Supporting Information

Iridium-Gold Cluster Compounds: Syntheses, Structures and an Unusual Ligand-Induced Skeletal Rearrangement

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Table 1. Crystallographic Data for Compounds 1 - 5.

Compound	**1**	**2**	**3**
Empirical formula	$Ir_4AuC_{35}H_{20}O_{11}P$	$Ir_4Au_2C_{46}H_{30}O_{10}P_2$	$Ir_4Au_2C_{47}H_{30}O_{11}P_2$
Formula weight	1613.33	1967.47	1995.48
Crystal system	Monoclinic	Triclinic	Hexagonal
Lattice parameters			
a (Å)	13.5055(6)	10.2250(4)	13.3377(3)
b (Å)	16.7314(8)	15.1704(6)	13.3377(3)
c (Å)	17.2324(8)	19.2345(7)	48.755(2)
α (deg)	90	94.858(1)	90
β (deg)	97.638(1)	102.439(1)	90
γ (deg)	90	98.277(1)	120
V ($Å^3$)	3859.4(3)	2862.48(19)	7511.2(4)
Space group	$P2_1/c$	P-*1*	$P6_5$
Z value	4	2	6
ρ_{calc} (g / cm^3)	2.776	2.464	2.647

μ (Mo Kα) (mm^{-1})	17.628	14.480	16.546
Temperature (K)	294(2)	294(2)	294(2)
$2\Theta_{max}$ (°)	51.36	56.14	56.02
No. Obs. (I > 2σ(I))	7330	10096	8761
No. Parameters	427	625	547
Goodness of fit (GOF)	1.002	1.081	1.058
Max. shift in cycle	0.001	0.001	0.001
Residuals*: R1; wR2	0.0297; 0.0727	0.0613; 0.1634	0.0519; 0.1146
Absorption Correction,	Multi-scan	Multi-scan	Multi-scan
Max/min	1.000 / 0.435	1.000 /0.686	1.000 / 0.522
Largest peak in Final Diff. Map (e^- / Å^3)	2.11	1.08	1.29

[a] $R = \Sigma_{hkl}(||F_{obs}|-|F_{calc}||)/\Sigma_{hkl}|F_{obs}|$; $R_w = [\Sigma_{hkl}w(|F_{obs}|-|F_{calc}|)^2/\Sigma_{hkl}wF^2_{obs}]^{1/2}$; $w = 1/\sigma^2(F_{obs})$; GOF = $[\Sigma_{hkl}w(|F_{obs}|-|F_{calc}|)^2/(n_{data} - n_{vari})]^{1/2}$.

Table 1. Crystallographic Data for Compounds 1 – 5 (continued).

Compound	**4**	**5**
Empirical formula	$Ir_4Au_2C_{65}H_{45}O_{11}P_3$	$Ir_4Au_2C_{57}H_{39}O_9P_3$
Formula weight	2257.76	2123.63
Crystal system	Monoclinic	Triclinic
Lattice parameters		
a (Å)	15.8580(8)	13.7892(14)
b (Å)	23.8550(13)	13.9054(14)
c (Å)	17.3821(9)	17.8443(18)
α (deg)	90	85.321(2)
β (deg)	95.644(1)	75.087(2)
γ (deg)	90	65.024(2)

V (Å^3)	6543.6(6)	2995.7(5)
Space group	P$2_1/c$	P-*1*
Z value	4	2
ρ_{calc} (g / cm^3)	2.348	2.397
μ (Mo Kα) (mm^{-1})	12.781	13.863
Temperature (K)	294(2)	294(2)
$2\Theta_{max}$ (°)	56.86	56.48
No. Obs. (I > 2σ(I))	16466	9873
No. Parameters	735	688
Goodness of fit (GOF)	1.061	1.087
Max. shift in cycle	0.001	0.001
Residuals*: R1; wR2	0.0432; 0.1065	0.0580; 0.1280
Absorption Correction,	Multi-scan	Multi-scan
Max/min	1.000 / 0.382	1.000 / 0.388
Largest peak in Final Diff. Map (e$^-$ / Å^3)	2.71	2.36

[a] $R = \Sigma_{hkl}(||F_{obs}| - |F_{calc}||)/\Sigma_{hkl}|F_{obs}|$; $R_w = [\Sigma_{hkl}w(|F_{obs}| - |F_{calc}|)^2/\Sigma_{hkl}wF^2_{obs}]^{1/2}$; $w = 1/\sigma^2(F_{obs})$; GOF = $[\Sigma_{hkl}w(|F_{obs}| - |F_{calc}|)^2/(n_{data} - n_{vari})]^{1/2}$.

