Electronic Supplementary Material (ESI) for Dalton Transactions.

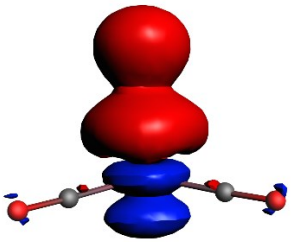
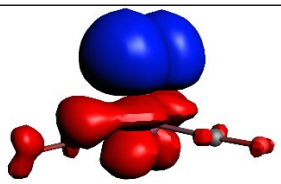
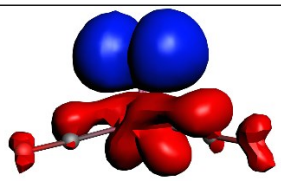
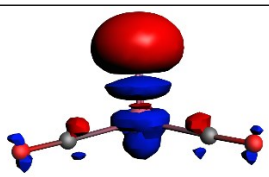
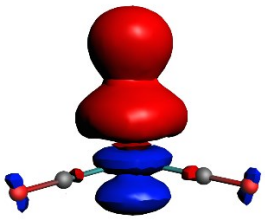
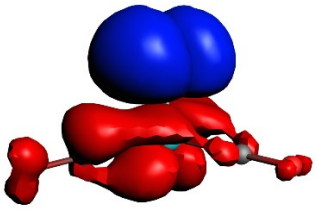
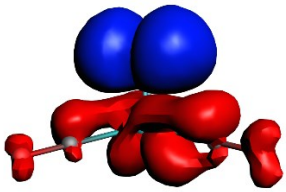
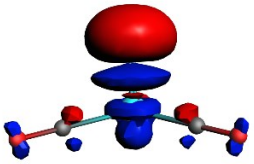
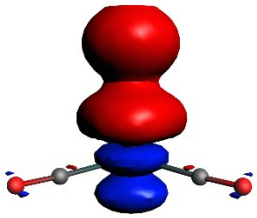
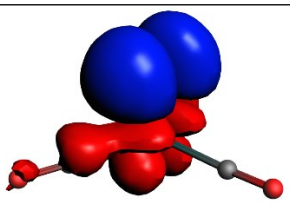
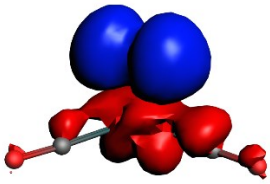
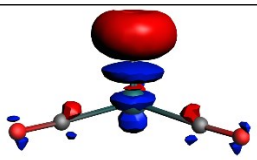
Supporting Information for

Quadruple Bonding of Bare Group-13 Atoms in Transition Metal Complexes

Sudip Pan, Sai Manoj, and Gernot Frenking

Figures S1 and S2

Tables S1 and S2

$BRu(CO)_3^-$			
 $\Delta E_{orb(1)}$ = -103.0; $\lvert\nu_1\rvert$ = 0.33[a]	 $\Delta E_{orb(2)}$ = -45.4; $\lvert\nu_2\rvert$ = 0.62	 $\Delta E_{orb(3)}$ = -45.4; $\lvert\nu_3\rvert$ = 0.62	 $\Delta E_{orb(4)}$ = -10.9; $\lvert\nu_4\rvert$ = 0.34
$BOs(CO)_3^-$			
 $\Delta E_{orb(1)}$ = -104.4; $\lvert\nu_1\rvert$ = 0.30[a]	 $\Delta E_{orb(2)}$ = -44.7; $\lvert\nu_2\rvert$ = 0.62	 $\Delta E_{orb(3)}$ = -44.7; $\lvert\nu_3\rvert$ = 0.62	 $\Delta E_{orb(4)}$ = -13.9; $\lvert\nu_4\rvert$ = 0.36
$BRh(CO)_3$			
 $\Delta E_{orb(1)}$ = -113.0; $\lvert\nu_1\rvert$ = 0.43[a]	 $\Delta E_{orb(2)}$ = -38.6; $\lvert\nu_2\rvert$ = 0.56	 $\Delta E_{orb(3)}$ = -38.6; $\lvert\nu_3\rvert$ = 0.56	 $\Delta E_{orb(4)}$ = -8.8; $\lvert\nu_4\rvert$ = 0.28
$BIr(CO)_3$			

