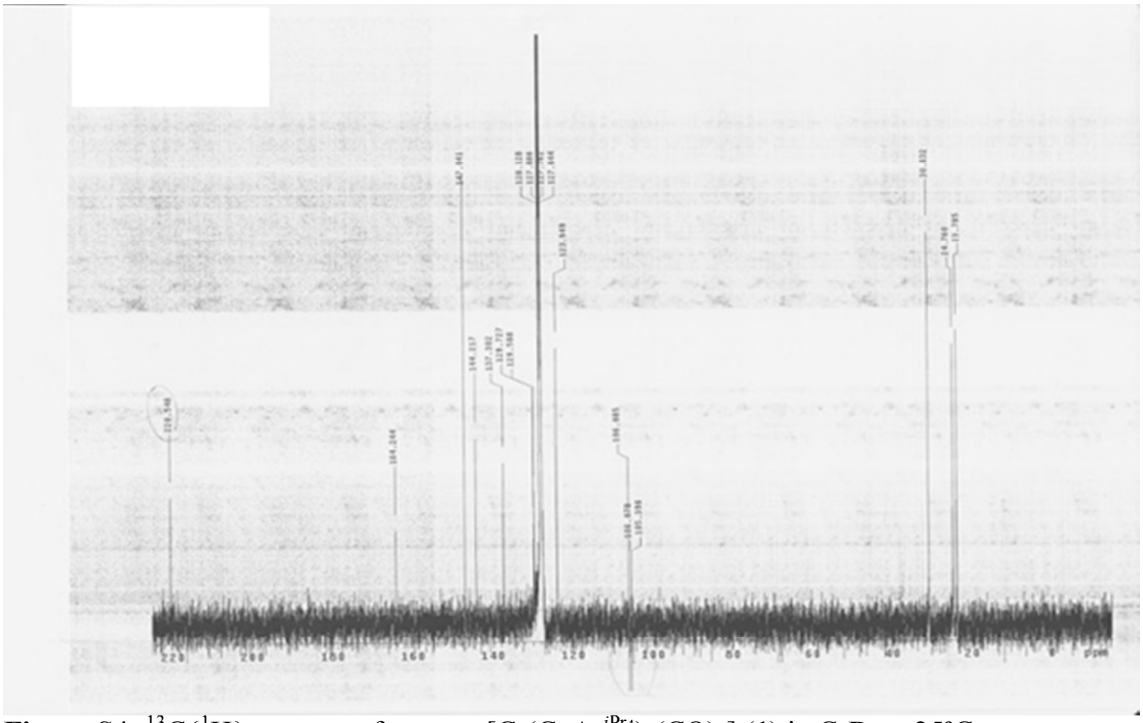


Figure S4: $^{13}C\{^{1}H\}$ spectrum for *trans*-[Cr(GaAr^{iPr4})$_2$(CO)$_4$] (**1**) in C_6D_6 at 25ºC

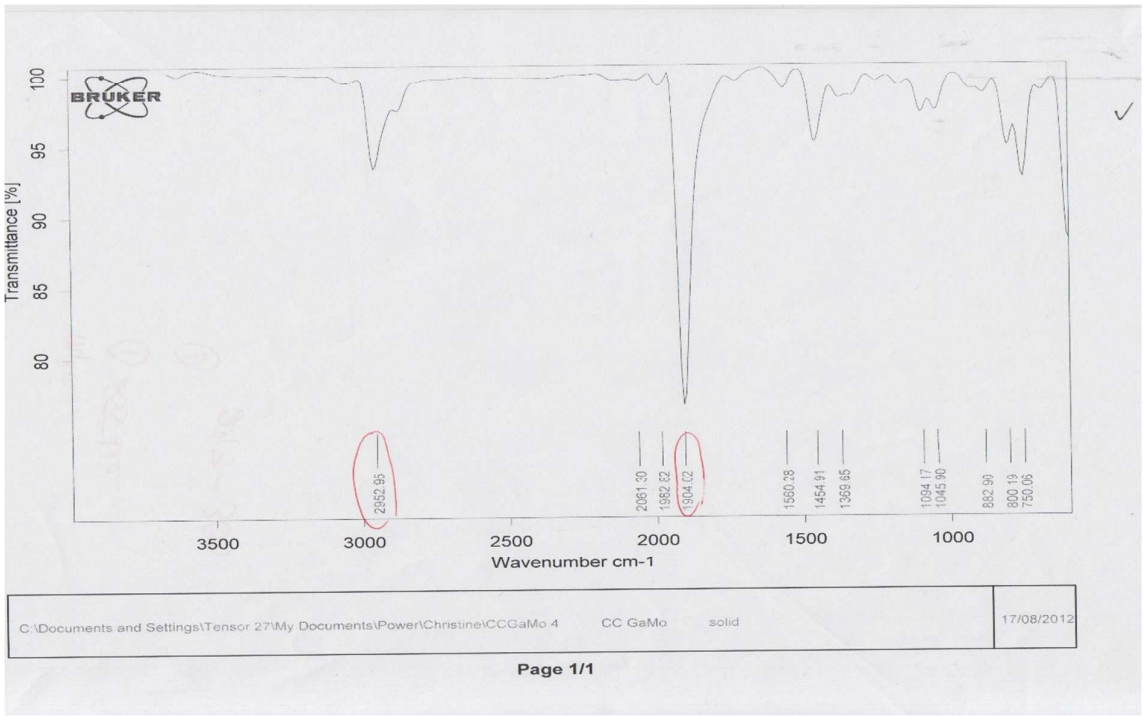
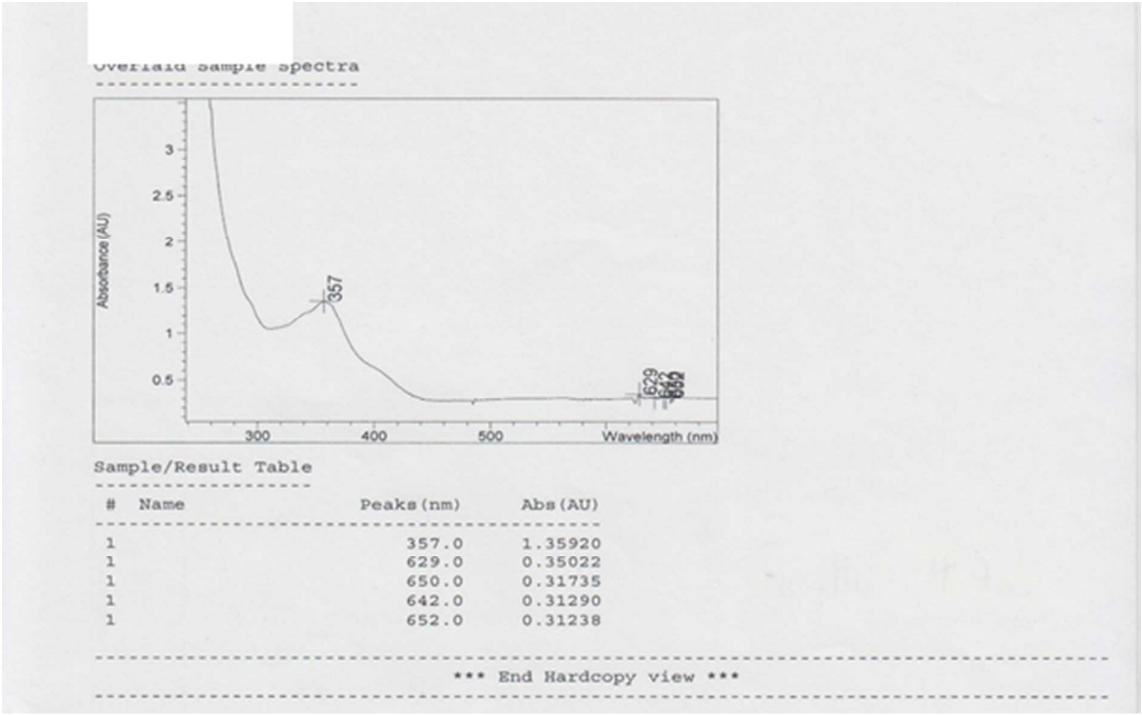