Results of the Computational Analyses.

Metal-metal bond lengths in the optimized structure of 3*, 2′* and 2*. Atoms are labeled in Figure 7 in the text.

metal – metal bond	Bond length (Å)		
	3*	**2′***	**2***
Ir(1)–Ir(2)	2.75807	2.71052	2.74363
Ir(1)–Ir(3)	2.75874	2.71738	2.75418
Ir(1)–Ir(4)	2.77812	2.78338	2.79901
Ir(1)–Au(6)	3.96487	2.78779	2.75512
Ir(2)–Ir(3)	3.07619	3.09590	3.87838
Ir(2)–Ir(4)	2.83193	2.81968	2.75216
Ir(2)–Au(5)	2.78387	2.82015	2.85781
Ir(2)–Au(6)	2.79379	2.78770	2.82113
Ir(3)–Ir(4)	2.83292	2.78779	2.74447
Ir(3)–Au(5)	2.78589	2.81181	2.81578
Ir(3)–Au(6)	2.79345	2.82201	2.85432
Ir(4)–Au(5)	3.00383	2.87593	2.76044
Au(5)–Au(6)	3.27322	4.25045	3.05309

Cartesian coordinates (Ångström) of all optimized geometric structures

$Ir_4(CO)_{10}(AuPPh_3)_2$, **2**

```
Ir                 0.03484300   -0.02202600   -0.15418000
Ir                 0.10775300   -0.01148300    3.70967900
Ir                 2.02909500   -0.05371900    1.73732500
Ir                -0.01846700   -1.97276100    1.78908700
Au                 0.26759100    2.07345200    1.73115000
Au                -2.02403500   -0.07335900    1.85151200
P                 -0.15722700    4.36934900    2.20093500
P                 -4.26831000    0.59693000    1.42411600
C                  0.26658200   -2.08348200    3.83441900
C                  2.08788300   -0.33273800   -0.31030700
C                 -0.89738900   -1.28557200   -1.19543100
C                 -0.02362200    1.43013200   -1.35793600
C                  1.45693400    0.79545000    4.74701200
C                 -1.31741300    0.14626900    4.93613700
C                  3.28099400    1.37958500    1.84881500
C                  3.20431400   -1.31410800    2.52068300
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C	1.15803200	-3.21359200	0.97632500
C	-1.52899000	-3.12748700	1.66125500
C	-1.32136100	4.72423300	3.57618900
C	-2.23080200	3.72932400	3.97971900
H	-2.23179500	2.76523600	3.47145200
C	-3.11038900	3.96851600	5.04453900
H	-3.80174900	3.18889200	5.35504300
C	-3.08422100	5.20101400	5.71042700
H	-3.76205300	5.38371800	6.54266700
C	-2.17583700	6.19541400	5.31711500
H	-2.14702300	7.14915400	5.84157300
C	-1.29205100	5.95943900	4.25777200
H	-0.57141800	6.72309000	3.96850800
C	-0.70635400	5.40131000	0.77712700
C	-1.76524100	6.32458200	0.86973400
H	-2.30798300	6.43838600	1.80582100
C	-2.12150400	7.10011400	-0.24279400
H	-2.94280800	7.81021400	-0.16109600
C	-1.42501400	6.96540300	-1.45109800
H	-1.70175200	7.57223400	-2.31163600
C	-0.37427100	6.04036300	-1.55265300
H	0.16392700	5.92002600	-2.49090000
C	-0.02095200	5.25602000	-0.44815500
H	0.78468800	4.52865900	-0.53679300
C	1.41250400	5.16357300	2.75603500
C	2.13231100	4.52758300	3.78854900
H	1.76767300	3.59244300	4.20826100
C	3.31883900	5.08870600	4.27115400
H	3.86718300	4.58396700	5.06409200
