Supporting Information

Weakly Interacting Solvation Spheres Surrounding a Calixarene-Protected Tetrairidium Carbonyl Cluster: Contrasting Effects on Reactivity of Alkane Solvent and Silica Support

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^{31}P NMR Spectroscopy and ^{31}P CP/MAS NMR Spectroscopy

Spectra in Figures S1a and b characterize the calixarene-phosphine ligands for cluster $Ir_4L_3(CO)_9$, both when dispersed on the surface of silica (^{31}P CP/MAS NMR spectrum), and when dissolved in $CDCl_3$ solution (^{31}P NMR spectrum), respectively. Both spectra in Figures S1a and S1b consist of two identical resonances at 18.5±1 ppm and -11.5±1.5 ppm, which are assigned to calixarene-phosphine ligands in the equatorial and axial positions, respectively. When the ^{31}P NMR spectrum in Figure S1b was integrated, corresponding to the cluster in $CDCl_3$ solution, it exhibited a 2:1 ratio for the area of the equatorial to axial phosphine resonances, in agreement with the previously reported structure from single-crystal X-ray diffraction, assuming ^{31}P NMR signal intensity is proportional to concentration (an assumption that is not generally accurate for ^{31}P NMR spectroscopy due to NOE effects).[S1] In comparison, the ^{31}P CP/MAS NMR spectrum in Figure S2 exhibits a ratio of equatorial to axial phosphine ligands of 1.72. Within experimental uncertainty (CP spectra cannot be quantitatively integrated because resonances can possess different degrees of cross polarization), this ratio is in near agreement with the ratio calculated from data in Figure S13b. Altogether, the identical chemical shifts of the equatorial and axial resonances and similarity of the integration demonstrate the supported $Ir_4L_3(CO)_9$ cluster's phosphorus ligand sphere and Ir_4 framework to be stable on silica, and identical with a solution in organic solvent.

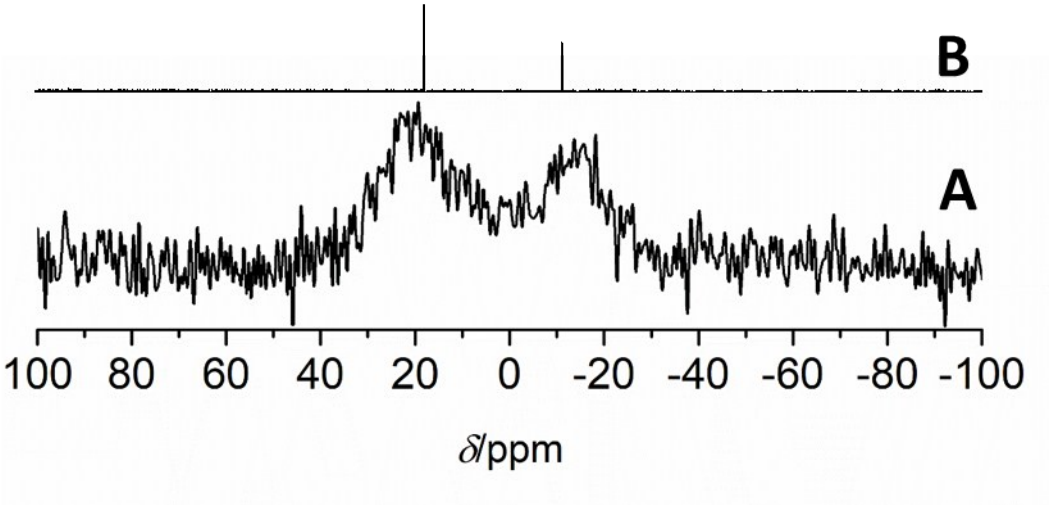


Figure S1. (A) ^{31}P CP MAS NMR data characterizing $Ir_4L_3(CO)_9$ on dehydrxylated silica and (B) ^{31}P NMR spectra $Ir_4L_3(CO)_9$ in $CDCl_3$ at room temperature.

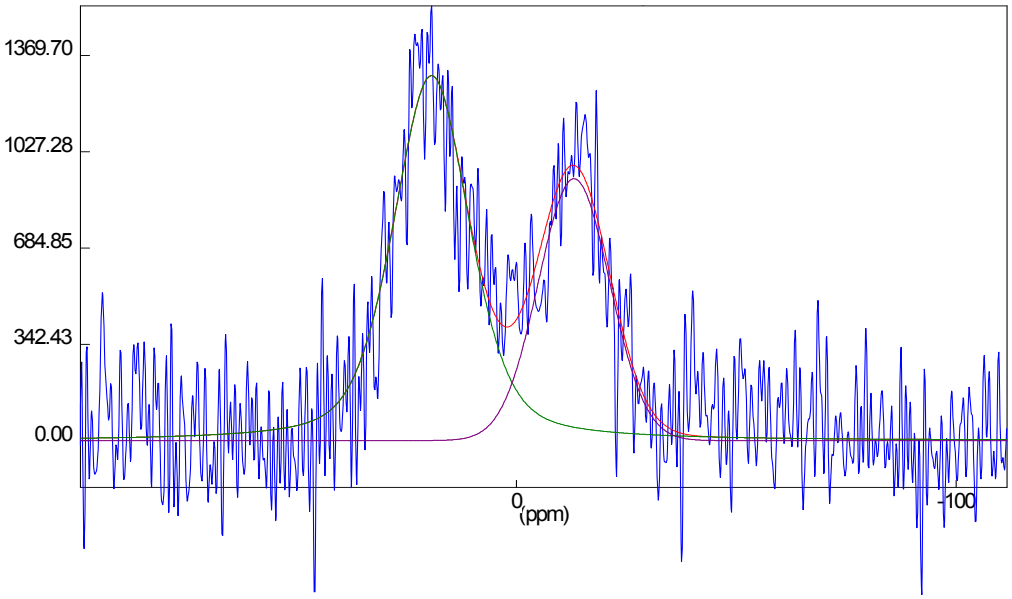


Figure S2. Decomposition of ^{31}P CP MAS NMR spectrum characterizing $Ir_4L_3(CO)_9$ on dehydroxylated silica shown in Figure S13. The two resonances at 19.29 ppm (equatorial) and -13.12 ppm (axial) had an area count of 63.2 a.u. and 36.8 a.u.

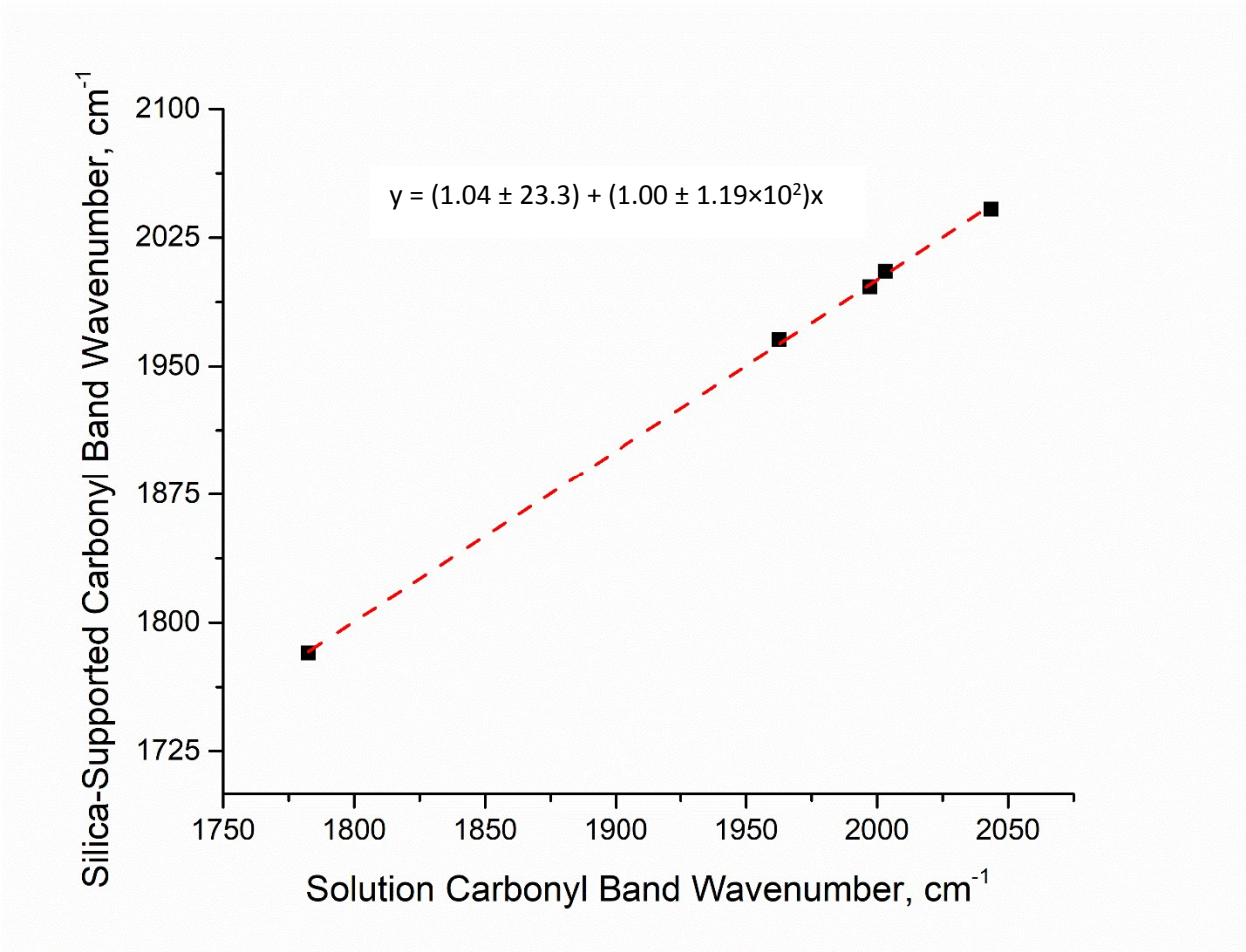


Figure S3. Parametric plot demonstrating the correlation between the carbonyl bands for the Ir4L3(CO)9 carbonyl cluster supported on dehydroxylated silica and the same clusters dissolved in anhydrous n-decane.

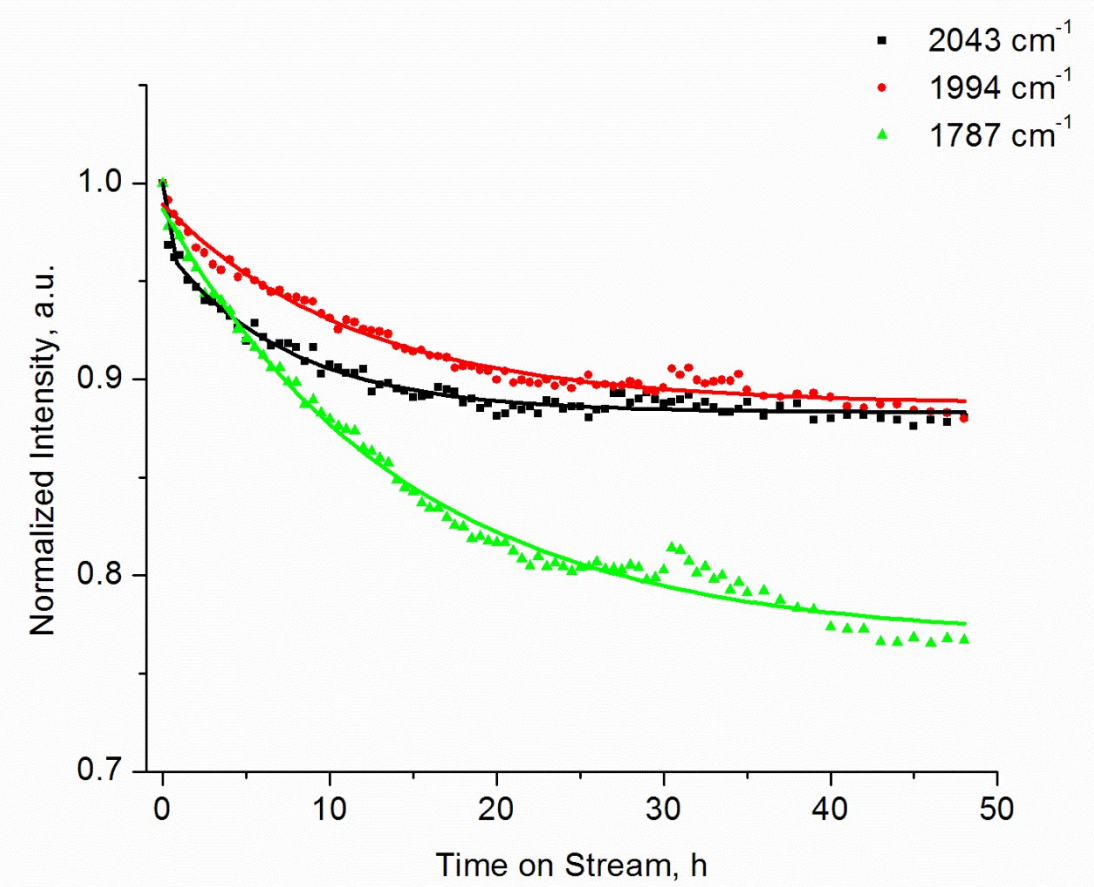


Figure S4. Decarbonylation of terminal (red circles and black squares) and bridging carbonyl (green triangles) bands for silica-supported $Ir_4L_3(CO)_9$ during decarbonylation treatment in flowing helium (helium flow rate = 50 mL/min, 323 K, 1 bar).