Figure S5: IR spectrum for *trans*-[Mo(GaAr^{iPr4})$_2$(CO)$_4$] (**2**)



Sample/Result Table

#	Name	Peaks(nm)	Abs(AU)
1		357.0	1.35920
1		629.0	0.35022
1		650.0	0.31735
1		642.0	0.31290
1		652.0	0.31238

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Figure S6: Electronic spectrum for *trans*-[Mo(GaAr$^{i\text{Pr}_4}$)$_2$(CO)$_4$] (**2**)

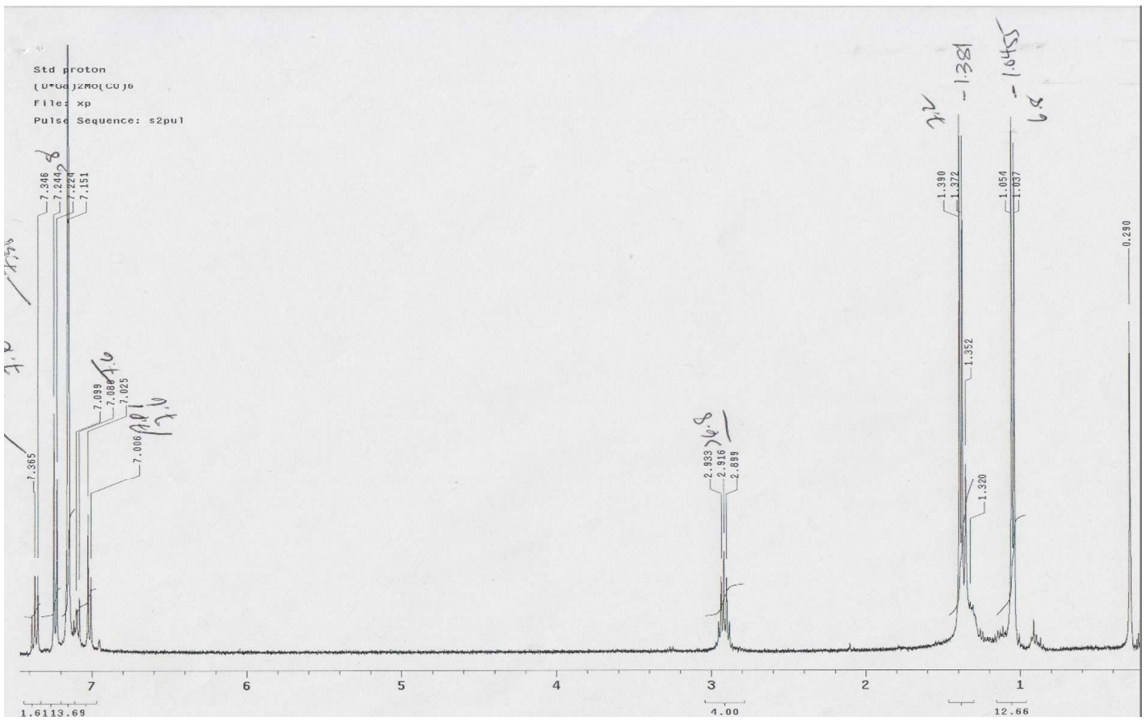

Figure S7: ^{1}H NMR spectrum for *trans*-[Mo(GaAr$^{i\text{Pr}_4}$)$_2$(CO)$_4$] (**2**) in C_6D_6 at 25ºC