C	3.80368900	6.28509700	3.72265400
H	4.73263300	6.71675000	4.09115100
C	3.09427000	6.92046200	2.69533100
H	3.46712500	7.84924200	2.26645000
C	1.90024900	6.36662700	2.21109600
H	1.35464900	6.86801600	1.41436900
C	-5.20146900	1.26611500	2.86513400
C	-5.09770800	0.57974600	4.09385500
H	-4.44821700	-0.29023300	4.17744500
C	-5.82525000	1.01214600	5.20895200
H	-5.73768800	0.47164600	6.14953000
C	-6.65185800	2.14239800	5.11422300
H	-7.21523200	2.47998700	5.98259300
C	-6.74442900	2.83907100	3.90199100
H	-7.37776200	3.72138100	3.82513100
C	-6.02565600	2.40445500	2.77894900
H	-6.10895200	2.94739000	1.83967900
C	-5.26595800	-0.86407200	0.90060600
C	-6.54738200	-1.12811900	1.42207000
H	-6.97773100	-0.47223200	2.17592900
C	-7.27163500	-2.24144100	0.97338300
H	-8.26004400	-2.44009400	1.38467000
C	-6.72743800	-3.09433600	0.00439400
H	-7.29051700	-3.96105300	-0.33740000
C	-5.45316800	-2.83385100	-0.52015100

H	-5.01996700	-3.49573800	-1.26743500
C	-4.72246900	-1.72754100	-0.07316300
H	-3.72887500	-1.53824100	-0.47465600
C	-4.50195700	1.80416200	0.05998600
C	-3.42932900	2.63863300	-0.30620300
H	-2.47386200	2.54461200	0.21061800
C	-3.58171300	3.56722400	-1.34485400
H	-2.74463600	4.20219500	-1.62485700
C	-4.80312700	3.66229300	-2.02515200
H	-4.91838200	4.37801600	-2.83752100
C	-5.87336700	2.82715300	-1.67160200
H	-6.81903500	2.89237500	-2.20728800
C	-5.72583500	1.89730700	-0.63548900
H	-6.55135800	1.23681300	-0.37458600
O	0.45662800	-2.86226800	4.70873200
O	2.83784900	-0.57451100	-1.19699400
O	-1.43313800	-2.04434100	-1.90909800
O	-0.08227400	2.25792500	-2.18549600
O	2.26550300	1.24682600	5.46456500
O	-2.12525000	0.26599300	5.77695200
O	4.09259600	2.21586400	1.91933800
O	3.94301800	-2.07389600	3.00942400
O	1.86395400	-3.99150100	0.46808400
O	-2.41529800	-3.88250500	1.57269700

$Ir_4(CO)_{11}(AuPPh_3)_2$, **3**

Ir	0.63708400	-0.09013100	-0.31361500
Ir	0.11676900	0.12609700	2.39263600
Ir	2.91908200	-0.02519300	1.23331100
Ir	1.16073500	-2.27584600	1.31621900
Au	2.27094100	-0.98714400	3.78110200
Au	2.00367900	2.16316800	2.73469200
P	3.25424400	-1.86833900	5.72857800
P	2.42036100	4.34672400	3.52463800
C	3.19066300	-1.95934100	0.58046500
C	-0.76778600	-1.71670000	2.12561200
C	1.53455100	-0.75522000	-1.88325700
C	-1.16761500	-0.57290300	-0.79115100
C	0.63404100	1.80832600	-0.63083900
C	-1.21509700	1.35214300	1.89778400
C	-0.20560300	0.32502300	4.25935400
C	3.64657400	1.04145200	-0.12280200
C	4.45730800	0.13498900	2.34788000
C	0.57045600	-3.37301700	-0.09486000
C	1.50241000	-3.70786300	2.53071100
C	3.63965400	-0.65372600	7.05721900
C	4.18710000	0.59189300	6.68700600
H	4.33901700	0.82565200	5.63411300
C	4.52913900	1.52889700	7.66833300
H	4.94425900	2.49060300	7.37372300
C	4.31594500	1.23791700	9.02384400
H	4.57360500	1.97275200	9.78479500
C	3.76284400	0.00613800	9.39690800