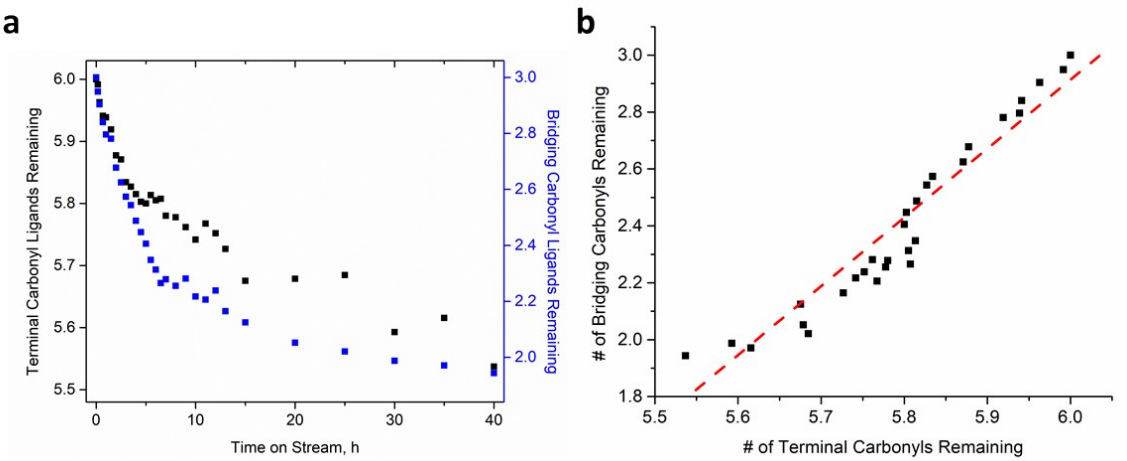


Figure S5. a) Number of terminal and bridging carbonyl ligands attached to silica-supported $Ir_4L_3(CO)_9$ as a function of time on stream during decarbonylation in helium (helium flow rate = 50 mL/min, 323 K, 1 bar, 99.999% purity). b) Data showing the linear relationship between bridging and terminal carbonyl loss during He treatment.

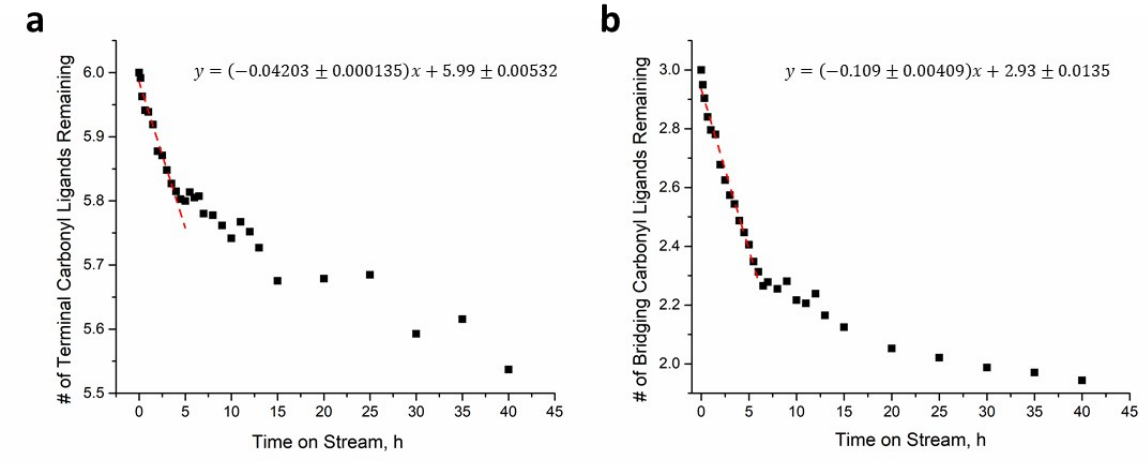


Figure S6. Initial rate of decarbonylation for terminal (a) and bridging (b) under helium flow at 323 K and 1 bar (helium flow rate = 50 mL/min) for silica-supported cluster $Ir_4L_3(CO)_9$.

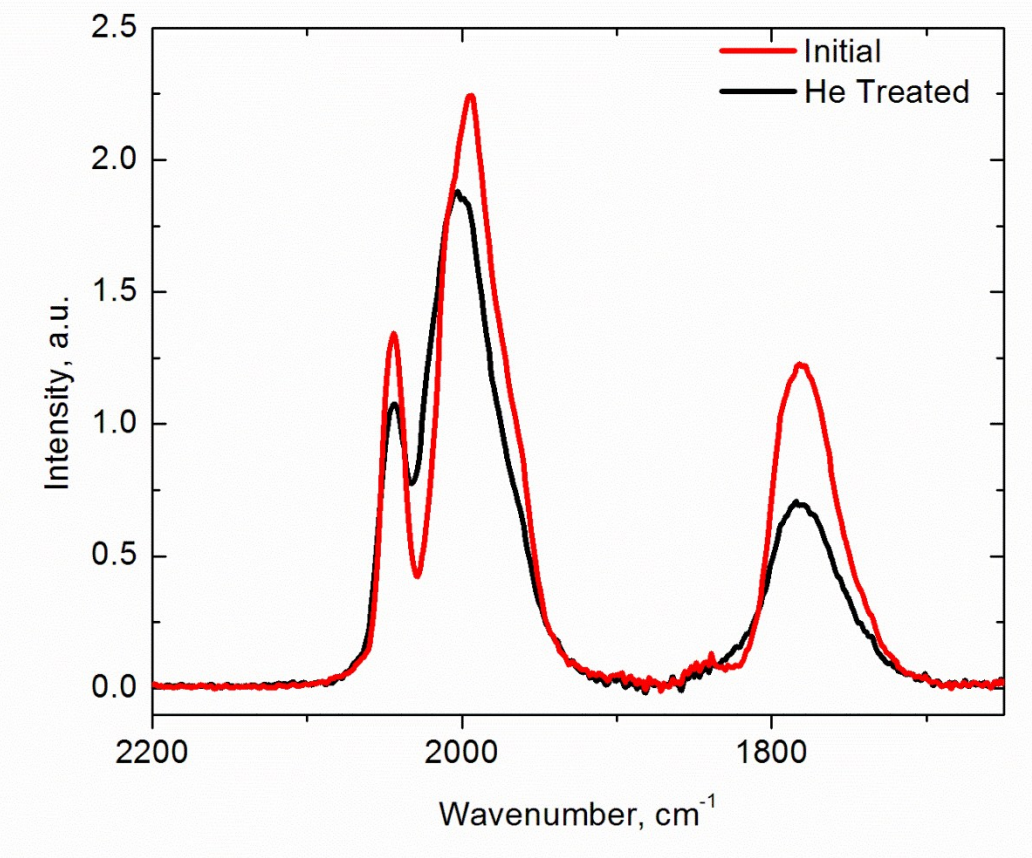


Figure S7. Difference spectra (difference spectra were used to substract the silica features) showing decarbonylation of silica-supported $Ir_4L_3(CO)_9$ in the carbonyl stretching region during He treatment. The red spectrum corresponds to the initial supported cluster before helium treatment, whereas the black spectrum corresponds to the supported cluster after 40 h of helium treatment (helium flow rate = 50 mL/min, 323 K, 1 bar). Bands corresponding to dehydroxylated silica support are absent in the spectra because they have been subtracted out.

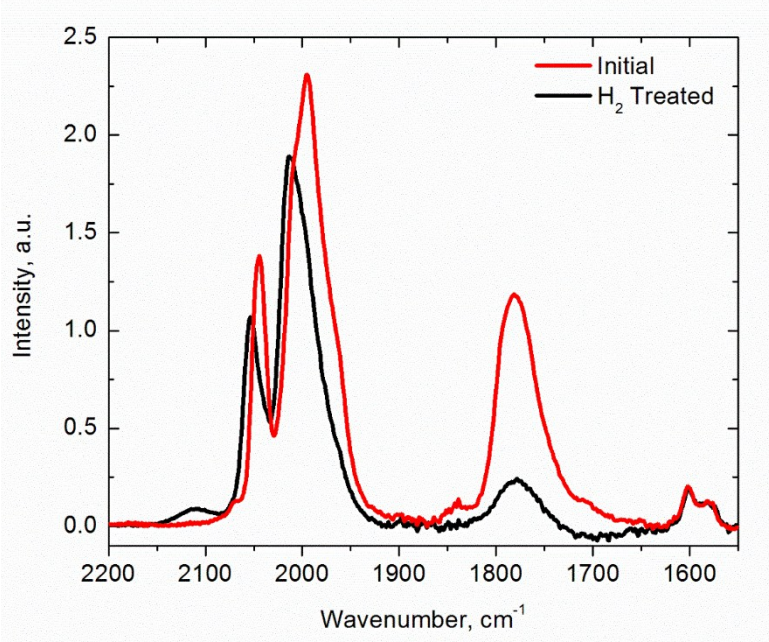


Figure S8. Difference spectra showing decarbonylation of silica-supported $Ir_4L_3(CO)_9$ in the carbonyl stretching region during H_2 treatment (H_2 flow rate = 10 mL/min and helium flow rate = 50 mL/min, 323 K, and 1 bar). Bands corresponding to dehydroxylated silica support are absent in the spectra because they have been subtracted out.

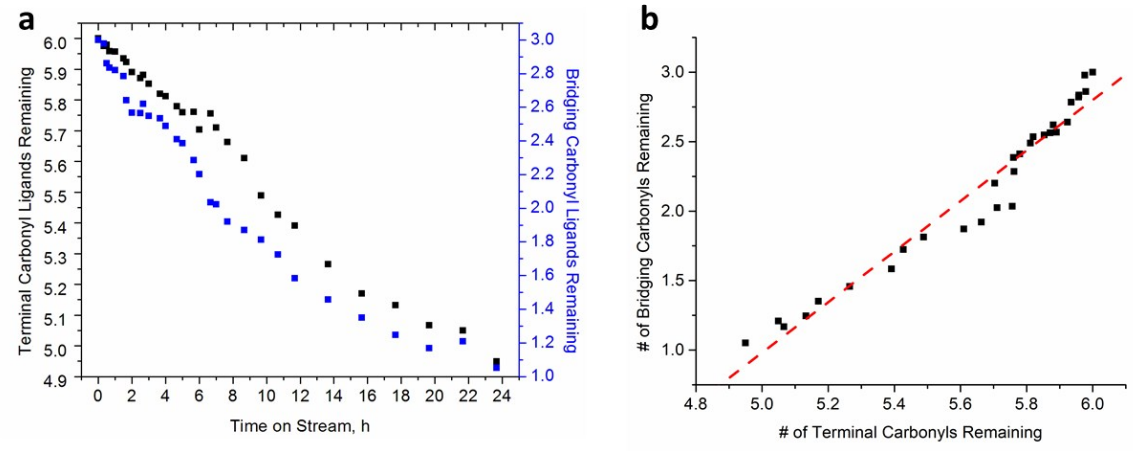


Figure S9. a) Number of terminal and bridging carbonyl ligands attached to silica-supported $Ir_4L_3(CO)_9$ as a function of time on stream during decarbonylation in hydrogen (helium flow rate = 50 mL/min, H_2=10 mL/min, 323 K, 1 bar). b) Parametric plot showing the linear relationship between bridging and terminal carbonyl loss during H_2 treatment.

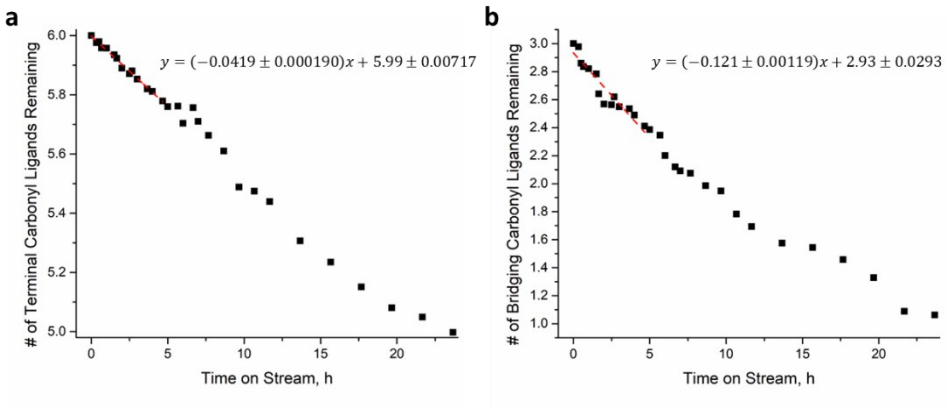


Figure S10. Initial rate of decarbonylation for terminal (a) and bridging (b) with sample in H_2 flowing at 323 K and 1 bar (H_2 flow rate = 10 mL/min and helium flow rate = 50 mL/min) for silica-supported cluster $Ir_4L_3(CO)_9$.

Table S1. Characteristic times for decarbonylation during treatments in helium and H_2 at 323 K and 1.0 bar.

Wavenumber of Carbonyl Band	Timescale for He Treatment (h)	Timescale for H_2 Treatment (h)
2043 cm^{-1}	3.14 ± 1.03	3.15 ± 0.52
1994 cm^{-1}	3.64 ± 0.54	3.90 ± 0.82
1787 cm^{-1}	5.25 ± 1.47	5.40 ± 0.34

Characterization of off-gas during CO treatment

To further characterize the process of synthesis of the original clusters via CO treatment after H_2 treatment, we used mass spectrometry to analyze the gas-phase effluents formed during the H_2 treatment of supported $Ir_4L_3(CO)_9$ with helium and then with CO at 323 K. The sample temperature was ramped up to 323 K when the helium was flowing, and a strong signal for H_2 was observed by mass spectrometry (Figure S9, SI). Once the temperature had reached 323 K, the flowing gas was switched from helium to CO, and subsequently the signal for effluent H_2 increased in intensity, followed by a decay to the baseline value. IR spectra of the solid sample recorded during these processes (Figure S10a and S10b, SI) demonstrate both the expected decrease in the hydride band intensity and a red shift in the terminal carbonyl band initially observed at 2052 cm^{-1}, and this band returned to its original position at 2043 cm^{-1}. Exposure of the sample to flowing CO following the helium treatment restored the other terminal carbonyl band, which was present at 2012 cm^{-1} initially and at 1994 cm^{-1} finally. This terminal carbonyl band remained essentially unchanged during the treatment in flowing helium that preceded the treatment in CO. We thus infer that the CO treatment following the helium treatment removed additional hydride ligands, which must have resided at bonding positions different from those characterizing the cluster to which hydride ligands were added by oxidative addition during the decarbonylation with the sample in flowing helium. The cluster with the hydride ligands in the different bonding positions after the CO treatment is characterized by the terminal CO band at 1994 cm^{-1}.