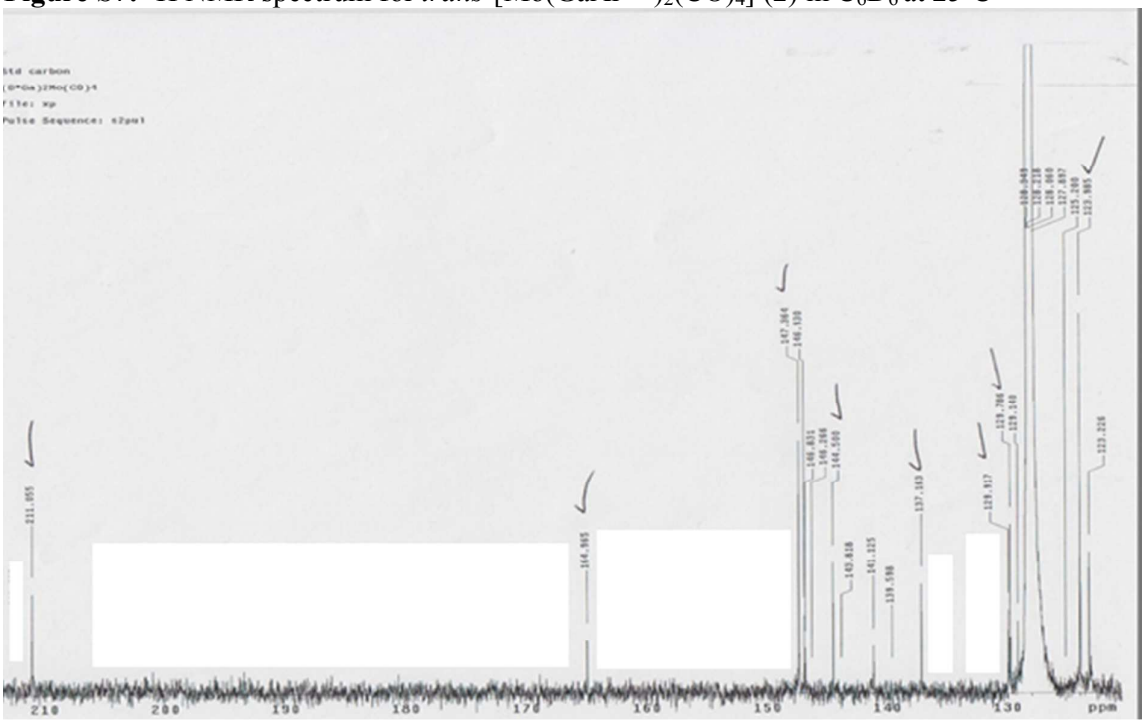

Figure S8: ^{13}C{^{1}H} spectrum for *trans*-[Mo(GaAr$^{i\text{Pr}_4}$)$_2$(CO)$_4$] (**2**) in C_6D_6 at 25ºC

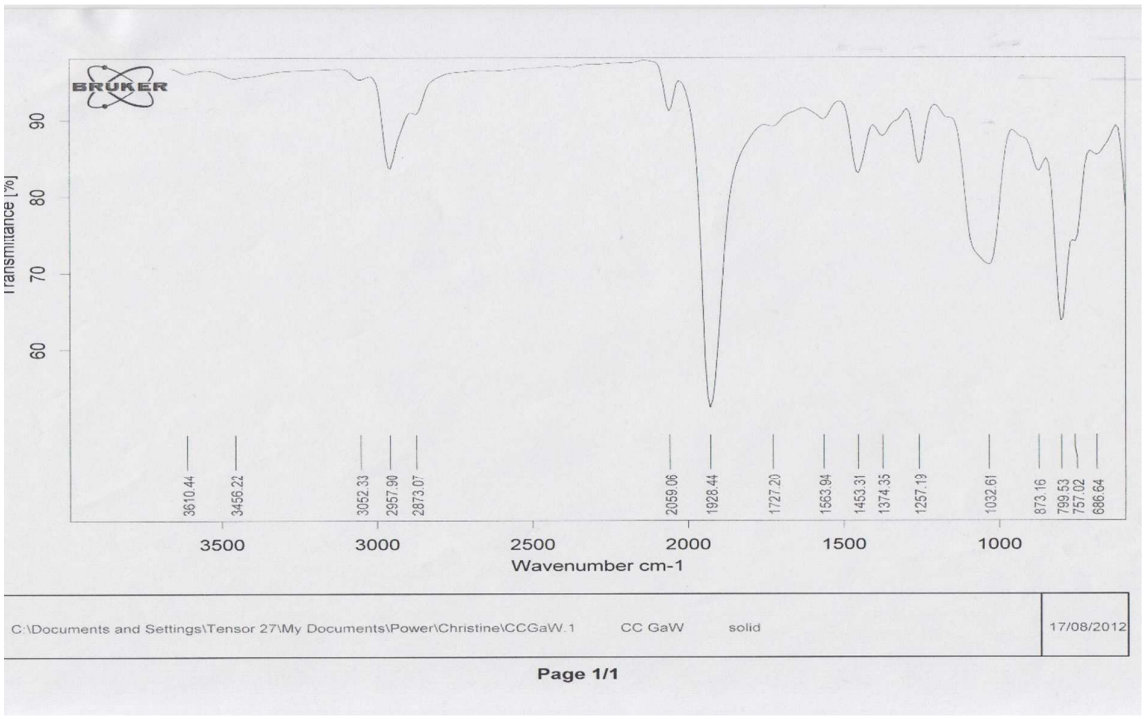

Figure S9: IR spectrum for *trans*-[W(GaAr$^{i\mathrm{Pr}_4}$)$_2$(CO)$_4$] (**3**) Nujol Mull