H	3.59149100	-0.22188600	10.44778100

C	3.42555800	-0.94044600	8.41904400
H	2.99621000	-1.89648600	8.71277000
C	4.86712800	-2.68443100	5.37773100
C	5.08203200	-3.24557600	4.10321600
H	4.30937500	-3.16543800	3.34034800
C	6.28979200	-3.88986900	3.80919500
H	6.44507200	-4.31358500	2.81887600
C	7.29569700	-3.97211300	4.78216300
H	8.23814200	-4.46551700	4.55079800
C	7.09215900	-3.40893300	6.04977100
H	7.87461800	-3.46420000	6.80492000
C	5.88409800	-2.76584300	6.35022000
H	5.73538700	-2.32059200	7.33262000
C	2.21328300	-3.15237700	6.53800800
C	0.82318700	-2.92941600	6.62355400
H	0.39217800	-2.01952500	6.20864500
C	-0.00582600	-3.87789500	7.23322100
H	-1.07786100	-3.69835400	7.28970700
C	0.54162000	-5.06063400	7.75150200
H	-0.10606700	-5.80345200	8.21395000
C	1.92095800	-5.29013000	7.66357200
H	2.34863400	-6.21056500	8.05754900
C	2.75779600	-4.34097200	7.06040700
H	3.82727400	-4.52855600	6.98706300
C	1.18309600	5.58230800	2.94560700
C	0.76896000	6.66874200	3.74143500
H	1.17517100	6.79583100	4.74337400
C	-0.17380400	7.58092800	3.24796000
H	-0.49242400	8.41541100	3.87075800
C	-0.70852100	7.41761800	1.96265100
H	-1.44557400	8.12471100	1.58564200
C	-0.30071800	6.33747000	1.16699900
H	-0.71937400	6.19836100	0.17202200
C	0.63668900	5.42014300	1.65626600
H	0.93748800	4.57214000	1.04368300
C	4.05090200	5.03317700	3.00799400
C	5.15286900	4.15490300	2.95151300
H	5.01509500	3.10121400	3.19096300
C	6.41445200	4.62758300	2.57138100
H	7.25681100	3.93944200	2.52747300
C	6.58526500	5.97728200	2.23012800
H	7.56376000	6.34176700	1.92196200
C	5.49226700	6.85319900	2.27359800
H	5.61924300	7.89977500	2.00120400
C	4.22836300	6.38700000	2.66178100
H	3.38077000	7.06974500	2.68646600
C	2.40023800	4.51680100	5.35977700
C	1.45618300	3.76083200	6.08499600
H	0.80019000	3.06876300	5.55912200
C	1.36648500	3.88937200	7.47596800
H	0.63412200	3.29972800	8.02428100
C	2.22551200	4.76309000	8.15832400
H	2.15763700	4.85946200	9.24082100
C	3.17659100	5.50662700	7.44578100

H	3.84828200	6.18355000	7.97189200
C	3.26638500	5.38668100	6.05145700
H	4.00561900	5.96757500	5.50232400
O	4.01662200	-2.64688200	0.07055600
O	-1.80480200	-2.26837000	2.31030300
O	2.06437700	-1.13906800	-2.84513000
O	-2.25439500	-0.84694800	-1.10196600
O	0.61122800	2.94485000	-0.88869800
O	-2.06816000	2.10541400	1.62780800
O	-0.53488300	0.50618800	5.36968300
O	4.14170900	1.69785600	-0.95498500
O	5.46825300	0.30143700	2.91651800
O	0.20361100	-4.07424400	-0.95132100
O	1.65793800	-4.65860600	3.19040300

$Ir_4(CO)_{10}(AuPMe_3)_2$, **2***

Ir	0.21324400	0.60885400	0.44415600
Ir	-0.15831900	-0.56313100	2.89689200
Ir	2.93539000	0.29431300	0.72075500
Ir	1.31546900	-1.90365500	0.99812000
Au	2.65222500	-0.96481100	3.22335900
Au	1.41494400	1.76420200	2.63773500
P	3.55007600	-1.36941500	5.36068000
P	2.36247100	3.56500300	3.81171200