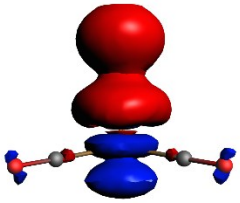
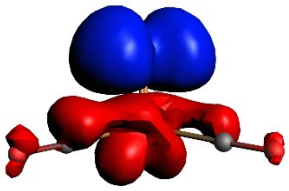
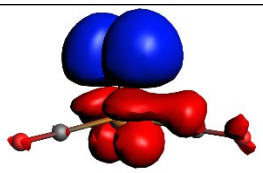
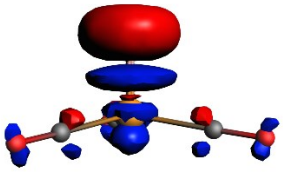
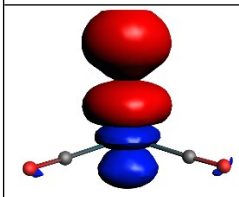
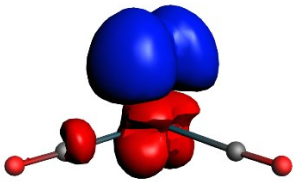
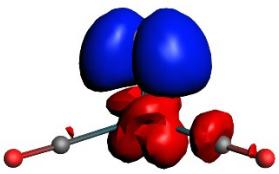
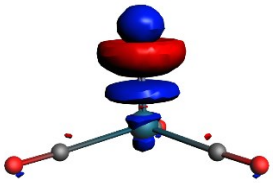
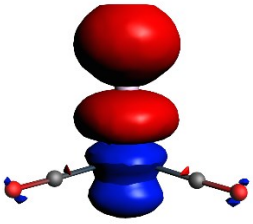
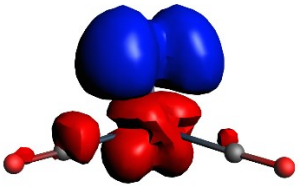
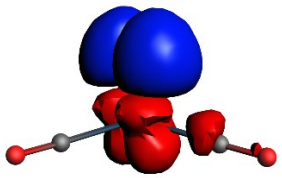
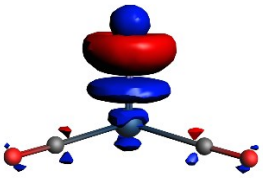
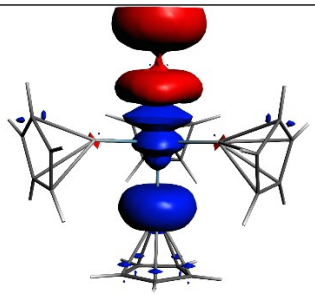
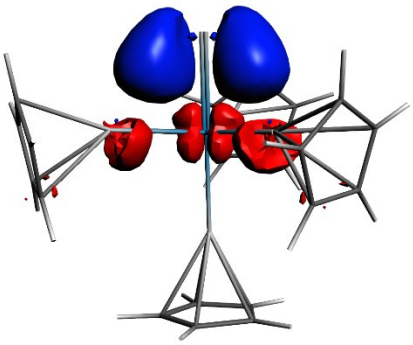
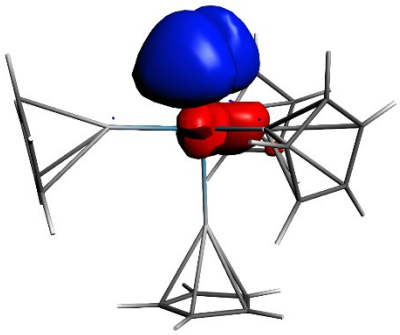
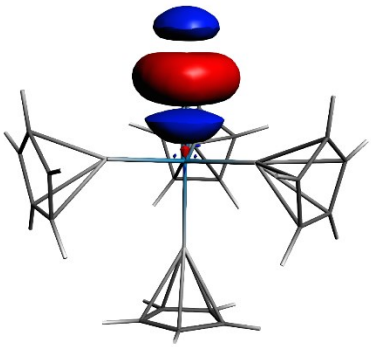
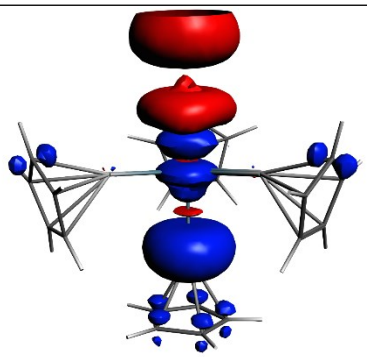
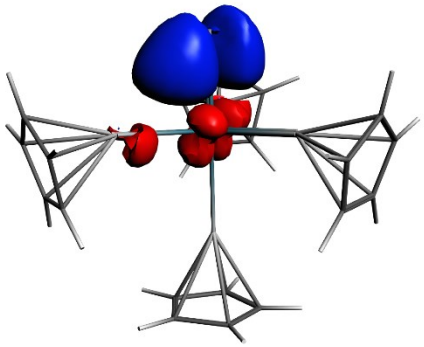
 $\Delta E_{orb(1)}$ = -117.5; $\|\nu_1\|$ = 0.39[a]	 $\Delta E_{orb(2)}$ = -37.6; $\|\nu_2\|$ = 0.56	 $\Delta E_{orb(3)}$ = -37.6; $\|\nu_3\|$ = 0.56	 $\Delta E_{orb(4)}$ = -13.1; $\|\nu_4\|$ = 0.32
$BPd(CO)_3^+$			
 $\Delta E_{orb(1)}$ = -120.8; $\|\nu_1\|$ = 0.53[a]	 $\Delta E_{orb(2)}$ = -28.2; $\|\nu_2\|$ = 0.50	 $\Delta E_{orb(3)}$ = -28.2; $\|\nu_3\|$ = 0.50	 $\Delta E_{orb(4)}$ = -6.3; $\|\nu_4\|$ = 0.18
$BPt(CO)_3^+$			
 $\Delta E_{orb(1)}$ = -131.4; $\|\nu_1\|$ = 0.49[a]	 $\Delta E_{orb(2)}$ = -29.4; $\|\nu_2\|$ = 0.50	 $\Delta E_{orb(3)}$ = -29.4; $\|\nu_3\|$ = 0.50	 $\Delta E_{orb(4)}$ = -11.9; $\|\nu_4\|$ = 0.26