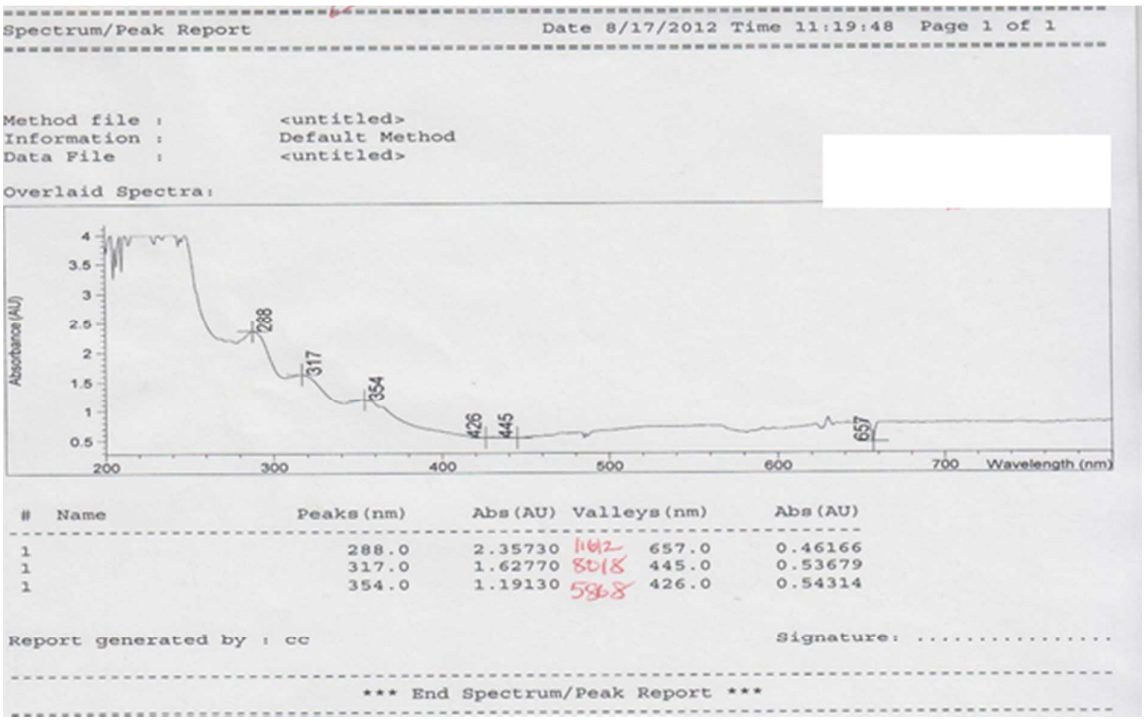

Figure S10: Electronic spectrum for *trans*-[W(GaAr$^{i\mathrm{Pr}_4}$)$_2$(CO)$_4$] (**3**) in hexanes at 25ºC

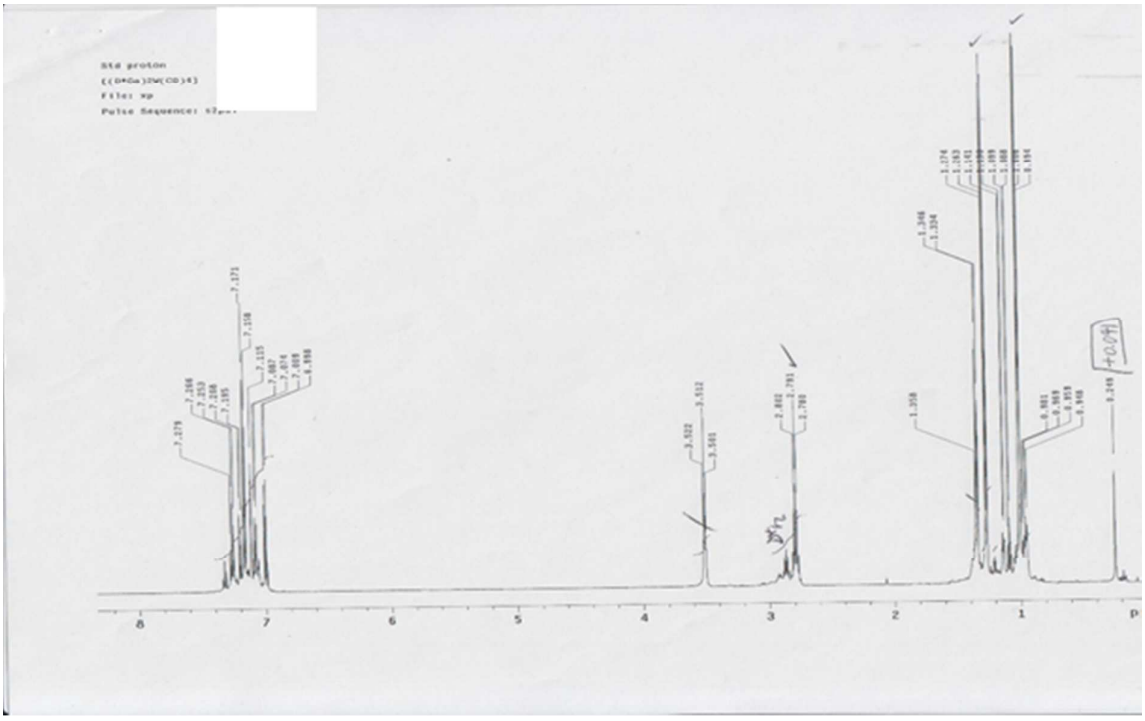

Figure S11: ^{1}H NMR spectrum for *trans*-[W(GaAr^{iPr4})$_2$(CO)$_4$] (**3**) in C_6D_6 at 25ºC