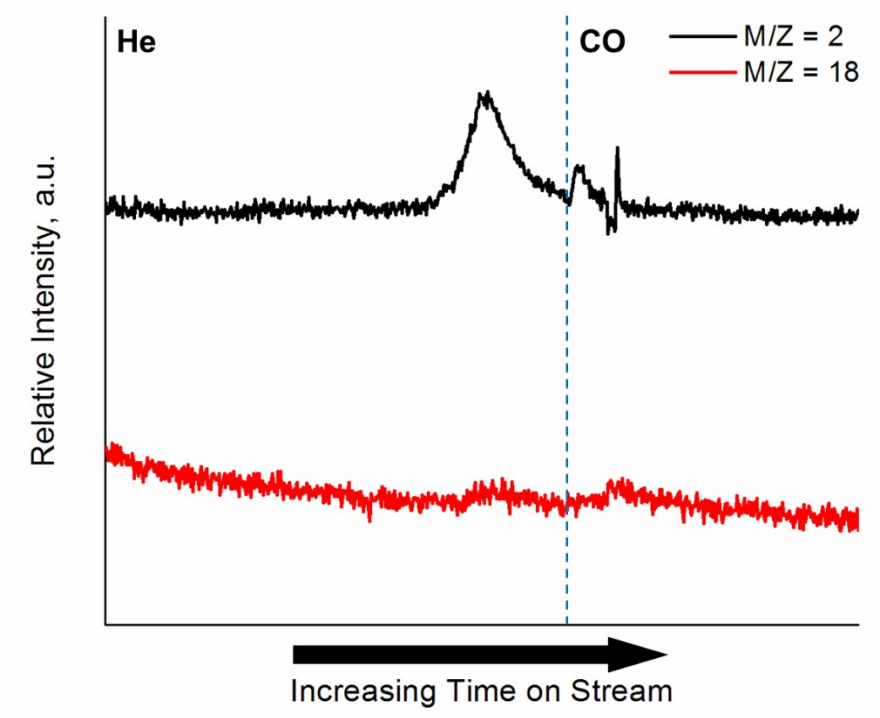


Figure S11. Water (red) and H_2 (black) mass intensities as a function of time on stream for SiO_2 supported $Ir_4L_3(CO)_9$ (treated with 10 mL/min of H_2 and 50 mL/min of helium for 24 h at 323 K and 1 bar) that underwent treatment in helium flowing at 50 mL/min during a temperature ramp from room temperature to 323 K (3 K/min ramp rate) followed by CO treatment (dashed line) once the temperature had reached 323 K (CO flow rate = 20 mL/min, helium flow rate = 50).

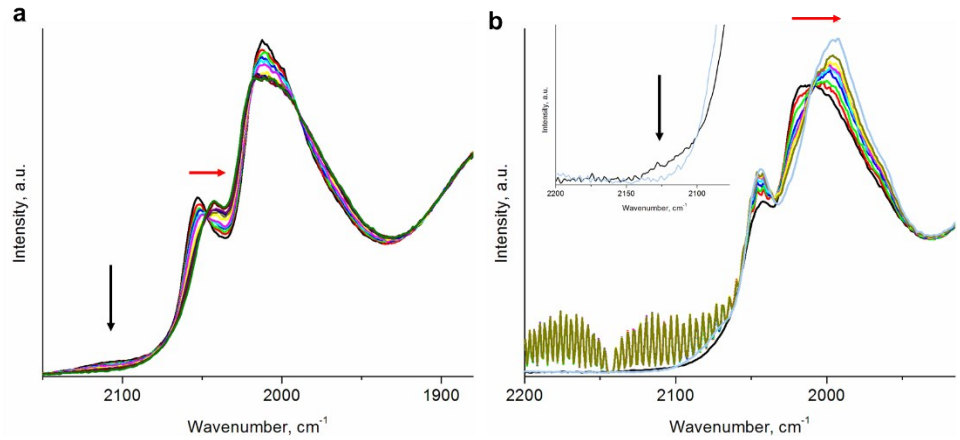


Figure S12. IR spectra of the carbonyl region of supported $Ir_4L_3(CO)_9$ (treated with H_2 flowing at 10 mL/min and helium flowing at 50 mL/min for 24 h at 323 K and 1 bar) during (a) helium (50 mL/min) followed by (b) CO treatment (20 mL/min and 50 mL/min of helium).

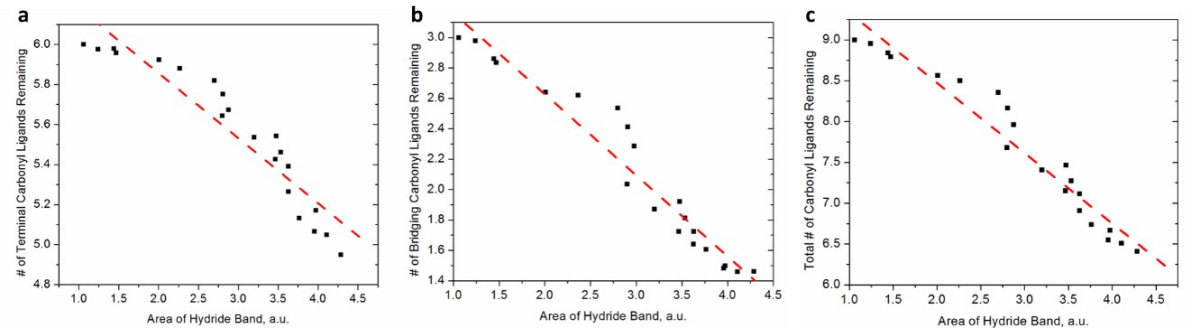


Figure S13. Number of terminal (a), bridging (b), and total carbonyls (c) remaining on silica-supported $Ir_4L_3(CO)_9$ as a function of hydride band area during H_2 treatment (helium flow rate = 50 mL/min, H_2 flow rate = 10 mL/min, 323 K, 1 bar).

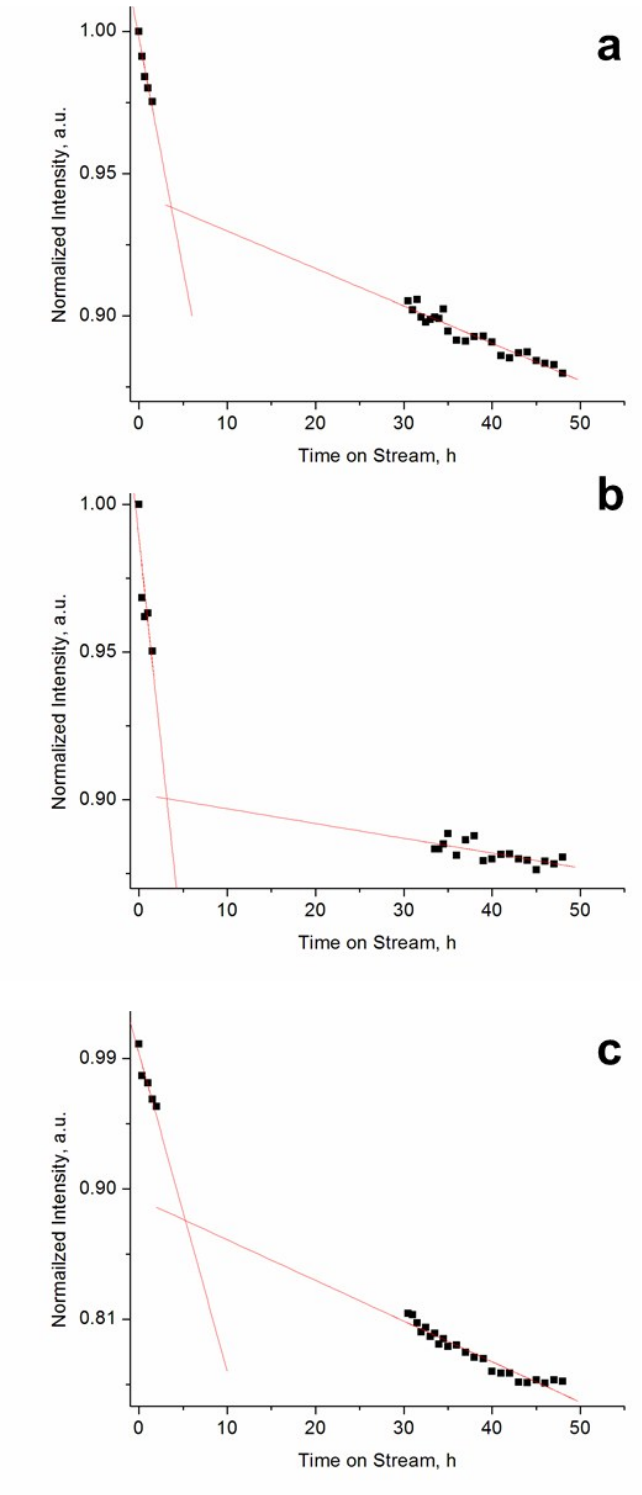


Figure S14. Removal of carbonyl bands at 2052 (a), 2043 (b), and 1787 cm^{-1} (c) during decarbonylation in flowing helium (helium flow rate = 50 mL/min, 323 K, 1 bar, 99.999% purity).

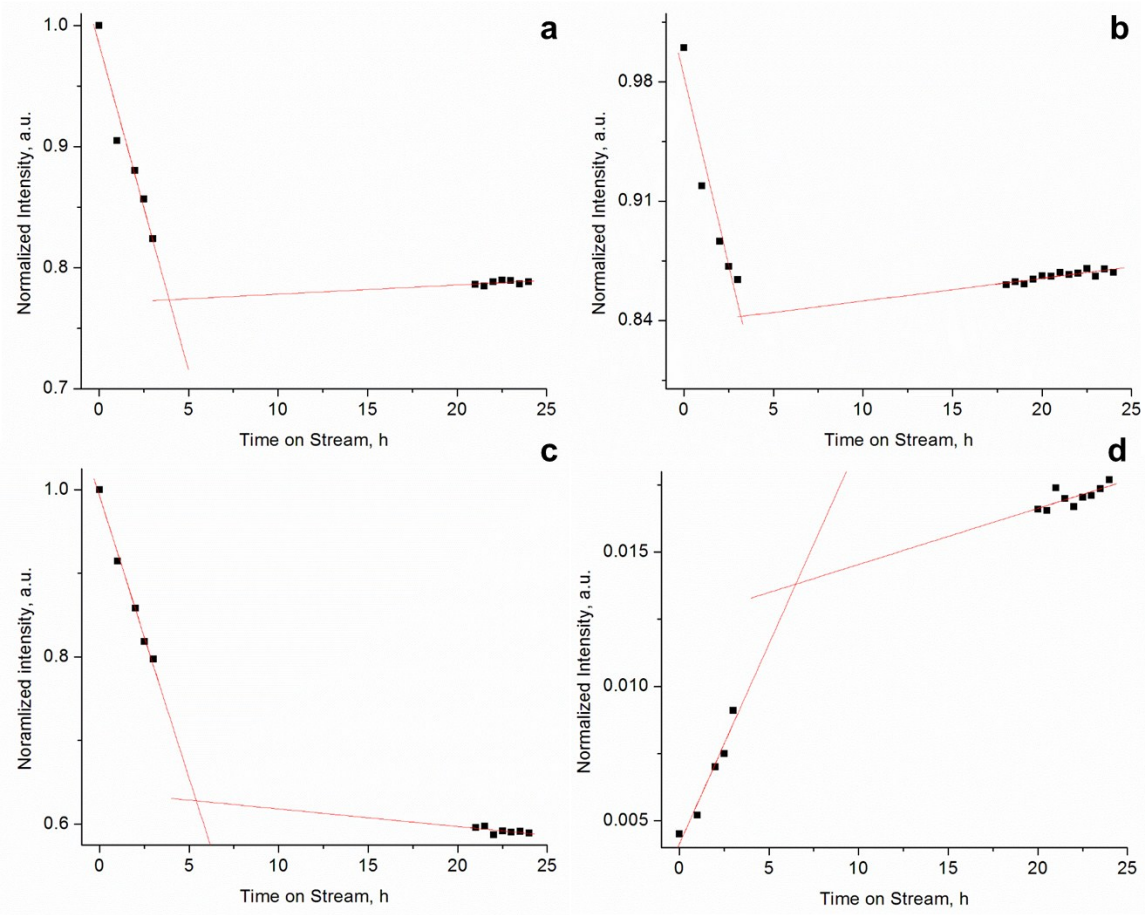


Figure S15. Declines in carbonyl band intensity for bands at 2043 cm^{-1} (a), 1994 cm^{-1} (b), and 1786 cm^{-1} (c), as well as hydride band growth at 2110 cm^{-1} (d) during H_2 treatment (flow rate H_2 flow rate = 10 mL/min (99.999% purity), helium flow rate = 50 mL/min (99.999% purity), 323 K, 1 bar)

NOTES REGARDING NMR SPECTROSCOPY

NMR spectroscopy for characterization of hydride ligands on single-site supported metals is highly informative,[S2-S6] but the simultaneous characterization of H and CO ligands by NMR spectroscopy on a sample such as ours is challenging because the spectra are complex, since they represent a mixture of compounds upon H_2 treatment, and as such are challenging to interpret. This complexity is compounded by the inherent asymmetry within the cluster (i.e. as discussed in elsewhere[S6] when describing the crystal structure, asymmetry results from having both equatorial as well as axial phosphine ligands, in addition to basal-plane and apical iridium atoms, which involve terminal and bridging CO ligands). This asymmetry creates a large number of sites where hydrogen can bond, and the multiplicity of metal hydride and carbonyl species that can subsequently form, resulting in broad and uninterpretable spectra comprising a complex mixture.