Figure S1. Shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$ of the complexes $BTM(CO)_3^q$ at the M06/TZ2P-ZORA//M06-D3/def2-TZVPPD level (Table 3). Isosurface values are 0.001 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow is red→blue.

$GaNi(GaCp)_4^+$	
 $\Delta E_{orb(1)} = -68.5$; $\lvert\nu_1\rvert = 0.49$	 $\Delta E_{orb(2)} = -14.6$; $\lvert\nu_2\rvert = 0.40$
 $\Delta E_{orb(3)} = -14.5$; $\lvert\nu_3\rvert = 0.40$	 $\Delta E_{orb(4)} = -4.6$; $\lvert\nu_4\rvert = 0.16$
$GaPd(GaCp)_4^+$	
 $\Delta E_{orb(1)} = -72.9$; $\lvert\nu_1\rvert = 0.53$	 $\Delta E_{orb(2)} = -9.7$; $\lvert\nu_2\rvert = 0.34$

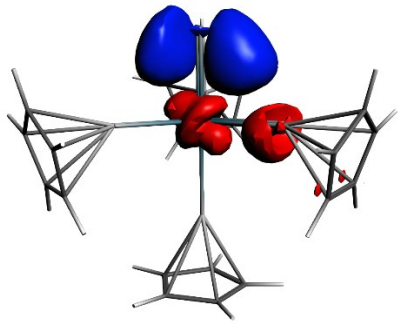
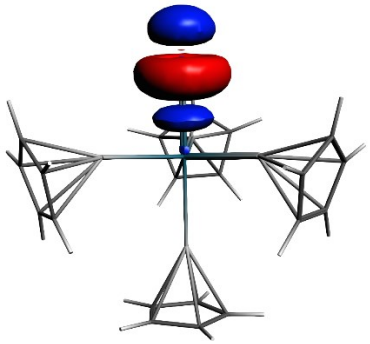
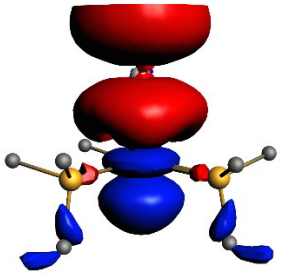
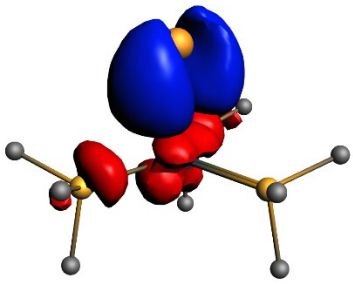
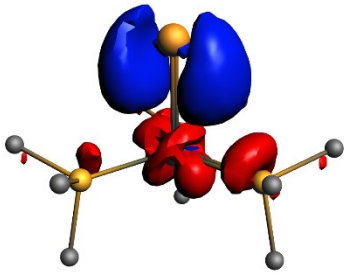
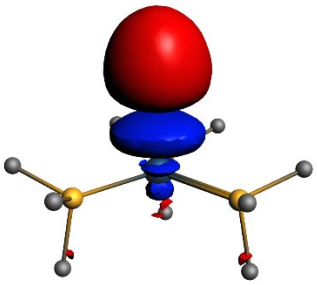
	
$\Delta E_{orb(3)}$ = **-9.7; $\lvert\nu_3\rvert$ = 0.34**	$\Delta E_{orb(4)}$ = **-3.1; $\lvert\nu_4\rvert$ = 0.12**
$InPt(PMe_3)_3^+$	
	
$\Delta E_{orb(1)}$ = **-89.6; $\lvert\nu_1\rvert$ = 0.50**	$\Delta E_{orb(2)}$ = **-10.1; $\lvert\nu_2\rvert$ = 0.44**
	
$\Delta E_{orb(3)}$ = **-10.1; $\lvert\nu_3\rvert$ = 0.44**	$\Delta E_{orb(4)}$ = **-4.1; $\lvert\nu_4\rvert$ = 0.14**

Figure S2. Shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$ of the complexes $GaTM(GaCp)_4^+$ (TM = Ni, Pd) and $InPt(PMe_3)_3^+$ at the M06/TZ2P-ZORA//M06-D3/def2-TZVPP level (Tables 4 and 5). Isosurface values are 0.001 au for $\Delta\rho_{(1)-(3)}$ and 0.0005 au for $\Delta\rho_{(4)}$. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow is red→blue.