C	2.80817800	-1.47456800	-0.37832000
C	-0.52089600	-2.26187600	3.62861400
C	0.05922300	0.13138400	-1.38312600
C	-0.22737700	2.44274200	0.17855800
C	-1.51504200	-0.01907700	1.40410000
C	-0.86644900	0.51112400	4.27829200
C	3.09306600	1.81012700	-0.39168800
C	4.73921400	0.12681300	1.25315100
C	-0.11016100	-2.72788500	0.06404200
C	2.00537300	-3.52706000	1.71551600
O	3.35732600	-1.92053500	-1.32905800
O	-0.79135700	-3.29160000	4.11577100
O	-0.02619100	-0.13918700	-2.51471800
O	-0.48642800	3.56541200	-0.01819300
O	-2.68895600	-0.09336600	1.26099600
O	-1.29748000	1.09811800	5.19777300
O	3.24953000	2.73263200	-1.09459000
O	5.87241200	0.11955500	1.55524900
O	-0.98736300	-3.25327600	-0.49768500
O	2.39472400	-4.53715900	2.15723100
C	4.20851300	3.61236900	3.90699100
H	4.57194700	2.74089400	4.46150900
H	4.62057300	3.56814800	2.89317200
H	4.55107600	4.52988400	4.40288900
C	1.94513400	5.17855500	3.01153500
H	2.31453700	5.17776700	1.98020900
H	0.85708800	5.30334400	2.98669100
H	2.39706800	6.01404400	3.56186700
C	1.83127100	3.81929800	5.56614500
H	2.29060000	4.72367700	5.98606300

H	0.74033900	3.91121100	5.60447600
H	2.12155800	2.95139200	6.16835900
C	4.54836400	-0.06825200	6.22116500
H	5.39091300	0.22719000	5.58615200
H	3.92150600	0.81080900	6.40821900
H	4.93111400	-0.44444400	7.17888600
C	2.28656200	-1.83140000	6.62799700
H	2.76579100	-2.08977700	7.58114400
H	1.59523900	-0.99510900	6.77920600
H	1.71032400	-2.68902100	6.26418700
C	4.69138700	-2.82458700	5.34959200
H	5.03996800	-3.05708400	6.36435500
H	4.16428200	-3.69200600	4.93721200
H	5.55250000	-2.60816000	4.70761200

$Ir_4(CO)_{11}(AuPMe_3)_2$, **3***

Ir	0.01175600	0.08383400	0.01796900
Ir	-0.00915200	0.02060300	2.77523200
Ir	2.55760200	0.07631400	1.08064000
Ir	0.90553200	-2.21483900	1.29672600
Au	2.41425200	-1.05669000	3.62168900
Au	1.86729300	2.08709800	2.89269900
P	3.60712100	-1.94077000	5.42508600
P	2.26992600	4.27651600	3.62308500
C	2.70331500	-1.75767600	0.15904100
C	-0.86263100	-1.83112100	2.50727100
C	0.59402400	-0.37222800	-1.76097900
C	-1.83774000	-0.42267900	-0.16658300
C	-0.07271600	2.00918100	-0.04830900
C	-1.42622500	1.24352300	2.69658400
C	0.06147100	0.01338100	4.68350800
C	3.00004400	1.34117300	-0.22900700
C	4.28684300	0.10737800	1.88914500
C	0.04782000	-3.23707400	-0.03752900
C	1.59718600	-3.67697500	2.30351900
O	3.39221600	-2.35494500	-0.60307700
O	-1.81927900	-2.46044100	2.82486400
O	0.93239000	-0.63158500	-2.84311900
O	-2.95716900	-0.71138700	-0.29456300
O	-0.15175900	3.16852900	-0.13314600
O	-2.32038200	1.99889800	2.68713300
O	-0.02478400	0.06276800	5.85115500
O	3.31660900	2.12523700	-1.03837700
O	5.39378700	0.18512700	2.26529000
O	-0.47438100	-3.88857900	-0.85055200
O	1.98062000	-4.63241600	2.85967600
C	4.03712100	4.82960500	3.68284700
H	4.59368200	4.19917100	4.38547300
H	4.48613300	4.71731300	2.68979400