ELECTRONIC STRUCTURE CALCULATIONS

Table S2. CO Dissociation Energies in kcal/mol for $Ir_4(CO)_9L_3$ clusters with L = $PMePh_2$ in the basal plane for the product CO in solution. See computational approach for details

CO Dissociated Energy[a]	$\Delta G_{(298,gas)}$	$\Delta G_{(298,water)}$	$\Delta G_{(298,n\text{-}hexane)}$
Eq	37.5	36.7	37.1
Ax	26.2	26.2	26.2
bri(1)	15.5	15.4	15.5
bri(1) → bri(1).ax(1) + CO	49.6	48.3	49.2
bri(1) → bri(1).ax(2)[b] + CO	23.6	22.4	23.2
bri(1) → bri(1).eq[b] + CO	44.9	42.9	44.0
bri(2)	20.0	18.6	19.5
bri(2) → bri(2).ax + CO	30.5	31.4	30.9
bri(2) → bri(2).eq[b] + CO	36.8	36.7	36.7

[a] eq = equatorial terminal, ax = axial terminal, br = bridge. [b] One of the three api CO's turns into a bri CO.

Table S3. CO Dissociation Energies in kcal/mol for $Ir_4(CO)_9L_3$ clusters with L = $PMePh_2$ in the basal plane for the product CO in the gas phase. See computational approach for details

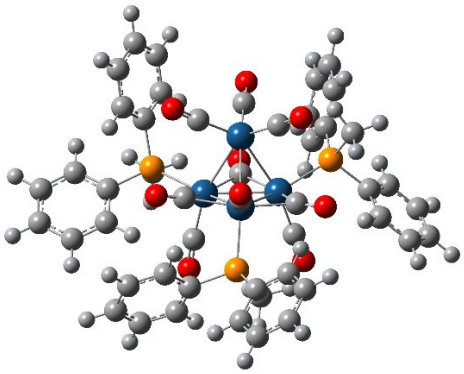
CO Dissociated Energy	$\Delta G_{(298,gas)}$	$\Delta G_{(298,water)}$	$\Delta G_{(298,n\text{-}hexane)}$
api (1)	12.5	12.8	12.7
api (2)	19.8	20.1	19.9
Eq	37.5	37.3	37.4
Ax	26.2	26.7	26.5
bri(1)	15.5	16.0	15.8
bri(1) → bri(1).ax(1) + CO	49.6	48.9	49.5
bri(1) → bri(1).ax(2)[b] + CO	23.6	22.9	23.4
bri(1) → bri(1).eq[b] + CO	44.9	43.5	44.2
bri(2)	20.0	19.2	19.8
bri(2) → bri(2).ax + CO	30.5	32.0	31.2
bri(2) → bri(2).eq[b] + CO	36.8	37.3	36.9

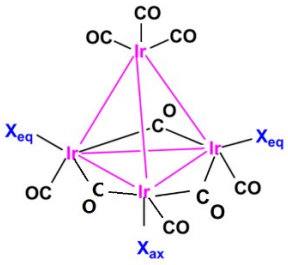
[a] eq = equatorial terminal, ax = axial terminal, br = bridge. [b] One of the three api CO's turns into a bri CO.

Computational Method

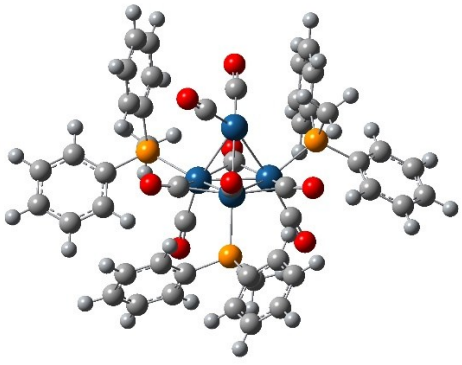
The geometries of $Ir_4(CO)_9L_3$ clusters were optimized using density functional theory (DFT)[S7] with the SVWN5[S8-9] functional as this has been shown to provide good geometries for such clusters. L = $PMePh_2$ was used for the phosphine ligands instead of the calixarene phosphines considering the calculation cost. The optimized geometries were used in single-point DFT calculations with the B3LYP[S10-11] function. We used the DZVP[S12] polarized double-zeta basis set for the light elements, and a relativistic pseudopotential correlation consistent double –zeta cc-pVDZ-pp[S13] basis set for Ir including 60 electrons in the pseudopotential ($1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}4f^{14}$) and 17 active electrons in the self-consistent field calculations ($5s^25p^66s^25d^7$). The reaction energies in water and n-hexane were calculated with COSMO[S14] solvation model. All the DFT calculations were performed using the Gaussian09 suite of programs.[S15]

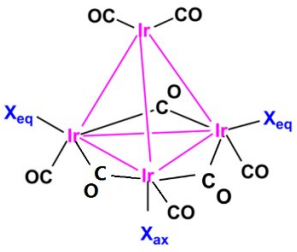
Structures of $Ir_4(CO)_9PL_3$, $Ir_4(CO)_8PL_3$and $Ir_4(CO)_7PL_3$ isomers.





$Ir_4(CO)_9[PCH_3(C_6H_5)_2]_3$





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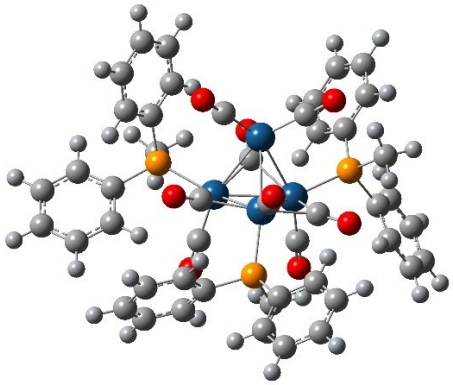

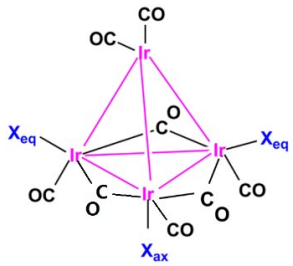

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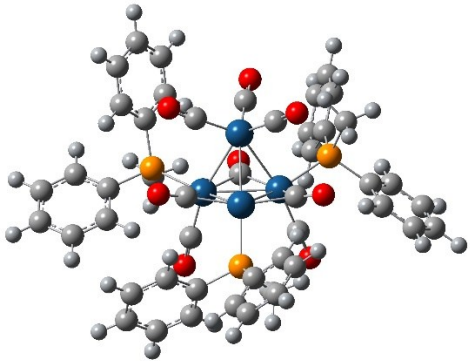

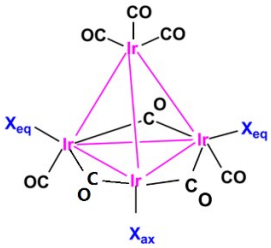

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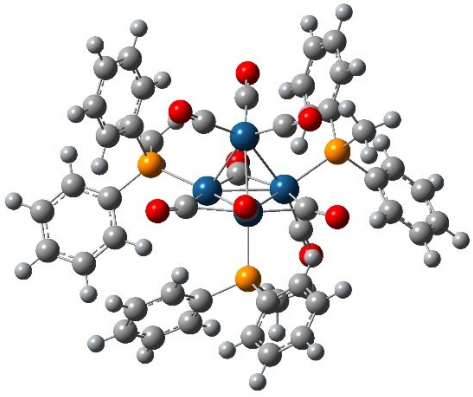

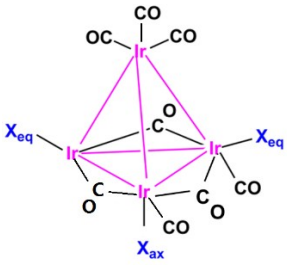

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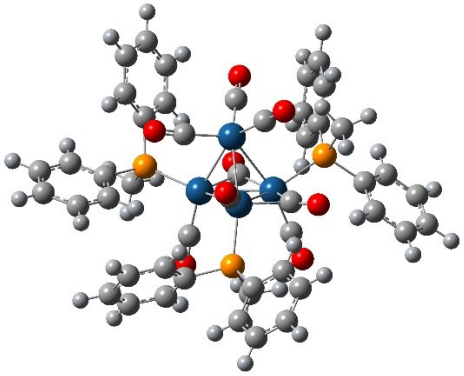

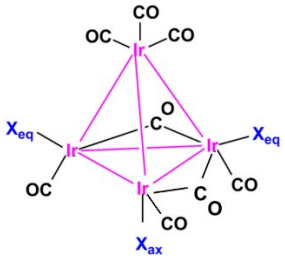

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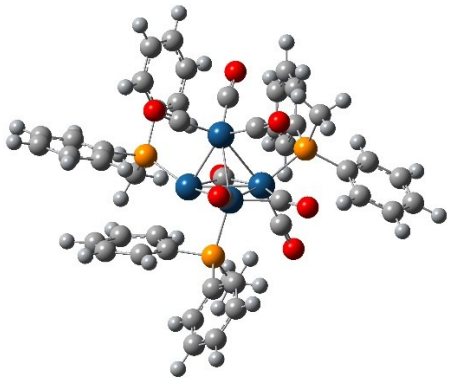

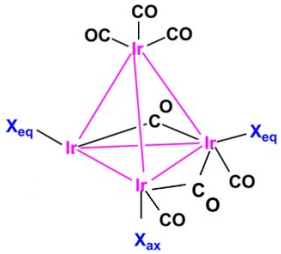

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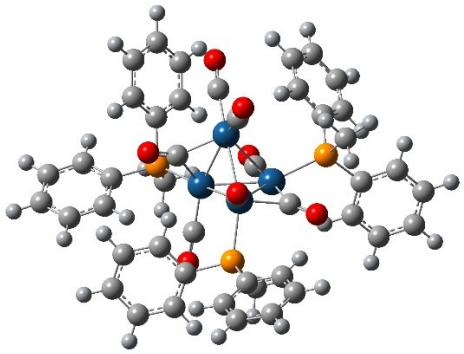
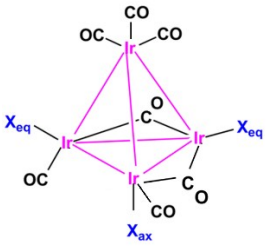
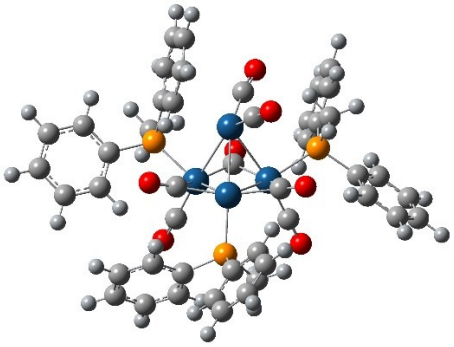
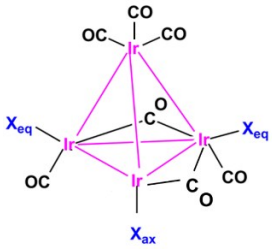


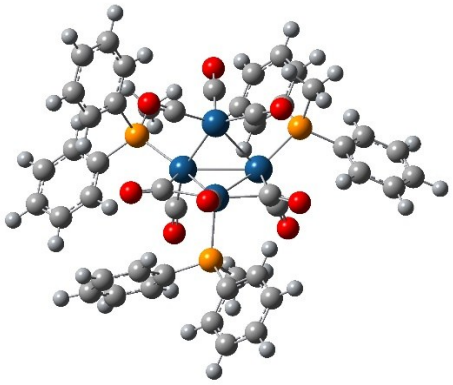


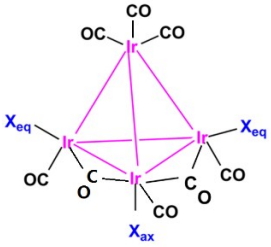
$Ir_4(CO)_7[PCH_3(C_6H_5)_2]_3$ bri CO(1) and ax CO(2) removed



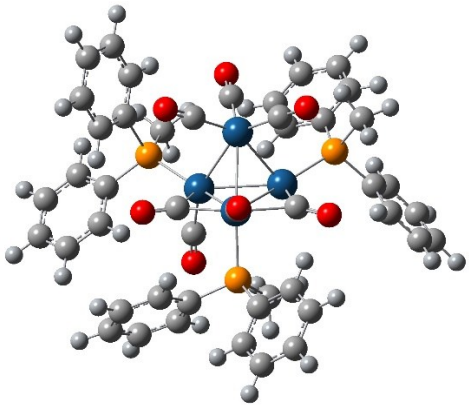


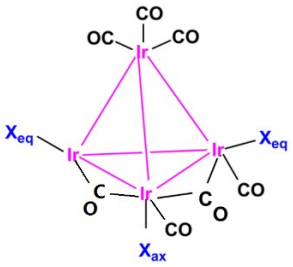
$Ir_4(CO)_7[PCH_3(C_6H_5)_2]_3$ bri CO(1) and eq CO removed



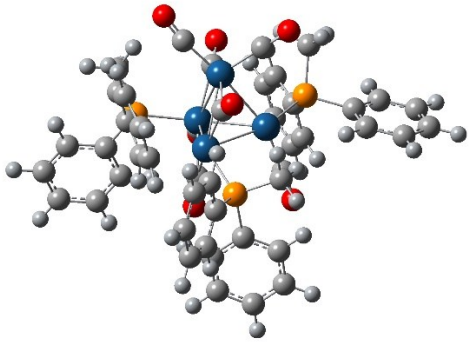


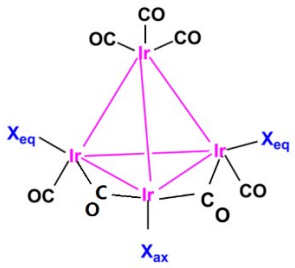
$Ir_4(CO)_8[PCH_3(C_6H_5)_2]_3$ bri CO(2) removed