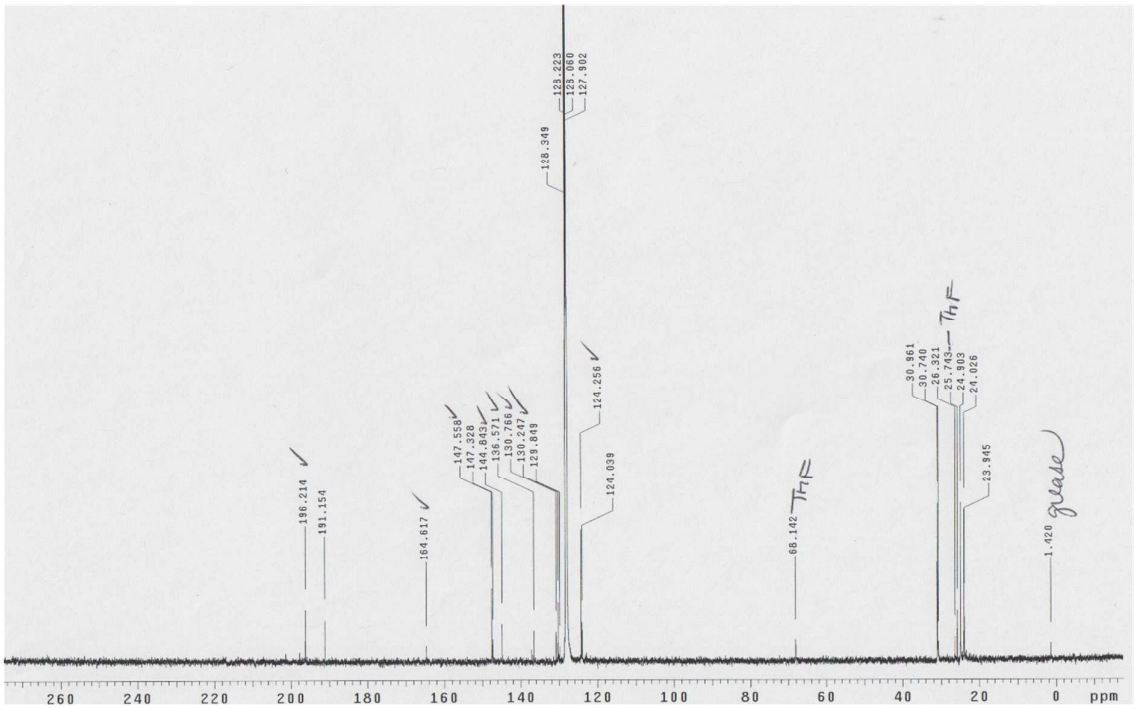

Figure S12: $^{13}C\{^{1}H\}$ spectrum for *trans*-[W(GaAr^{iPr4})$_2$(CO)$_4$] (**3**) in C_6D_6 at 25ºC

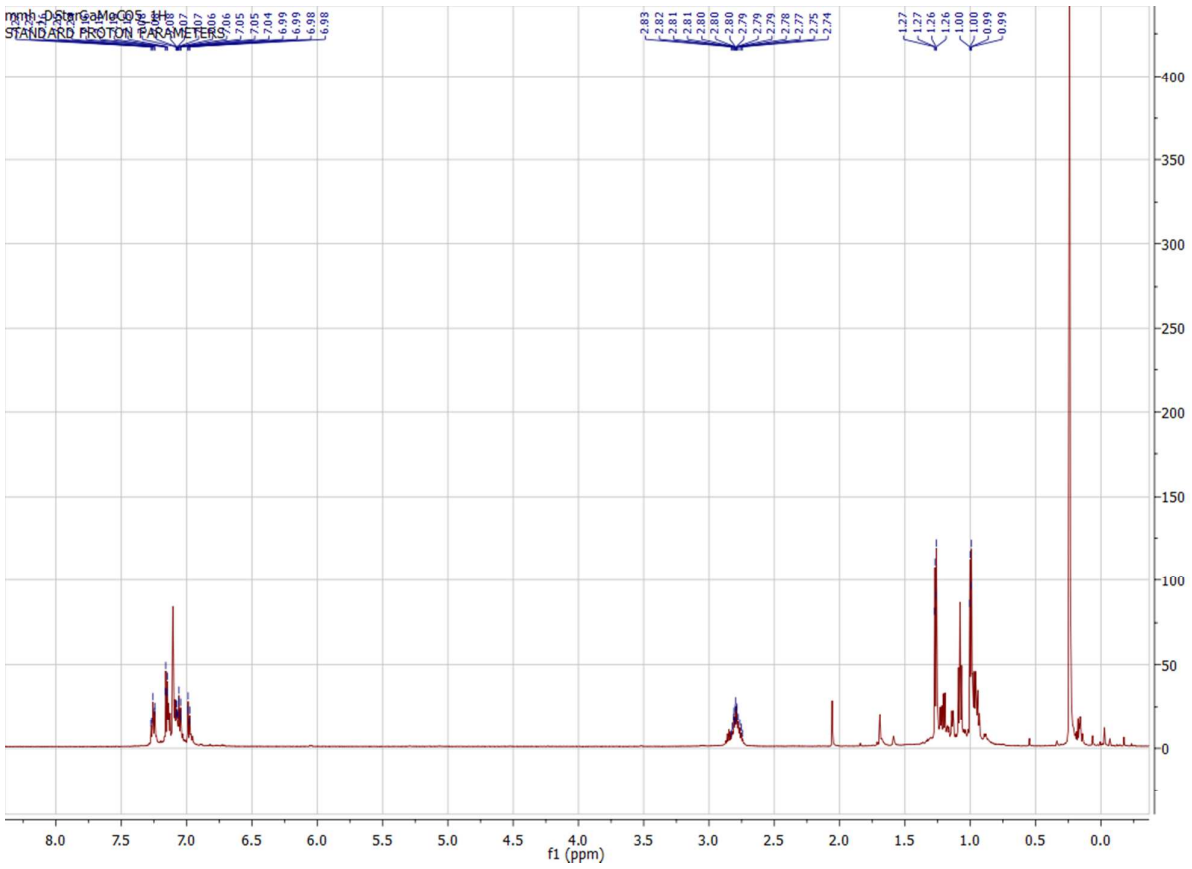

Figure S13: ^{1}H NMR spectrum for [Mo(GaAr^{iPr4})(CO)$_5$] (**4**) in C_6D_6 at 25ºC