H	4.10944400	5.87850100	3.99934400
C	1.47801300	5.55863800	2.54965200
H	1.85072900	5.45293200	1.52488200
H	0.39402800	5.40041000	2.53523300
H	1.69624300	6.56996300	2.91725800

C	1.65503600	4.71950700	5.31404800
H	1.85958200	5.77356800	5.54455600
H	0.57575500	4.53816500	5.36645400
H	2.14672100	4.08353600	6.05889300
C	4.18644800	-0.71898700	6.68719100
H	4.84384800	0.01357100	6.20572300
H	3.32207100	-0.19103300	7.10501700
H	4.73280800	-1.22277200	7.49516900
C	2.67157000	-3.17935900	6.42749300
H	3.28889900	-3.56045600	7.25133100
H	1.76882000	-2.71040200	6.83445000
H	2.37060000	-4.01091100	5.78119700
C	5.15555400	-2.83891100	4.96564100
H	5.65717700	-3.22883700	5.86079400
H	4.90708100	-3.66947800	4.29601300
H	5.82863900	-2.15553400	4.43628500

2′*

Ir	0.42576300	0.64424000	0.83153000
Ir	0.36361300	-0.07368000	3.44451000
Ir	2.92796500	0.05895300	1.71503300
Ir	1.04823200	-1.98746900	1.49020100
Au	2.62086200	-1.70676500	3.88164400
Au	1.68337800	2.31346400	2.86913200
P	3.77804000	-2.85533000	5.56691800
P	1.72366000	4.66896700	2.84518000
C	2.94701800	-1.50554900	0.44228600
C	-0.67496800	-1.72003100	2.94977600
C	0.86230000	0.88659900	-0.98522400
C	-1.43330400	0.77159900	0.54509900
C	-0.94765500	1.26535300	3.62517300
C	0.64651400	-0.32017700	5.33894700
C	3.48475300	1.53229100	0.68455900
C	4.61194400	-0.14748600	2.63482000
C	0.00360300	-2.52321900	0.01987700
C	1.47723800	-3.76327200	1.94611100
O	3.52603100	-2.03099000	-0.44991300
O	-1.64540000	-2.37694700	3.12643800
O	1.11011900	0.98660600	-2.12432800
O	-2.58356400	0.79711200	0.33287500
O	-1.81640800	2.03157300	3.79611200
O	0.71793900	-0.36302000	6.50846700
O	3.90331700	2.39288000	0.00828900
O	5.68140400	-0.16015200	3.11479400
O	-0.64411400	-2.82272200	-0.89964700
O	1.73684100	-4.87131900	2.21267400
C	3.39324800	5.45907000	2.95731700
H	3.86605200	5.18197600	3.90628700
H	4.02013900	5.09011300	2.13799400
H	3.31648400	6.55257900	2.89547700
C	1.03059000	5.37705700	1.28350300
H	1.60326300	4.99695200	0.43036100
H	-0.01048300	5.05510600	1.17053500
H	1.07484400	6.47399900	1.29548400

C	0.75836300	5.53721500	4.16438400
H	0.81529700	6.62700300	4.04239600
H	-0.28837300	5.21743600	4.11281000
H	1.15405900	5.26091900	5.14822000
C	4.45712100	-1.75006900	6.88149000
H	5.15177100	-1.03516700	6.42673200
H	3.63407700	-1.19267000	7.34194300
H	4.98186200	-2.33216400	7.64980700
C	2.77257400	-4.08728400	6.50764800
H	3.37861800	-4.57034700	7.28485100
H	1.91994400	-3.57961900	6.97183400
H	2.39082400	-4.84785300	5.81778100
C	5.24729200	-3.82486000	5.00515100
H	5.73641300	-4.31956600	5.85438800
H	4.92687000	-4.57997500	4.27882000
H	5.95809600	-3.15071400	4.51471800

$TS_{2'*,2*}$

Ir	0.13307400	0.38206100	0.52754300
Ir	-0.33488200	-0.57332400	3.04491100
Ir	2.81543000	-0.07760900	1.18586200
Ir	1.19047000	-2.15456200	1.19908600
Au	2.35516700	-1.32793200	3.64233000