$Ir_4(CO)_7[PCH_3(C_6H_5)_2]_3$ bri CO(2) and ax CO removed





$Ir_4(CO)_7[PCH_3(C_6H_5)_2]_3$ bri CO(2) and eq CO removed

Coordinates

$Ir_4(CO)_9[PCH_3(C_6H_5)_2]_3$

IR	0.825586	-0.819794	-0.734055
P	1.819592	-2.874243	-1.040329
C	-1.070116	-1.432262	-1.302432
C	1.189655	-3.693788	-2.535541
C	1.584010	-4.110923	0.261608
C	3.618409	-2.873969	-1.308581
C	1.433214	-0.224992	-2.371211
C	2.193931	-0.045547	0.612258
IR	-1.531356	0.428394	-0.484390
O	-1.582594	-2.367600	-1.838905
H	1.510670	-3.097486	-3.408092
H	0.083975	-3.700527	-2.512515
C	0.435955	-4.911687	0.260258
C	2.506555	-4.217138	1.308998
C	4.322025	-1.684236	-1.507572
C	4.295144	-4.099468	-1.383071
O	1.752260	0.181980	-3.424185
O	3.273647	-0.274418	1.055815
P	-3.782062	0.214843	-0.064207
C	-1.280849	2.037275	0.794713
C	-1.835327	1.323620	-2.072360
C	0.218790	-5.818660	1.295162
H	-0.312039	-4.813641	-0.540116
C	2.285903	-5.127979	2.339272
H	3.397673	-3.572965	1.323899
C	5.688311	-1.718712	-1.784830
H	3.801716	-0.718964	-1.430222
C	5.659093	-4.130900	-1.659147
H	3.749718	-5.038776	-1.206461
C	-4.308246	0.611217	1.626647
C	-4.497529	-1.408331	-0.409708
C	-4.812672	1.377967	-1.017439
IR	0.666634	1.353615	0.872864
O	-1.933017	2.927408	1.261199
O	-2.030882	1.868388	-3.089753
C	1.144267	-5.930847	2.333912
H	-0.690704	-6.433203	1.293841
H	3.008314	-5.198666	3.162653
C	6.358226	-2.938351	-1.862356
H	6.225524	-0.771022	-1.930602
H	6.182882	-5.094308	-1.713391
H	-3.920022	-0.129410	2.345723
H	-3.884445	1.597255	1.891935
C	-5.161238	-2.146822	0.575247

C	-4.364602	-1.939626	-1.698763
C	-5.895226	0.968406	-1.800096
C	-4.503138	2.741378	-0.917112
P	1.605888	2.986029	-0.438192
C	1.228464	2.125525	2.449934
H	0.969100	-6.642315	3.151538
H	7.434906	-2.964154	-2.076825
C	-5.693666	-3.399026	0.272710
H	-5.266449	-1.747192	1.592899
C	-4.910640	-3.183564	-2.002022
H	-3.821265	-1.376195	-2.470287
C	-6.656497	1.915004	-2.487389
H	-6.146542	-0.099429	-1.874577
C	-5.273535	3.681738	-1.596161
H	-3.654409	3.069266	-0.294424
C	0.706776	3.393156	-1.963016
C	3.288050	2.587492	-0.980764
C	1.769855	4.613593	0.354935
O	1.585573	2.582162	3.464708
C	-5.573307	-3.916925	-1.016531
H	-6.206089	-3.975395	1.053847
H	-4.800565	-3.590829	-3.015458
C	-6.348355	3.270815	-2.387400
H	-7.501027	1.585972	-3.107141
H	-5.027778	4.748366	-1.510124
H	0.611029	2.510465	-2.619382
H	-0.310336	3.718702	-1.681344
C	4.251994	2.332527	0.004132
C	3.631079	2.471178	-2.331588
C	2.849732	5.453630	0.061289
C	0.759564	5.049342	1.220518
H	-5.993173	-4.903301	-1.253693
H	-6.948963	4.013186	-2.929198
C	5.551760	1.995843	-0.360688
H	3.973734	2.381718	1.067172
C	4.932650	2.122316	-2.694571
H	2.879123	2.640522	-3.114484
C	2.919408	6.723166	0.632791
H	3.649378	5.104434	-0.608614
C	0.831858	6.322724	1.782581
H	-0.089800	4.389347	1.458858
C	5.894967	1.892329	-1.711168
H	6.298362	1.794302	0.418120
H	5.192604	2.027319	-3.756848
C	1.910291	7.159442	1.492154
H	3.773244	7.375879	0.408384

H	0.039453	6.659003	2.463792
H	6.923299	1.633197	-1.998754
H	1.968781	8.157977	1.944945
C	-1.561542	-2.502465	1.304215
IR	-0.536156	-0.963877	1.671964
O	-2.208732	-3.452936	1.104770
C	0.939463	-1.632273	2.647040
C	-1.432627	0.048301	2.986361
O	1.824142	-2.037806	3.286091
O	-1.950079	0.667180	3.830159
H	-5.410628	0.660781	1.680735
H	1.208778	4.218418	-2.500844
H	1.583902	-4.721590	-2.625971

$Ir_4(CO)_8[PCH_3(C_6H_5)_2]_3$ api CO(1) removed

IR	0.766882	-0.832017	-0.781958
P	1.665006	-2.948995	-0.929788
C	-1.167547	-1.298027	-1.471190
C	0.951060	-3.934299	-2.274685
C	1.431717	-3.932828	0.563792
C	3.457972	-3.049429	-1.216552
C	1.469640	-0.397235	-2.402879
C	2.180698	-0.130139	0.602694
IR	-1.520805	0.502330	-0.573921
O	-1.677417	-2.199727	-2.059624
H	1.278947	-3.486760	-3.229609
H	-0.152561	-3.868719	-2.235672
C	0.412787	-4.885411	0.656899
C	2.255780	-3.674126	1.667332
C	4.223250	-1.916559	-1.501971
C	4.072104	-4.308463	-1.170141
O	1.856823	-0.061968	-3.458968
O	3.235302	-0.468228	1.036898
P	-3.708355	0.223968	0.053403
C	-1.209699	1.988355	0.863389
C	-1.924237	1.583695	-2.048147
C	0.224560	-5.585259	1.847352
H	-0.257239	-5.072891	-0.193701
C	2.062500	-4.376176	2.852319
H	3.043966	-2.908477	1.599418
C	5.588823	-2.044027	-1.754215
H	3.760493	-0.918872	-1.507056
C	5.435013	-4.432631	-1.424789
H	3.479457	-5.198581	-0.910065
C	-3.954093	0.397797	1.844816
C	-4.459309	-1.357567	-0.395115

C	-4.871510	1.463437	-0.605594
IR	0.717211	1.279917	0.862986
O	-1.851030	2.829617	1.427614
O	-2.209249	2.254593	-2.964160
C	1.048312	-5.332018	2.943962
H	-0.585531	-6.322040	1.921368
H	2.698750	-4.157955	3.719417
C	6.195283	-3.298518	-1.720536
H	6.177069	-1.140339	-1.966574
H	5.910284	-5.421516	-1.384656
H	-3.334281	-0.351210	2.379899
H	-3.596619	1.404657	2.129524
C	-5.030314	-2.202058	0.560667
C	-4.465632	-1.736457	-1.742701
C	-6.092091	1.110834	-1.190129
C	-4.528052	2.815733	-0.477444
P	1.713420	2.934479	-0.439075
C	1.270815	1.954911	2.491057
H	0.891417	-5.876576	3.883789
H	7.271670	-3.396431	-1.915149
C	-5.614250	-3.407054	0.172780
H	-5.016094	-1.923923	1.622580
C	-5.065097	-2.931919	-2.130264
H	-3.992550	-1.088504	-2.492768
C	-6.960867	2.104442	-1.644202
H	-6.365533	0.050942	-1.293996
C	-5.404542	3.802816	-0.921917
H	-3.569451	3.096962	-0.012795
C	0.835224	3.405053	-1.958667
C	3.373290	2.466738	-0.998967
C	1.953790	4.533774	0.389218
O	1.634066	2.354433	3.527790
C	-5.638037	-3.770543	-1.173002
H	-6.049340	-4.069251	0.932264
H	-5.069154	-3.218896	-3.189557
C	-6.621176	3.449801	-1.509637
H	-7.914290	1.820198	-2.109023
H	-5.130332	4.860215	-0.813532
H	0.662812	2.523496	-2.601664
H	-0.151766	3.809180	-1.673432
C	4.342580	2.186036	-0.025434
C	3.677584	2.274053	-2.350105
C	3.038654	5.358689	0.071945
C	0.999928	4.961225	1.319871
H	-6.101884	-4.718557	-1.477532
H	-7.306944	4.229239	-1.866171

C	5.608039	1.748125	-0.402671
H	4.093756	2.295450	1.040404
C	4.943716	1.821899	-2.725339
H	2.921281	2.462064	-3.124675
C	3.168752	6.604061	0.684138
H	3.794595	5.014268	-0.649433
C	1.130214	6.211417	1.922342
H	0.150675	4.308165	1.575992
C	5.911465	1.565304	-1.754299
H	6.358132	1.528010	0.367911
H	5.170344	1.666990	-3.788077
C	2.214125	7.032251	1.607953
H	4.026447	7.244831	0.440766
H	0.381121	6.541186	2.653870
H	6.912850	1.224771	-2.052076
H	2.320165	8.011770	2.092483
C	-1.696017	-2.420896	1.473509
IR	-0.667656	-0.877451	1.569251
O	-2.269023	-3.441275	1.414528
C	0.470229	-1.280053	2.991069
O	1.198097	-1.520653	3.873566
H	1.393911	4.182307	-2.511934
H	-5.018972	0.298052	2.122798
H	1.286458	-4.985947	-2.231212

$Ir_4(CO)_8[PCH_3(C_6H_5)_2]_3$ api CO(2) removed

IR	-0.899954	-0.751064	0.747841
P	-2.107607	-2.679497	1.030590
C	0.935886	-1.722851	0.573203
C	-1.320505	-3.810084	2.216545
C	-2.318918	-3.706170	-0.447618
C	-3.804060	-2.489184	1.653052
C	-1.320012	-0.151584	2.454469
C	-2.174480	0.130518	-0.564298
IR	1.630415	0.237466	0.450002
O	1.339609	-2.870548	0.597693
H	-1.339855	-3.337352	3.213794
H	-0.265039	-3.942931	1.914144
C	-1.247286	-4.500635	-0.881370
C	-3.503219	-3.665643	-1.190852
C	-4.373812	-1.225578	1.823363
C	-4.552108	-3.633975	1.961438
O	-1.533828	0.240563	3.540775
O	-3.286528	0.024937	-0.976605
P	3.878632	-0.068620	0.080729
C	1.524446	1.873812	-0.755540

C	1.926037	0.942101	2.143822
C	-1.378990	-5.272171	-2.033771
H	-0.296662	-4.501205	-0.324786
C	-3.623395	-4.434864	-2.347541
H	-4.333104	-3.018646	-0.868686
C	-5.677138	-1.108092	2.305516
H	-3.797820	-0.325052	1.562640
C	-5.851077	-3.513331	2.447061
H	-4.118567	-4.633077	1.805712
C	4.535857	0.630582	-1.461109
C	4.487130	-1.770776	0.129499
C	4.912146	0.805960	1.301439
IR	-0.468860	1.317757	-0.921571
O	2.229719	2.765138	-1.143155
O	2.092208	1.348268	3.229652
C	-2.567587	-5.245133	-2.765448
H	-0.537788	-5.895054	-2.366937
H	-4.551547	-4.392472	-2.932081
C	-6.415961	-2.247192	2.620376
H	-6.112910	-0.106236	2.423741
H	-6.430453	-4.414390	2.688184
H	4.156341	0.088496	-2.344479
H	4.184091	1.676757	-1.528754
C	5.329014	-2.284818	-0.862350
C	4.120689	-2.577930	1.213498
C	5.862385	0.160547	2.096004
C	4.734268	2.191570	1.416753
P	-1.248376	3.080611	0.274208
C	-0.948637	2.087272	-2.529539
H	-2.665077	-5.848314	-3.677615
H	-7.442113	-2.152364	2.999466
C	5.810644	-3.589975	-0.763508
H	5.615274	-1.663760	-1.722564
C	4.616586	-3.874702	1.318264
H	3.434897	-2.182115	1.976520
C	6.625394	0.894879	3.005594
H	6.006535	-0.925918	2.005335
C	5.505911	2.920889	2.317137
H	3.979576	2.701666	0.795323
C	-0.311740	3.405883	1.793916
C	-2.963776	2.867682	0.805040
C	-1.231785	4.689322	-0.568583
O	-1.267038	2.524798	-3.565079
C	5.461292	-4.383285	0.329970
H	6.467808	-3.988812	-1.547468
H	4.327223	-4.499519	2.173562

C	6.450629	2.273369	3.116788
H	7.365205	0.380999	3.633761
H	5.362997	4.006282	2.401068
H	-0.310681	2.524830	2.458764
H	0.734553	3.618040	1.511036
C	-3.964715	2.843919	-0.175535
C	-3.298609	2.644312	2.144596
C	-2.206255	5.655181	-0.291787
C	-0.188762	4.981551	-1.454751
H	5.844567	-5.409374	0.408210
H	7.052260	2.848266	3.833027
C	-5.290968	2.631753	0.187024
H	-3.700375	2.980472	-1.234803
C	-4.628625	2.420550	2.502814
H	-2.522400	2.631873	2.922023
C	-2.141422	6.904401	-0.906912
H	-3.030199	5.422618	0.398522
C	-0.127616	6.234748	-2.061535
H	0.586207	4.228445	-1.666886
C	-5.625561	2.422186	1.526967
H	-6.068460	2.611510	-0.587284
H	-4.881892	2.241164	3.556064
C	-1.103182	7.195068	-1.792770
H	-2.913473	7.655703	-0.695975
H	0.689907	6.457725	-2.759201
H	-6.674241	2.258091	1.810679
H	-1.057185	8.177500	-2.280999
IR	0.481469	-1.179652	-1.543594
C	-0.934290	-1.799300	-2.602945
C	1.752001	-0.851528	-2.858785
O	-1.816868	-2.067492	-3.315305
O	2.509195	-0.610624	-3.718832
H	-0.731600	4.284517	2.317248
H	5.640103	0.621259	-1.443790
H	-1.828946	-4.789924	2.255606