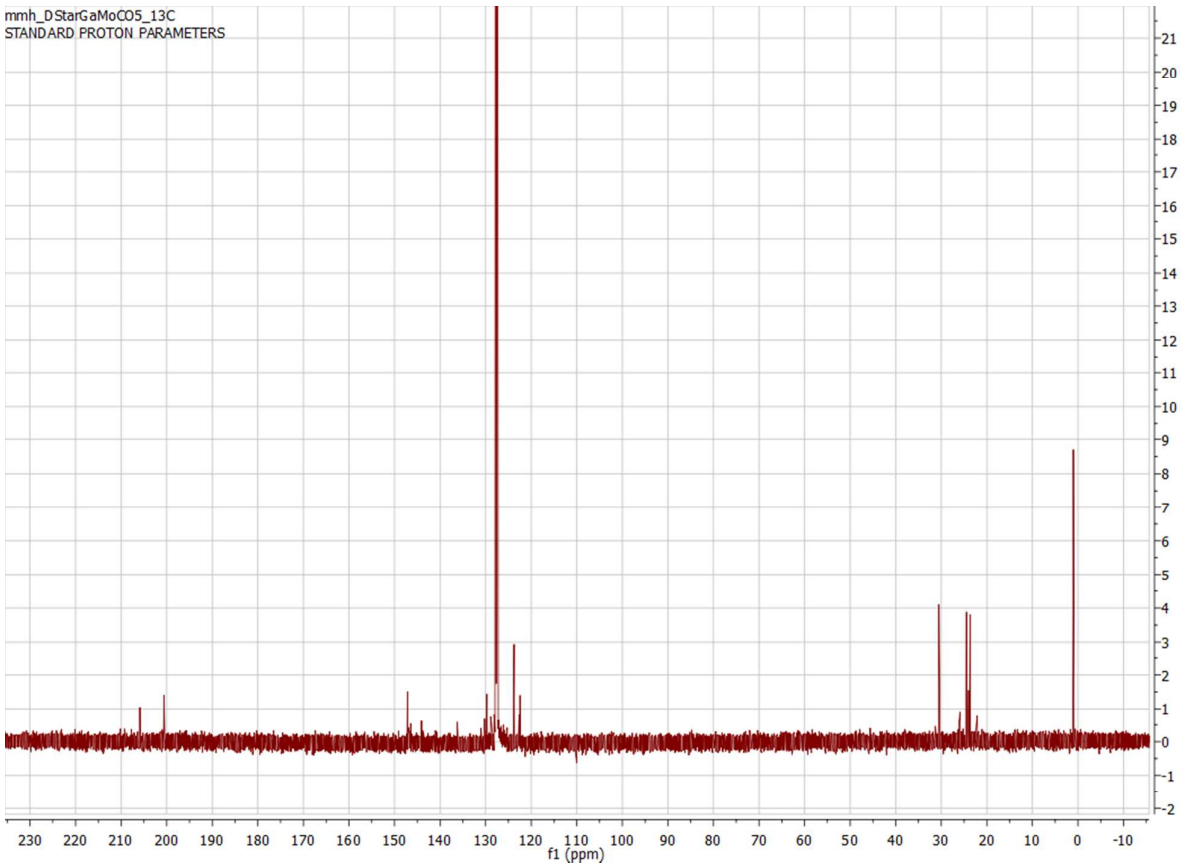

Figure S14: $^{13}C\{^{1}H\}$ spectrum for [Mo(GaAr^{iPr4})(CO)$_5$] (**4**) in C_6D_6 at 25ºC

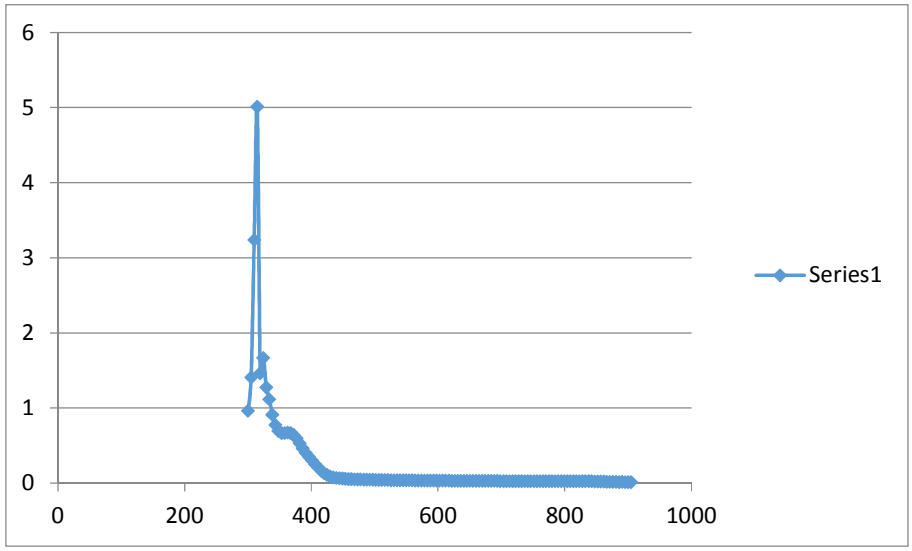

Figure S15: Electronic spectrum for Mo(GaAr^{iPr4})(CO)$_5$ (**4**) in hexanes at 25ºC