Au	1.30173400	1.60140900	2.96682100
P	3.67198800	-1.80105000	5.53547300
P	2.12049900	3.79268100	3.29708800
C	2.97730300	-1.92184500	0.22662100
C	-1.66603600	-1.65056700	2.18730700
C	0.54043900	0.52348300	-1.29108300
C	-1.43840900	1.40858800	0.36448000
C	-1.20397400	1.03657600	3.58647400
C	-0.21626100	-1.42677100	4.78243800
C	3.09911700	1.46817900	0.13442100
C	4.54160500	0.02617200	1.94688900
C	0.03971200	-2.79979600	-0.16256900
C	1.26221900	-3.85338100	2.03616900
O	3.73003800	-2.49178500	-0.49205400
O	-2.58053600	-2.24814400	1.77268000
O	0.75778400	0.54971700	-2.44200000
O	-2.40142300	2.06216500	0.25755800
O	-1.91865500	1.89677300	3.94043900
O	-0.31531000	-1.92751400	5.83716700
O	3.32215500	2.40532700	-0.52888100
O	5.60406600	0.12049400	2.43173800
O	-0.64075600	-3.17242000	-1.03127400
O	1.32483300	-4.88352800	2.58400800
C	3.95210300	4.04217700	3.21089000
H	4.44359600	3.43705000	3.98089300
H	4.31717400	3.71709600	2.23068600
H	4.20809300	5.09900200	3.36085000
C	1.47788200	4.99560900	2.04847400
H	1.78670500	4.67582600	1.04736600
H	0.38296000	5.00516300	2.08510800
H	1.85973200	6.00594500	2.24534900

C	1.67061500	4.58315600	4.90990900
H	2.05381900	5.61061200	4.96351100
H	0.58004500	4.59535300	5.01479400
H	2.08927900	3.99648800	5.73554000
C	3.84980800	-0.43436300	6.77061800
H	4.32558100	0.42795700	6.29011200
H	2.85722200	-0.13377000	7.12379200
H	4.45990700	-0.75649700	7.62458000
C	3.02615900	-3.20555500	6.54908700
H	3.67624000	-3.39033800	7.41415400
H	2.01250200	-2.97148600	6.89083800
H	2.98055100	-4.10767000	5.92885400
C	5.42344700	-2.29310400	5.20400900
H	5.95114000	-2.50362400	6.14339500
H	5.43248600	-3.18897500	4.57328200
H	5.93562600	-1.48880300	4.66553000

$TS_{CO\text{-}12}$

Ir	0.25870800	0.52764400	0.44840900
Ir	-0.44016300	-0.46874100	2.90875900
Ir	2.84871800	0.23868500	1.09165900
Ir	1.24417500	-1.95755500	1.09201300
Au	2.19880500	-1.06415400	3.60738900
Au	1.14884300	1.71432500	2.97922100
P	3.66569300	-1.59413000	5.36111400
P	2.09643100	3.77051000	3.63339000
C	2.88931100	-1.59297500	-0.00455100
C	-1.17891200	-2.24262600	2.80051000
C	0.62018300	0.27672200	-1.36087100
C	-2.59662700	-0.05732700	-0.69680600
C	-0.22091500	2.36056700	0.26508500
C	-1.93726600	0.61909500	2.49102000
C	-0.21380400	-0.24261300	4.81506400
C	3.34736700	1.83651900	0.21947700
C	4.52602600	-0.03467500	1.86523600
C	-0.00523200	-2.76676700	-0.08664400
C	1.83517200	-3.57885400	1.93785300
O	3.62208300	-2.03381600	-0.82651300
O	-1.74330300	-3.26530600	2.85419600
O	0.81606100	0.11061800	-2.50125700
O	-3.23736300	-1.00852300	-0.65342500
O	-0.42777300	3.49944200	0.09898400
O	-2.90493700	1.26466800	2.35826900
O	-0.30746200	-0.07421100	5.97335200
O	3.66633100	2.79847900	-0.36546400
O	5.58808000	-0.15630300	2.34906900
O	-0.72503400	-3.27203600	-0.85444100
O	2.15069600	-4.58869300	2.43288800