$Ir_4(CO)_8[PCH_3(C_6H_5)_2]_3$ eq CO removed

IR	1.010432	-0.688965	-0.607960
P	2.117907	-2.644535	-0.919317
C	-0.839181	-1.422638	-1.215026
C	1.623336	-3.470087	-2.460281
C	1.888341	-3.920948	0.341762
C	3.923381	-2.499681	-1.089967
C	1.652318	-0.151337	-2.250175
C	2.228285	0.354177	0.837364
IR	-1.543149	0.369830	-0.426047

O	-1.244481	-2.404574	-1.767797
H	1.963443	-2.849000	-3.308109
H	0.518940	-3.530558	-2.492122
C	0.733334	-4.712050	0.305307
C	2.810785	-4.077139	1.381880
C	4.549391	-1.252901	-1.151109
C	4.686741	-3.667218	-1.233319
O	1.985452	0.151390	-3.332959
O	3.301353	0.252644	1.347782
P	-3.728626	-0.122690	-0.074719
C	-1.406792	1.951753	0.967460
C	-1.960885	1.253478	-1.995931
C	0.511833	-5.662544	1.298301
H	-0.016522	-4.564826	-0.486679
C	2.585407	-5.033066	2.370181
H	3.703934	-3.437962	1.426510
C	5.925050	-1.173600	-1.364950
H	3.960237	-0.334423	-1.017249
C	6.060164	-3.584015	-1.444527
H	4.201472	-4.652571	-1.165832
C	-4.259044	-0.055067	1.656813
C	-4.287132	-1.722435	-0.696979
C	-4.857655	1.082487	-0.843168
IR	0.530881	1.431107	0.808697
O	-2.125193	2.704891	1.570546
O	-2.238054	1.790179	-3.000337
C	1.439198	-5.827176	2.329479
H	-0.403896	-6.267294	1.273084
H	3.307322	-5.145000	3.189386
C	6.681579	-2.334409	-1.513656
H	6.401519	-0.184322	-1.411509
H	6.651822	-4.502187	-1.555743
H	-3.774040	-0.856646	2.239501
H	-3.935605	0.916565	2.075208
C	-4.959728	-2.641595	0.114070
C	-4.029527	-2.037605	-2.036741
C	-5.882280	0.706041	-1.715226
C	-4.685112	2.433257	-0.509714
P	1.271910	3.182126	-0.389507
H	1.259803	-6.573036	3.114969
H	7.765180	-2.270113	-1.680344
C	-5.390856	-3.856273	-0.416823
H	-5.150421	-2.414194	1.171693
C	-4.476716	-3.243567	-2.568460
H	-3.468745	-1.330326	-2.664995
C	-6.725018	1.676342	-2.259758

H	-6.021942	-0.353420	-1.974067
C	-5.535918	3.394550	-1.049395
H	-3.880527	2.734464	0.181252
C	0.182389	3.780753	-1.716186
C	2.884867	2.963261	-1.190037
C	1.481021	4.650517	0.668894
C	-5.157074	-4.154816	-1.759231
H	-5.913449	-4.576336	0.226151
H	-4.273619	-3.481180	-3.620806
C	-6.554082	3.019619	-1.928849
H	-7.523645	1.376007	-2.950710
H	-5.398979	4.450589	-0.781853
H	0.023498	2.994746	-2.474718
H	-0.799553	4.018929	-1.270509
C	3.997393	2.687513	-0.381058
C	3.033895	2.977569	-2.579999
C	2.576549	5.514053	0.556100
C	0.476884	4.916869	1.611395
H	-5.499732	-5.111139	-2.176070
H	-7.218346	3.780938	-2.358560
C	5.238778	2.437340	-0.958934
H	3.889028	2.651921	0.712467
C	4.276852	2.715826	-3.156963
H	2.170520	3.173945	-3.230287
C	2.662110	6.639734	1.373973
H	3.369749	5.300547	-0.175183
C	0.567678	6.046223	2.422901
H	-0.386623	4.238924	1.711418
C	5.380666	2.446789	-2.349210
H	6.101154	2.223600	-0.312976
H	4.377200	2.710801	-4.249874
C	1.658789	6.908288	2.306735
H	3.523327	7.314614	1.281944
H	-0.222451	6.249494	3.157545
H	6.358013	2.240431	-2.805908
H	1.730498	7.795402	2.949636
C	-1.425070	-2.558019	1.373019
IR	-0.457104	-0.972509	1.718620
O	-2.060565	-3.527195	1.220269
C	1.092516	-1.523656	2.647408
C	-1.379053	-0.002429	3.046325
O	2.021196	-1.873615	3.258944
O	-1.922964	0.579314	3.901349
H	-5.359586	-0.128752	1.724414
H	0.596298	4.688691	-2.191674
H	2.070907	-4.476772	-2.535658

$Ir_4(CO)_8[PCH_3(C_6H_5)_2]_3$ ax CO removed

IR	0.790515	-0.877125	-0.709630
P	1.853404	-2.839511	-1.010449
C	-0.908725	-1.430140	-1.581817
C	0.948034	-4.108089	-1.949725
C	2.280760	-3.701486	0.533033
C	3.455928	-2.746000	-1.870391
C	2.248759	-0.084654	0.395640
IR	-1.539320	0.378154	-0.527013
O	-1.428315	-2.217903	-2.315048
H	0.816799	-3.754801	-2.986832
H	-0.063778	-4.240168	-1.527000
C	1.367503	-4.583437	1.123587
C	3.490945	-3.421659	1.178588
C	3.937871	-1.507783	-2.302862
C	4.207312	-3.902886	-2.110224
O	3.373195	-0.190456	0.779500
P	-3.789216	0.113331	-0.105265
C	-1.286798	2.029615	0.681453
C	-1.863718	1.251799	-2.119890
C	1.672372	-5.197268	2.337129
H	0.405308	-4.796739	0.634893
C	3.790057	-4.036494	2.392577
H	4.194173	-2.704068	0.731538
C	5.153039	-1.428089	-2.983028
H	3.360787	-0.593284	-2.087265
C	5.420369	-3.822716	-2.789085
H	3.847661	-4.875680	-1.742738
C	-4.328869	0.665722	1.541119
C	-4.485863	-1.547999	-0.278212
C	-4.847893	1.160875	-1.155028
IR	0.634644	1.312349	0.841889
O	-1.925229	2.987407	1.021364
O	-2.066179	1.801668	-3.134315
C	2.885491	-4.927308	2.971955
H	0.951314	-5.888433	2.793190
H	4.737541	-3.807264	2.897378
C	5.892828	-2.583591	-3.230207
H	5.521805	-0.445345	-3.308072
H	6.006297	-4.732981	-2.972758
H	-3.952372	-0.004262	2.331983
H	-3.907086	1.671970	1.719601
C	-5.222392	-2.153933	0.745755
C	-4.253189	-2.246271	-1.469332
C	-5.893467	0.653272	-1.930097

C	-4.593667	2.539338	-1.144019
P	1.503162	3.010334	-0.434544
C	1.296363	2.004458	2.421960
H	3.122458	-5.405828	3.931079
H	6.850000	-2.521347	-3.764476
C	-5.718101	-3.446591	0.580670
H	-5.410321	-1.618513	1.686305
C	-4.759947	-3.532549	-1.634741
H	-3.640413	-1.793271	-2.260917
C	-6.678025	1.518934	-2.693212
H	-6.095089	-0.427856	-1.937724
C	-5.387505	3.398839	-1.898086
H	-3.766218	2.941851	-0.535115
C	0.476910	3.519560	-1.843643
C	3.120165	2.645752	-1.160944
C	1.751036	4.583457	0.442389
O	1.711819	2.407802	3.438473
C	-5.489848	-4.136683	-0.608991
H	-6.287588	-3.918627	1.392065
H	-4.566159	-4.073786	-2.569945
C	-6.429152	2.890583	-2.677399
H	-7.493910	1.113984	-3.306274
H	-5.186123	4.478100	-1.882017
H	0.315125	2.675597	-2.535950
H	-0.509204	3.828532	-1.453296
C	4.196855	2.403548	-0.297270
C	3.308700	2.547439	-2.544298
C	2.833223	5.421936	0.152342
C	0.789570	4.981419	1.379265
H	-5.877609	-5.156359	-0.736282
H	-7.048957	3.569287	-3.278175
C	5.451250	2.095434	-0.814128
H	4.044621	2.442538	0.791098
C	4.566546	2.229981	-3.059415
H	2.471855	2.728367	-3.232915
C	2.956580	6.649451	0.802233
H	3.591787	5.106693	-0.578782
C	0.914497	6.213507	2.018412
H	-0.064845	4.323642	1.604560
C	5.639967	2.011666	-2.195685
H	6.287215	1.903098	-0.129187
H	4.707405	2.162722	-4.146501
C	1.997773	7.046639	1.734673
H	3.812830	7.299689	0.579975
H	0.159479	6.520321	2.753819
H	6.632909	1.773289	-2.600190

H	2.098355	8.011756	2.248417
C	-1.573181	-2.544734	1.214587
IR	-0.520498	-1.010618	1.606757
O	-2.208103	-3.497315	0.997571
C	0.901007	-1.596731	2.744948
C	-1.433253	-0.078548	2.926226
O	1.724185	-1.941597	3.486936
O	-1.992506	0.515886	3.760614
H	0.936875	4.372166	-2.374714
H	-5.431362	0.722866	1.585671
H	1.487264	-5.072108	-1.946480

$Ir_4(CO)_8[PCH_3(C_6H_5)_2]_3$ bri CO(1) removed

IR	0.697103	-0.961417	-0.911718
P	1.698483	-3.009978	-1.084291
C	-1.270823	-1.185283	-1.349450
C	1.555934	-3.647576	-2.784760
C	0.941913	-4.345067	-0.115738
C	3.472968	-3.102952	-0.728483
C	1.277154	-0.432266	-2.566816
IR	-1.449603	0.612746	-0.479276
O	-1.757055	-2.114450	-1.931134
H	2.135716	-2.996017	-3.461627
H	0.492905	-3.604538	-3.082456
C	-0.336173	-4.779183	-0.492204
C	1.572399	-4.913887	0.996813
C	4.158748	-1.946648	-0.347649
C	4.162761	-4.316113	-0.848297
O	1.590390	-0.036961	-3.630182
P	-3.665457	0.564526	0.186034
C	-0.987309	2.174480	0.780756
C	-1.781329	1.612833	-2.002973
C	-0.966801	-5.790499	0.227677
H	-0.865308	-4.291336	-1.325734
C	0.932785	-5.923888	1.713699
H	2.562837	-4.555821	1.311626
C	5.526146	-2.004410	-0.082211
H	3.608659	-0.994689	-0.253033
C	5.529219	-4.369939	-0.586384
H	3.622080	-5.230800	-1.134335
C	-3.941514	0.939093	1.940004
C	-4.525596	-0.994929	-0.116266
C	-4.701691	1.827737	-0.615658
IR	0.795293	1.338995	0.802753
O	-1.464462	3.128321	1.339197
O	-1.995505	2.237304	-2.969539

C	-0.332203	-6.368726	1.327638
H	-1.975200	-6.112394	-0.062244
H	1.429195	-6.363604	2.588784
C	6.210769	-3.213261	-0.199664
H	6.052442	-1.090687	0.224428
H	6.066634	-5.323020	-0.677302
H	-3.504874	0.152759	2.578751
H	-3.423181	1.888639	2.167757
C	-5.128950	-1.718726	0.916749
C	-4.551919	-1.499565	-1.422672
C	-5.943690	1.535093	-1.185807
C	-4.229428	3.146891	-0.610089
P	1.881561	2.827818	-0.536490
C	1.747495	1.862575	2.282571
H	-0.833952	-7.161300	1.898092
H	7.286494	-3.258998	0.016241
C	-5.760735	-2.931670	0.645007
H	-5.103579	-1.340372	1.947629
C	-5.195248	-2.703602	-1.692813
H	-4.053031	-0.949326	-2.233253
C	-6.706373	2.556467	-1.753631
H	-6.315425	0.500115	-1.190169
C	-5.000889	4.163299	-1.167405
H	-3.251746	3.377784	-0.155486
C	1.127292	3.197438	-2.146024
C	3.535288	2.194382	-0.932411
C	2.207067	4.476714	0.154225
O	2.320966	2.222244	3.240992
C	-5.798569	-3.423108	-0.659207
H	-6.222726	-3.499240	1.463108
H	-5.208911	-3.091861	-2.719474
C	-6.238248	3.869933	-1.744454
H	-7.677740	2.320769	-2.208044
H	-4.627666	5.195744	-1.156557
H	0.945067	2.271265	-2.719062
H	0.151054	3.679506	-1.962612
C	4.471300	2.090980	0.108034
C	3.881049	1.765184	-2.217470
C	3.280659	5.247393	-0.307674
C	1.340337	4.991407	1.123722
H	-6.296033	-4.378585	-0.871766
H	-6.840393	4.671276	-2.192463
C	5.745943	1.593995	-0.146263
H	4.201039	2.415157	1.124637
C	5.154647	1.250083	-2.463664
H	3.154138	1.819884	-3.039884

C	3.484985	6.528930	0.198928
H	3.973111	4.831922	-1.055401
C	1.546814	6.277348	1.622271
H	0.499134	4.381081	1.488769
C	6.090027	1.170441	-1.433555
H	6.478304	1.535692	0.670399
H	5.414154	0.906315	-3.473336
C	2.616708	7.045493	1.163173
H	4.332998	7.128436	-0.157405
H	0.866903	6.677231	2.385766
H	7.093041	0.770157	-1.632553
H	2.781844	8.053966	1.564820
C	-1.576471	-2.397015	1.478275
IR	-0.371119	-0.941502	1.575365
O	-2.342208	-3.276698	1.441020
C	1.322624	-1.657774	1.946549
C	-0.974900	-0.009425	3.101560
O	2.360305	-2.122108	2.227330
O	-1.302270	0.569952	4.061817
H	-5.021239	1.052133	2.146422
H	1.766130	3.888112	-2.726831
H	1.923093	-4.687035	-2.857334