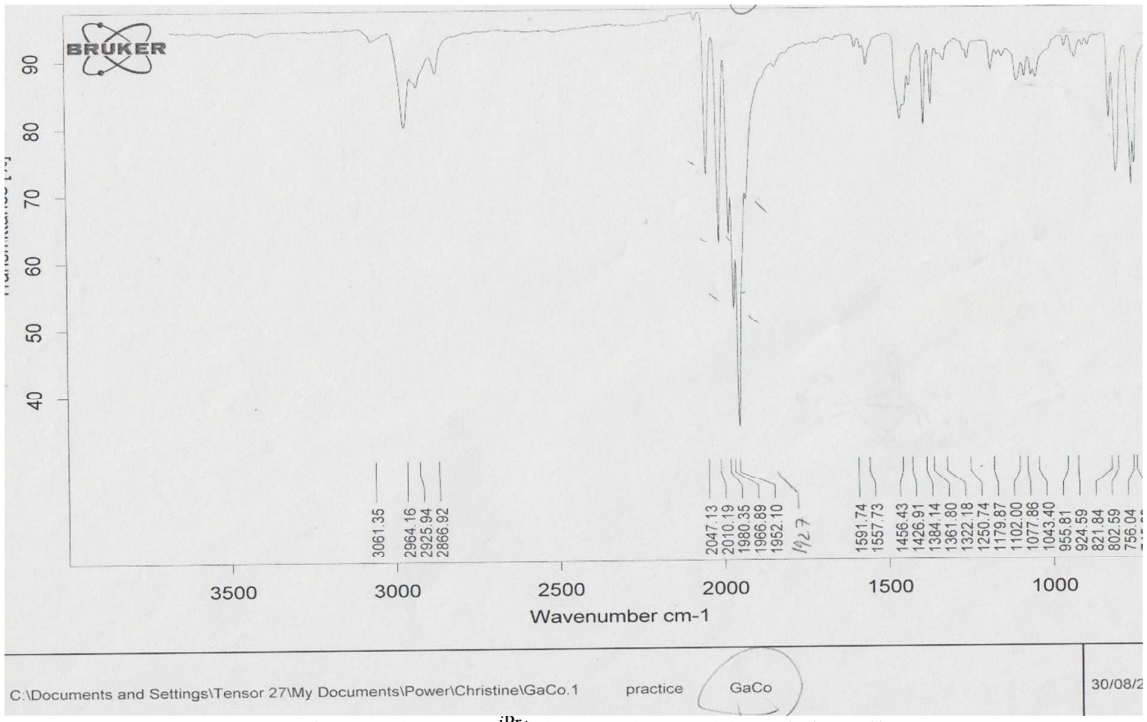

Figure S16: IR spectrum for $Co_2(\mu\text{-}GaAr^{i\text{Pr}_4})(\mu\text{-}CO)(CO)_6$ (**5**) Nujol Mull

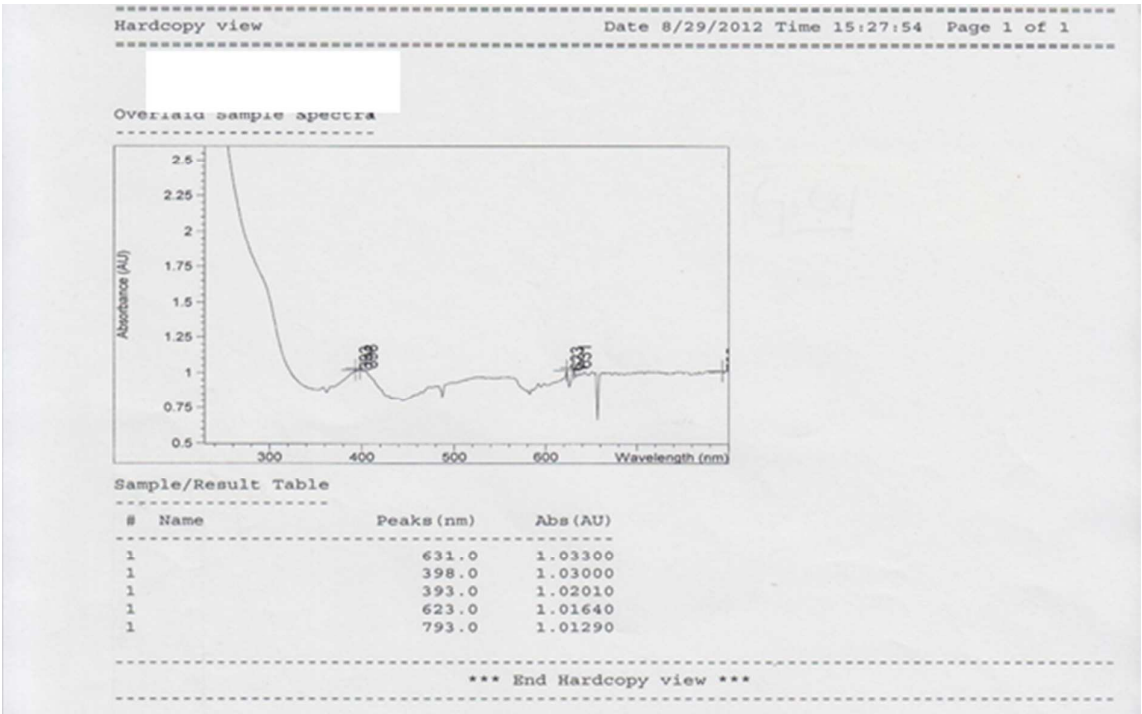

Figure S17: Electronic spectrum for $Co_2(\mu\text{-}GaAr^{i\text{Pr}_4})(\mu\text{-}CO)(CO)_6$ (**5**) in hexanes at 25ºC