C	3.89943100	3.75286200	4.05037500
H	4.07520000	3.07207500	4.89061800
H	4.46620200	3.38859300	3.18633500
H	4.24952100	4.75828700	4.31807300
C	1.97822600	5.11292500	2.36820400
H	2.52620400	4.81343300	1.46836400

H	0.92908800	5.26650000	2.09467300
H	2.39810500	6.04959500	2.75723000
C	1.32430100	4.53364900	5.13164900
H	1.80173200	5.49107300	5.37829200
H	0.25760400	4.69768200	4.94250700
H	1.41936800	3.84809700	5.98111200
C	4.68615300	-0.22591200	6.07693300
H	5.34154900	0.18056200	5.29896600
H	4.02690500	0.57110700	6.43811900
H	5.29796700	-0.59590200	6.90992000
C	2.81315600	-2.29835500	6.84431000
H	3.53799100	-2.55302600	7.62879900
H	2.09146100	-1.57056500	7.23072400
H	2.26602800	-3.20095400	6.54979400
C	4.93381000	-2.87939300	4.96163000
H	5.53907600	-3.11711500	5.84633700
H	4.43178300	-3.78635100	4.60730500
H	5.58363300	-2.50715400	4.16246900

$TS_{CO\text{-}13}$

Ir	0.52025500	0.37236500	0.47108300
Ir	0.24681200	-0.05206700	3.13547600
Ir	2.93813800	-0.08634100	1.60152900
Ir	1.03932200	-2.16055500	1.48798600
Au	2.46053000	-1.58983500	3.93566400
Au	1.73100700	2.24880300	2.52063000
P	3.52046800	-2.64148700	5.74167000
P	1.87876400	4.56800500	2.90348900
C	3.08598100	-1.80262100	0.57070000
C	-0.78127800	-1.72864000	2.69336600
C	1.06960800	0.36883900	-1.33255300
C	-1.32085500	0.41753200	0.06284700
C	-0.17699400	3.59564100	-0.79273100
C	-1.03268700	1.33038500	3.08010800
C	0.31678700	-0.14511900	5.06203100
C	3.55964300	1.22342100	0.39911800
C	4.53154200	-0.12852700	2.69063100
C	0.22833900	-2.89879200	-0.04087600
C	1.40357100	-3.85722000	2.21671200
O	3.72947000	-2.46720500	-0.17024500
O	-1.79452000	-2.32493300	2.85168100
O	1.38266700	0.29700500	-2.45750500
O	-2.45670100	0.38244600	-0.21011500
O	0.74751800	4.18919400	-1.12836000
O	-1.88676100	2.13073000	3.10292400
O	0.24809300	-0.09728400	6.23132600
O	4.02631400	1.97551300	-0.36637400
O	5.55221300	-0.04522500	3.26154600
O	-0.28384900	-3.31845700	-0.99797600
O	1.62115800	-4.91590700	2.66277600
C	2.98586100	5.53723700	1.78023200
H	4.00137400	5.12943500	1.83401600
H	2.63265200	5.44073500	0.74814000
H	3.00202100	6.59785100	2.06445800

C	0.29408400	5.52399400	2.84840500
H	-0.14419800	5.44704400	1.84766900
H	-0.41457900	5.09400200	3.56441400
H	0.46625300	6.58131000	3.08981000
C	2.54221600	4.97992900	4.58240200
H	2.59796900	6.06685400	4.72591500
H	1.89035800	4.54480200	5.34815700
H	3.54275100	4.54724600	4.69418900
C	4.11715000	-1.50081900	7.06734900
H	4.82995000	-0.78986800	6.63493200
H	3.26898200	-0.94088900	7.47616300
H	4.60661800	-2.06407000	7.87233700
C	2.47316400	-3.86289200	6.64905800
H	3.03503200	-4.32286600	7.47210600
H	1.58862100	-3.35455400	7.04828200
H	2.14158200	-4.64085800	5.95265400
C	5.03229600	-3.60567900	5.29498700
H	5.47571400	-4.06859000	6.18609000
H	4.76677100	-4.38555800	4.57279600
H	5.76239600	-2.93510300	4.82869700