$Ir_4(CO)_7[PCH_3(C_6H_5)_2]_3$ bri CO(1) and ax CO(1) removed

IR	-0.787149	0.810713	-0.829612
P	-0.888287	3.044724	-1.107789
C	1.046994	0.662987	-1.455116
C	-0.604613	3.553899	-2.839825
C	0.404743	4.029651	-0.277922
C	-2.414829	3.893775	-0.607288
IR	1.209733	-1.031162	-0.345630
O	1.645389	1.280983	-2.309326
H	-1.466816	3.283406	-3.472482
H	0.283061	2.996869	-3.195565
C	1.698669	4.061375	-0.815921
C	0.123439	4.747359	0.890576
C	-3.325473	3.215031	0.205996
C	-2.689870	5.206895	-1.006974
P	3.448035	-0.973838	0.193181
C	0.496053	-2.619716	0.826529
C	1.514148	-2.119564	-1.810217
C	2.694020	4.812085	-0.193916
H	1.945431	3.461514	-1.704183
C	1.123222	5.499973	1.504837
H	-0.888342	4.721572	1.322239
C	-4.495614	3.843150	0.628504

H	-3.108980	2.176314	0.503922
C	-3.867233	5.830225	-0.598780
H	-1.969613	5.754124	-1.632686
C	3.806042	-1.003346	1.974928
C	4.373054	0.443305	-0.449959
C	4.404921	-2.416632	-0.372407
IR	-1.117392	-1.476231	0.864553
O	0.797292	-3.693462	1.256674
O	1.734870	-2.796454	-2.740737
C	2.408387	5.538488	0.962250
H	3.710762	4.803470	-0.611060
H	0.893921	6.058753	2.421805
C	-4.769414	5.149385	0.223221
H	-5.198202	3.302764	1.276402
H	-4.080030	6.859437	-0.916593
H	3.411154	-0.098133	2.466389
H	3.292723	-1.879528	2.409738
C	5.046956	1.338832	0.386443
C	4.365395	0.662696	-1.833875
C	5.700274	-2.288384	-0.883750
C	3.840677	-3.688310	-0.211075
P	-2.355054	-2.249652	-0.837433
C	-2.228575	-1.965534	2.258020
H	3.195073	6.126170	1.453165
H	-5.692668	5.645207	0.551189
C	5.713090	2.438003	-0.155074
H	5.049628	1.189029	1.474344
C	5.042279	1.752962	-2.373073
H	3.815287	-0.022239	-2.494491
C	6.425551	-3.426083	-1.237222
H	6.141737	-1.289181	-1.011414
C	4.574701	-4.821031	-0.556254
H	2.821091	-3.795368	0.194776
C	-1.570881	-2.766423	-2.394462
C	-3.270492	-0.742156	-1.250107
C	-3.617634	-3.532198	-0.600542
O	-2.934295	-2.276355	3.143610
C	5.714179	2.645502	-1.534589
H	6.234353	3.138226	0.510876
H	5.030365	1.914688	-3.458813
C	5.865291	-4.692907	-1.072833
H	7.439120	-3.319998	-1.645976
H	4.128461	-5.815446	-0.424515
H	-0.923236	-1.962271	-2.781204
H	-0.934645	-3.646978	-2.197756
C	-4.587014	-0.581622	-0.786580

C	-2.648304	0.331945	-1.959146
C	-4.641686	-3.709406	-1.540429
C	-3.525189	-4.390092	0.497463
H	6.243156	3.508727	-1.960655
H	6.437657	-5.587399	-1.351968
C	-5.338987	0.529379	-1.146706
H	-5.037452	-1.371417	-0.168143
C	-3.476454	1.390208	-2.411722
H	-1.692735	0.128223	-2.552430
C	-5.570607	-4.732885	-1.373979
H	-4.723756	-3.027557	-2.400430
C	-4.453657	-5.419022	0.658139
H	-2.714667	-4.245558	1.226950
C	-4.791229	1.501474	-1.998082
H	-6.373382	0.624457	-0.791738
H	-3.049990	2.153544	-3.075103
C	-5.476009	-5.589717	-0.274203
H	-6.377170	-4.863792	-2.107254
H	-4.376970	-6.089035	1.524140
H	-5.392434	2.363030	-2.316280
H	-6.209062	-6.396644	-0.143946
C	1.747032	1.875549	1.656060
IR	0.281450	0.690043	1.608079
O	2.698333	2.522889	1.859318
C	-1.088668	1.728189	2.398600
C	0.706291	-0.549894	2.946378
O	-1.895884	2.392453	2.916867
O	1.011503	-1.289829	3.798199
H	4.893684	-1.097458	2.149093
H	-2.341000	-3.034320	-3.140170
H	-0.412807	4.639182	-2.920899

$Ir_4(CO)_7[PCH_3(C_6H_5)_2]_3$ bri CO(1) and ax CO(2) removed

IR	-0.636692	1.038612	-0.679173
P	-0.945584	3.232322	-1.239162
C	1.834095	0.869979	-1.399509
C	-0.362806	3.587797	-2.924684
C	0.001008	4.361808	-0.187193
C	-2.633710	3.892856	-1.231039
C	-1.525519	0.485906	-2.199157
IR	1.357922	-0.700129	-0.507049
O	2.273472	1.793163	-1.986913
H	-1.013434	3.042741	-3.631088
H	0.671322	3.219634	-3.048174
C	1.354232	4.595763	-0.463184
C	-0.588541	4.930771	0.949326

C	-3.714902	3.013159	-1.153996
C	-2.858595	5.267651	-1.377389
O	-2.192929	0.092029	-3.084789
P	3.521776	-1.298835	-0.175248
C	0.765862	-2.496718	0.269014
C	2.100640	5.422642	0.373439
H	1.840111	4.109598	-1.321853
C	0.165006	5.756283	1.780487
H	-1.642024	4.720553	1.185167
C	-5.016755	3.503685	-1.237681
H	-3.527054	1.936283	-1.019881
C	-4.161261	5.754260	-1.453713
H	-2.007385	5.964050	-1.417749
C	3.800568	-2.189104	1.386753
C	4.601323	0.155141	-0.020129
C	4.314524	-2.343131	-1.431910
IR	-0.800607	-1.470909	0.832231
O	1.129998	-3.637385	0.399688
C	1.506963	6.008186	1.491888
H	3.162197	5.597542	0.154013
H	-0.299884	6.197034	2.671866
C	-5.242301	4.871463	-1.387855
H	-5.861383	2.802040	-1.184184
H	-4.336122	6.832506	-1.564076
H	3.383323	-1.586727	2.213175
H	3.264410	-3.153757	1.347356
C	4.235839	1.107903	0.939623
C	5.705217	0.392479	-0.843081
C	5.571406	-2.929063	-1.237569
C	3.627053	-2.564832	-2.628240
P	-2.213906	-2.655024	-0.541996
C	-1.507668	-2.237800	2.358679
H	2.099794	6.650559	2.155774
H	-6.268379	5.257670	-1.449095
C	4.967678	2.282031	1.083297
H	3.338054	0.941495	1.558622
C	6.440515	1.570379	-0.695881
H	5.985308	-0.339859	-1.614233
C	6.132147	-3.725235	-2.234257
H	6.121810	-2.763889	-0.299487
C	4.189257	-3.359287	-3.626324
H	2.632810	-2.103988	-2.752963
C	-1.551074	-3.121304	-2.169648
C	-3.708370	-1.684921	-0.881000
C	-2.813944	-4.237312	0.116393
O	-1.894972	-2.792057	3.313408

C	6.076070	2.513826	0.264696
H	4.652329	3.023214	1.831066
H	7.303978	1.755525	-1.348464
C	5.442357	-3.939819	-3.429747
H	7.116992	-4.184540	-2.077167
H	3.642740	-3.530065	-4.563089
H	-1.318140	-2.207590	-2.744388
H	-0.619515	-3.691101	-2.001289
C	-4.047659	-0.657521	0.006995
C	-4.514069	-1.928197	-1.998793
C	-4.174731	-4.538896	0.222969
C	-1.854582	-5.166709	0.542852
H	6.655017	3.440885	0.370651
H	5.885903	-4.569263	-4.212403
C	-5.191262	0.109374	-0.212189
H	-3.397543	-0.450285	0.874026
C	-5.655462	-1.159436	-2.217999
H	-4.248093	-2.719447	-2.714056
C	-4.575283	-5.771176	0.740714
H	-4.927215	-3.800226	-0.089545
C	-2.262759	-6.397641	1.050062
H	-0.781931	-4.914411	0.500755
C	-5.997089	-0.143257	-1.322916
H	-5.444271	0.913519	0.492684
H	-6.282244	-1.351937	-3.098443
C	-3.621935	-6.703052	1.148992
H	-5.645070	-6.001196	0.831149
H	-1.508892	-7.121496	1.386258
H	-6.900174	0.457924	-1.497308
H	-3.939766	-7.670496	1.559451
C	1.361114	2.237185	2.250192
IR	0.411038	0.691599	1.766544
O	1.983539	3.151634	2.632796
C	-1.302678	1.527753	1.163996
C	0.393418	-0.105427	3.449266
O	-2.265908	2.031172	1.660223
O	0.317982	-0.564380	4.522259
H	4.877558	-2.353147	1.567517
H	-2.258143	-3.757325	-2.731825
H	-0.408644	4.670651	-3.139882

$Ir_4(CO)_7[PCH_3(C_6H_5)_2]_3$ bri CO(1) and eq CO removed

IR	0.948211	-0.804480	-0.907637
P	1.655648	-2.915782	-0.669488
C	-0.957673	-1.235957	-1.501281
C	1.046351	-4.090702	-1.903341

C	1.082902	-3.539970	0.932264
C	3.455084	-3.162002	-0.643158
C	1.770466	-0.518498	-2.551259
IR	-1.411159	0.543174	-0.432469
O	-1.547204	-2.073321	-2.117581
H	1.459567	-3.781195	-2.879502
H	-0.056268	-4.014205	-1.957853
C	0.396354	-4.751541	1.063056
C	1.260441	-2.700810	2.069755
C	4.321388	-2.178564	-1.125729
C	3.969940	-4.364088	-0.143595
O	2.250727	-0.435348	-3.619478
P	-3.620943	0.288942	0.042256
C	-1.009586	1.938854	1.159604
C	-1.833530	1.647693	-1.838498
C	-0.104138	-5.143664	2.304417
H	0.216790	-5.383359	0.182811
C	0.759375	-3.130536	3.315795
H	2.008013	-1.893623	2.046160
C	5.695444	-2.409808	-1.135544
H	3.918015	-1.217253	-1.476722
C	5.344169	-4.590526	-0.152381
H	3.288179	-5.121012	0.274596
C	-3.963083	0.204494	1.821172
C	-4.461549	-1.126877	-0.698301
C	-4.629075	1.714585	-0.479334
IR	0.800711	1.187061	0.794076
O	-1.631111	2.657538	1.892043
O	-2.107226	2.328927	-2.753414
C	0.070509	-4.335133	3.430512
H	-0.644883	-6.095078	2.391891
H	0.933203	-2.500399	4.198038
C	6.208128	-3.614107	-0.654008
H	6.369613	-1.628975	-1.513676
H	5.746181	-5.532590	0.242911
H	-3.566961	-0.736347	2.240676
H	-3.435265	1.045962	2.307551
C	-5.291643	-1.967898	0.048888
C	-4.290380	-1.356624	-2.068211
C	-5.685997	1.589277	-1.385089
C	-4.315482	2.972016	0.056233
P	1.727218	2.937825	-0.298349
H	-0.333193	-4.647274	4.401756
H	7.291757	-3.791562	-0.655730
C	-5.961410	-3.018977	-0.574157
H	-5.413589	-1.809515	1.128980

C	-4.969730	-2.400871	-2.690138
H	-3.613209	-0.713676	-2.648195
C	-6.421288	2.714635	-1.759315
H	-5.936916	0.603678	-1.802522
C	-5.059402	4.088983	-0.315764
H	-3.482286	3.079901	0.769476
C	0.667663	3.780553	-1.511670
C	3.226518	2.513704	-1.228106
C	2.243731	4.286245	0.809177
C	-5.806116	-3.232638	-1.944405
H	-6.607396	-3.680057	0.018044
H	-4.829016	-2.575456	-3.764651
C	-6.110502	3.964710	-1.226839
H	-7.246470	2.609996	-2.476003
H	-4.811067	5.070513	0.109209
H	0.326014	3.070878	-2.285159
H	-0.227138	4.157501	-0.985944
C	4.342027	2.047108	-0.517520
C	3.254299	2.513119	-2.625814
C	3.391609	5.048601	0.566275
C	1.433929	4.576307	1.915497
H	-6.334380	-4.061824	-2.433360
H	-6.690282	4.848837	-1.523041
C	5.466016	1.589810	-1.199216
H	4.322853	2.018082	0.581480
C	4.378484	2.045374	-3.307260
H	2.383035	2.856680	-3.200237
C	3.723973	6.098115	1.420862
H	4.031645	4.812742	-0.296678
C	1.769112	5.630188	2.764304
H	0.532346	3.972045	2.108723
C	5.485021	1.583009	-2.596682
H	6.329741	1.220869	-0.629928
H	4.378662	2.027201	-4.404561
C	2.913623	6.390537	2.519443
H	4.626328	6.693411	1.228299
H	1.131692	5.853655	3.629717
H	6.366599	1.209541	-3.134604
H	3.179622	7.215892	3.192916
C	-1.761523	-2.508505	1.170026
IR	-0.473450	-1.177403	1.416838
O	-2.669718	-3.247878	1.102857
C	2.320430	-0.080248	0.573432
C	-0.863747	-0.310966	3.015493
O	3.372900	-0.391298	1.054232
O	-1.183156	0.251476	3.995418