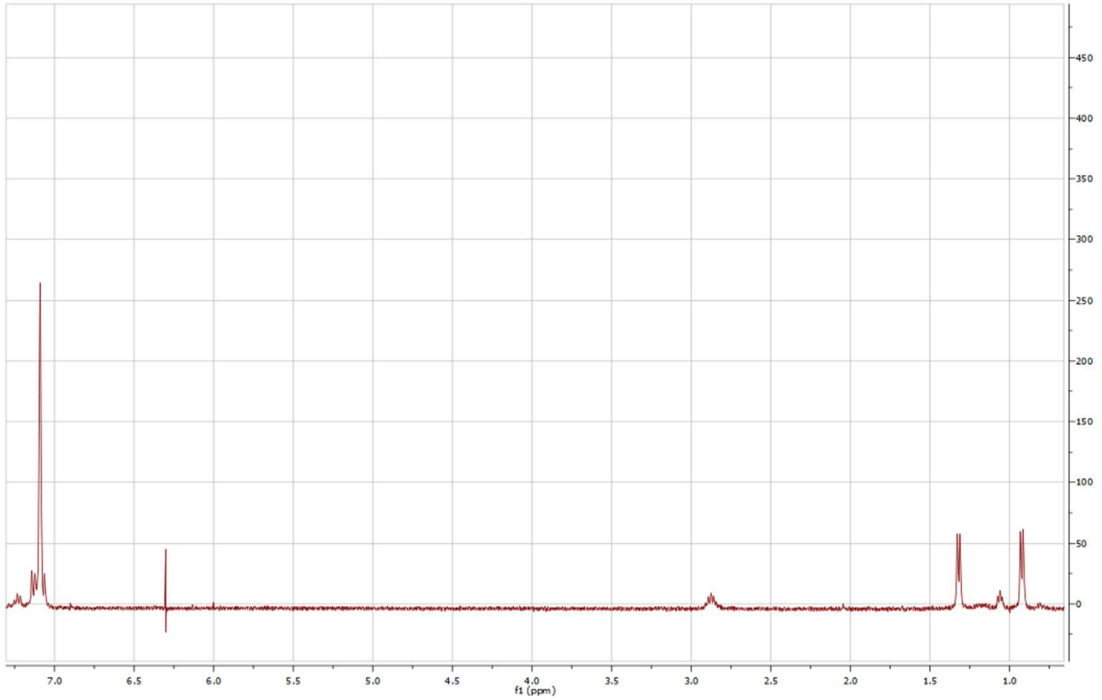

Figure S18: ^{1}H NMR spectrum for $Co_2(\mu\text{-}GaAr^{iPr_4})(\mu\text{-}CO)(CO)_6$ (**5**) in C_6D_6 at 25ºC

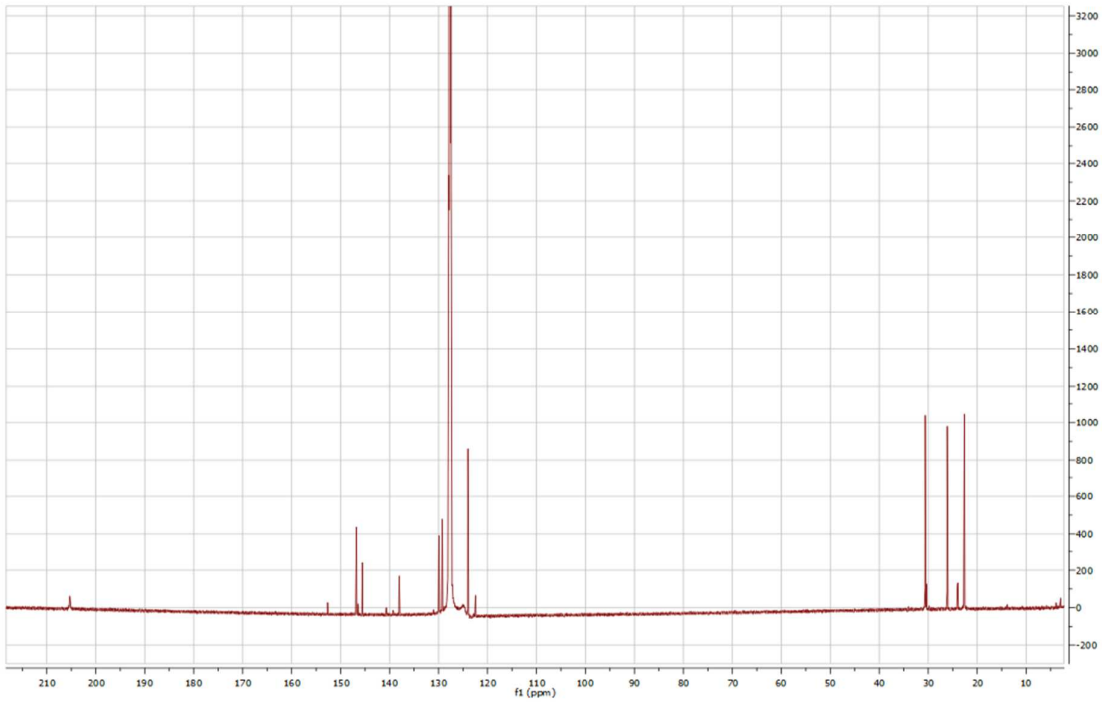

Figure S19: $^{13}C\{^{1}H\}$ spectrum for $Co_2(\mu\text{-}GaAr^{iPr_4})(\mu\text{-}CO)(CO)_6$ (**5**) in C_6D_6 at 25ºC