H	-5.047567	0.296218	2.011936
H	1.199494	4.627867	-1.981453
H	1.367135	-5.127136	-1.693987

$Ir_4(CO)_8[PCH_3(C_6H_5)_2]_3$ bri CO(2) removed

IR	0.762535	-0.850978	-0.544022
P	1.684019	-2.933551	-0.613418
C	0.623510	-4.261773	-1.265468
C	2.260086	-3.569733	0.986071
C	3.197744	-3.023100	-1.628377
C	1.216755	-0.468155	-2.280004
C	2.069322	0.281480	0.493536
IR	-1.705694	0.403545	-0.291828
H	0.480421	-4.091456	-2.347336
H	-0.364982	-4.217715	-0.772269
C	1.496999	-4.484712	1.720625
C	3.475419	-3.102207	1.499556
C	3.971248	-1.873248	-1.822660
C	3.626230	-4.240061	-2.170881
O	1.418263	-0.162550	-3.397066
O	3.229458	0.069177	0.706110
P	-3.769505	-0.548970	-0.109507
C	-1.395476	2.171305	0.628048
C	-2.124732	1.127678	-1.930759
C	1.955258	-4.934970	2.957717
H	0.530940	-4.841795	1.335742
C	3.928014	-3.559299	2.734495
H	4.061948	-2.362373	0.935515
C	5.156918	-1.942073	-2.551913
H	3.652035	-0.915759	-1.384176
C	4.806515	-4.303439	-2.909331
H	3.037450	-5.155034	-2.014999
C	-4.449722	-0.877348	1.546096
C	-3.795237	-2.169828	-0.931137
C	-5.107085	0.420239	-0.874074
IR	0.522551	1.550339	0.755449
O	-2.194035	3.037884	0.850321
O	-2.358612	1.557805	-2.996871
C	3.171667	-4.476536	3.464638
H	1.350916	-5.648669	3.532920
H	4.877159	-3.182883	3.137063
C	5.575442	-3.154025	-3.100448
H	5.752616	-1.028059	-2.687430
H	5.130759	-5.260933	-3.337791
H	-3.816549	-1.612008	2.073402
H	-4.455385	0.062983	2.124743

C	-4.742744	-3.154677	-0.632696
C	-2.787851	-2.444299	-1.864079
C	-6.126838	-0.170285	-1.625779
C	-5.107971	1.803666	-0.654881
P	1.353515	3.058236	-0.776107
C	1.111642	2.487455	2.243970
H	3.527610	-4.828975	4.441435
H	6.506033	-3.206860	-3.680910
C	-4.691050	-4.393114	-1.271165
H	-5.522332	-2.963660	0.118837
C	-2.739819	-3.679650	-2.505233
H	-2.021730	-1.673473	-2.064900
C	-7.149909	0.619855	-2.150295
H	-6.110291	-1.252774	-1.821531
C	-6.139347	2.584819	-1.171515
H	-4.282503	2.272439	-0.092696
C	0.418898	3.196597	-2.326465
C	3.046023	2.666903	-1.284553
C	1.440283	4.779460	-0.200516
O	1.466575	3.047926	3.205083
C	-3.693158	-4.655209	-2.211177
H	-5.434525	-5.163514	-1.028284
H	-1.947814	-3.883963	-3.238476
C	-7.160629	1.995484	-1.919143
H	-7.942686	0.156118	-2.751967
H	-6.137133	3.668795	-0.997472
H	0.353061	2.219246	-2.836056
H	-0.607403	3.523555	-2.083913
C	4.056686	2.714493	-0.314357
C	3.344156	2.201819	-2.569247
C	2.433623	5.643883	-0.674840
C	0.460323	5.256306	0.677117
H	-3.653370	-5.631936	-2.711048
H	-7.965750	2.615427	-2.335007
C	5.353693	2.327212	-0.635168
H	3.819243	3.042993	0.708457
C	4.642566	1.797955	-2.883213
H	2.559869	2.131144	-3.334912
C	2.449068	6.976749	-0.268032
H	3.209743	5.264672	-1.355866
C	0.476363	6.592396	1.073912
H	-0.323202	4.578988	1.050647
C	5.648805	1.863667	-1.919471
H	6.136492	2.364271	0.133208
H	4.863459	1.427318	-3.893060
C	1.470371	7.452542	0.605847

H	3.236381	7.649058	-0.633502
H	-0.293645	6.960957	1.764010
H	6.671944	1.550665	-2.168539
H	1.486382	8.501754	0.928984
C	-1.190442	-2.447969	1.321292
IR	-0.521313	-0.787540	1.829786
O	-1.616653	-3.506208	1.033284
C	0.951640	-1.191351	2.964491
C	-1.713969	0.139303	2.969276
O	1.842695	-1.440715	3.670437
O	-2.491733	0.700859	3.636498
H	-5.488376	-1.247038	1.467653
H	0.885209	3.944685	-2.993817
H	1.062136	-5.263785	-1.105040

$Ir_4(CO)_7[PCH_3(C_6H_5)_2]_3$ bri CO(2) and ax CO removed

IR	-0.992140	-0.602306	0.548691
P	-2.354344	-2.412123	0.799439
C	-1.604214	-3.883320	1.572222
C	-3.080529	-3.040598	-0.740780
C	-3.838713	-2.088333	1.814689
C	-1.259541	-0.049491	2.274142
C	-2.019799	0.815719	-0.522130
IR	1.716944	-0.090400	0.263429
H	-1.340099	-3.623336	2.612677
H	-0.678639	-4.144907	1.026989
C	-2.661932	-4.243486	-1.319585
C	-4.057500	-2.263153	-1.376427
C	-4.285663	-0.774609	1.992139
C	-4.565467	-3.143338	2.379097
O	-1.305017	0.311492	3.393292
O	-3.206150	0.892468	-0.656073
P	3.683653	-1.118429	0.270496
C	1.876447	1.566014	-0.659690
C	-3.221539	-4.667507	-2.524828
H	-1.882345	-4.852008	-0.840440
C	-4.615587	-2.695440	-2.576048
H	-4.364475	-1.300155	-0.939459
C	-5.438707	-0.519931	2.733078
H	-3.734359	0.058663	1.531445
C	-5.712807	-2.885959	3.126371
H	-4.240344	-4.183189	2.231882
C	4.579614	-1.149831	-1.315411
C	3.629684	-2.849367	0.820683
C	4.873497	-0.310571	1.389120
IR	-0.178419	1.535421	-0.875921

O	2.844084	2.259787	-0.912694
C	-4.200186	-3.897122	-3.152653
H	-2.884989	-5.609287	-2.978007
H	-5.372753	-2.077189	-3.075131
C	-6.151383	-1.572388	3.306216
H	-5.773462	0.519532	2.858816
H	-6.272509	-3.719356	3.571086
H	4.027555	-1.776984	-2.036713
H	4.613983	-0.117587	-1.708495
C	4.677166	-3.754608	0.618630
C	2.466633	-3.276309	1.472087
C	5.468097	-0.964567	2.473547
C	5.154240	1.043625	1.149056
P	-0.407759	3.250702	0.638706
C	-0.344982	2.580678	-2.404634
H	-4.636420	-4.230817	-4.103193
H	-7.056117	-1.372223	3.895434
C	4.561524	-5.069278	1.067897
H	5.594641	-3.430753	0.105793
C	2.351555	-4.588704	1.924684
H	1.637207	-2.557000	1.607938
C	6.355607	-0.275451	3.300262
H	5.234495	-2.020984	2.672343
C	6.045878	1.722814	1.976411
H	4.651362	1.570180	0.319266
C	0.687185	3.088360	2.078991
C	-2.080966	3.391405	1.312428
C	-0.014975	4.909822	0.013297
O	-0.442777	3.211008	-3.384211
C	3.400300	-5.486511	1.722264
H	5.384539	-5.777381	0.904494
H	1.431897	-4.915625	2.429407
C	6.649419	1.065612	3.051094
H	6.822148	-0.792690	4.149173
H	6.266674	2.780871	1.782602
H	0.468767	2.152158	2.623498
H	1.724015	3.035778	1.699050
C	-3.128058	3.657496	0.418933
C	-2.369833	3.130990	2.655658
C	-0.736054	6.035213	0.427158
C	1.068316	5.053037	-0.862611
H	3.311233	-6.523865	2.070730
H	7.348980	1.604983	3.703238
C	-4.444010	3.681219	0.869772
H	-2.908216	3.825166	-0.645724
C	-3.692117	3.138090	3.101344

H	-1.564543	2.898583	3.365507
C	-0.376671	7.300110	-0.036446
H	-1.592872	5.917988	1.106849
C	1.426634	6.321892	-1.313932
H	1.639862	4.167455	-1.186951
C	-4.729707	3.415576	2.211281
H	-5.256537	3.884167	0.160387
H	-3.908716	2.919227	4.155180
C	0.704768	7.444848	-0.906116
H	-0.950603	8.180410	0.281744
H	2.275664	6.430808	-2.001313
H	-5.769998	3.425278	2.564052
H	0.983799	8.441200	-1.273660
C	0.479457	-2.827310	-1.277122
IR	0.347293	-1.016373	-1.761439
O	0.532889	-3.960808	-0.988233
C	-1.164829	-1.075690	-2.861435
C	1.654011	-0.465760	-3.040885
O	-2.112894	-1.089764	-3.535742
O	2.480227	-0.143263	-3.795053
H	5.611879	-1.525897	-1.197008
H	0.591941	3.957858	2.754929
H	-2.277631	-4.760318	1.574301

$Ir_4(CO)_7[PCH_3(C_6H_5)_2]_3$ bri CO(2) and eq CO removed

IR	0.176915	-1.602285	0.329967
P	-1.560938	-3.035945	0.087029
C	-1.267639	-4.433483	-1.024044
C	-2.855632	-2.040640	-0.687101
C	-2.317507	-3.737632	1.579784
C	1.115209	-2.597285	1.589698
C	-0.949712	-0.283340	1.598255
IR	1.333793	0.776776	-0.155650
H	-0.508888	-5.089294	-0.563742
H	-0.860474	-4.050731	-1.978059
C	-3.205405	-2.179364	-2.016809
C	-3.205055	-0.852370	0.031520
C	-1.808009	-3.456386	2.849359
C	-3.457149	-4.542281	1.446488
O	1.697161	-3.224623	2.387553
O	-1.106825	-0.228331	2.776251
P	3.559033	0.358458	-0.366910
C	-1.128810	1.139546	-2.106402
C	1.605852	1.462293	1.521825
C	-3.857046	-1.124775	-2.690271
H	-2.924806	-3.080697	-2.579110

C	-3.799291	0.217537	-0.665639
H	-3.259855	-0.888948	1.129161
C	-2.422843	-3.996532	3.979203
H	-0.936897	-2.794807	2.955408
C	-4.065934	-5.081180	2.576191
H	-3.885183	-4.734535	0.451123
C	4.234020	-0.284341	-1.930103
C	4.128681	-0.861733	0.855100
C	4.648026	1.787890	-0.067134
IR	-1.320928	0.529811	-0.207747
O	-1.425895	1.971816	-2.909448
O	1.770014	1.862208	2.614576
C	-4.106306	0.069427	-2.041688
H	-4.121444	-1.244813	-3.748724
H	-4.213889	1.072365	-0.116412
C	-3.545378	-4.811713	3.844643
H	-2.018770	-3.770558	4.974417
H	-4.958030	-5.711851	2.468513
H	3.668702	-1.172163	-2.265752
H	4.146413	0.497859	-2.702821
C	4.373280	-2.189896	0.489205
C	4.260403	-0.478260	2.196749
C	6.009050	1.614786	0.208682
C	4.124131	3.077848	-0.177604
P	-1.759596	2.663421	0.488221
H	-4.570209	0.910989	-2.573831
H	-4.027353	-5.235594	4.735436
C	4.759860	-3.120005	1.453810
H	4.236851	-2.516343	-0.551218
C	4.649876	-1.410170	3.154449
H	4.057739	0.560835	2.495976
C	6.835585	2.724821	0.367107
H	6.419076	0.599325	0.319369
C	4.952150	4.189287	-0.025723
H	3.046687	3.198419	-0.379035
C	-0.613617	3.830244	-0.309046
C	-1.578612	2.973665	2.261584
C	-3.374837	3.423896	0.085186
C	4.900532	-2.733587	2.785372
H	4.938496	-4.162354	1.159287
H	4.749310	-1.100632	4.203062
C	6.308831	4.013059	0.246509
H	7.901457	2.585000	0.590617
H	4.534154	5.200543	-0.115708
H	0.424477	3.494413	-0.107315
H	-0.779955	3.772339	-1.399747

C	-2.389578	2.259134	3.152753
C	-0.640015	3.878329	2.766305
C	-4.247556	3.928448	1.054716
C	-3.746477	3.472664	-1.267839
H	5.195258	-3.470130	3.544064
H	6.962243	4.886399	0.372272
C	-2.288786	2.475015	4.524103
H	-3.101671	1.514765	2.766996
C	-0.525927	4.079797	4.140957
H	0.023445	4.427711	2.084707
C	-5.478185	4.470171	0.678850
H	-3.959203	3.906320	2.115539
C	-4.971213	4.023662	-1.637446
H	-3.068790	3.069355	-2.038791
C	-1.354950	3.385839	5.021054
H	-2.929605	1.908442	5.212082
H	0.225333	4.781059	4.526581
C	-5.843870	4.519256	-0.665508
H	-6.155484	4.863077	1.448744
H	-5.247552	4.065968	-2.699721
H	-1.263576	3.544699	6.103547
H	-6.810998	4.948192	-0.958896
C	1.249778	-2.109101	-1.350597
IR	0.215901	-0.535488	-2.214237
O	2.097235	-2.888484	-1.663687
C	-0.697575	-1.577604	-3.508074
C	1.430501	0.331571	-3.316045
O	-1.097108	-2.212354	-4.407202
O	2.172511	0.899785	-4.021345
H	5.299643	-0.547303	-1.796186
H	-0.767444	4.870957	0.028749
H	-2.187980	-5.015216	-1.213264

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