Table S1. Calculated bond dissociation energies of the E-TM bonds D_e, ZPE corrected values D_0 and free energy changes at 298 K ΔG^{298} at the M06-D3/def2-TZVPPD level. The atoms E were calculated in the doublet electronic ground state, the atomic ions E^+ in the singlet ground state and E^- in the triplet ground state. The energy values are given in kcal/mol.

Dissociation	D_e	D_0	ΔG^{298}
$BFe(CO)_3^- \rightarrow B + Fe(CO)_3^-$ (D_{3h}, $^2A_1'$)	96.2	93.7	85.0
$AlFe(CO)_3^- \rightarrow Al + Fe(CO)_3^-$ (D_{3h}, $^2A_1'$)	61.7	60.5	52.2
$GaFe(CO)_3^- \rightarrow Ga + Fe(CO)_3^-$ (D_{3h}, $^2A_1'$)	58.9	57.9	49.3
$InFe(CO)_3^- \rightarrow In + Fe(CO)_3^-$ (D_{3h}, $^2A_1'$)	51.0	50.2	41.9
$TlFe(CO)_3^- \rightarrow Tl + Fe(CO)_3^-$ (D_{3h}, $^2A_1'$)	45.7	45.0	36.7
$BFe(CO)_3^- \rightarrow B + Fe(CO)_3^-$ (D_{3h}, $^2A_1'$)	96.2	93.7	85.0
$BRu(CO)_3^- \rightarrow B + Ru(CO)_3^-$ (C_s, $^2A'$)	120.3	118.7	110.8
$BOs(CO)_3^- \rightarrow B + Os(CO)_3^-$ (C_s, $^2A'$)	126.6	124.7	116.7
$BCo(CO)_3 \rightarrow B + Co(CO)_3$ (D_{3h}, $^2A_1'$)	81.1	78.9	70.1
$BRh(CO)_3 \rightarrow B + Rh(CO)_3$ (C_{2v}, $^2A_1$)	93.8	92.5	84.1
$BIr(CO)_3 \rightarrow B + Ir(CO)_3$ (C_{2v}, $^2A_1$)	98.0	96.7	88.3
$BNi(CO)_3^+ \rightarrow B + Ni(CO)_3^+$ (C_{2v}, $^2A_1$)	66.6	65.0	56.2
$BPd(CO)_3^+ \rightarrow B + Pd(CO)_3^+$ (C_{2v}, $^2A_1$)	84.6	83.8	76.2
$BPt(CO)_3^+ \rightarrow B + Pt(CO)_3^+$ (C_{2v}, $^2A_1$)	87.0	86.1	78.4
$BNi(CO)_3^+ \rightarrow B^+ + Ni(CO)_3$ (D_{3h}, $^1A_1'$)	78.9	77.5	70.5
$BPd(CO)_3^+ \rightarrow B^+ + Pd(CO)_3$ (D_{3h}, $^1A_1'$)	83.6	82.3	75.9
$BPt(CO)_3^+ \rightarrow B^+ + Pt(CO)_3$ (D_{3h}, $^1A_1'$)	85.5	84.3	77.6
$BFe(CO)_3^- \rightarrow B^- + Fe(CO)_3$ (C_{2v}, $^3A_1$)	132.9	130.5	120.8
$AlFe(CO)_3^- \rightarrow Al^- + Fe(CO)_3$ (C_{2v}, $^3A_1$)	100.7	99.5	90.3

$GaFe(CO)_3^- \rightarrow Ga^- + Fe(CO)_3$ (C_{2v}, $^3A_1$)	102.6	101.6	92.2
$InFe(CO)_3^- \rightarrow In^- + Fe(CO)_3$ (C_{2v}, $^3A_1$)	83.8	83.0	73.8
$TlFe(CO)_3^- \rightarrow Tl^- + Fe(CO)_3$ (C_{2v}, $^3A_1$)	80.1	79.4	70.3
$BFe(CO)_3^- \rightarrow B^- + Fe(CO)_3$ (C_{2v}, $^3A_1$)	132.9	130.5	120.8
$BRu(CO)_3^- \rightarrow B^- + Ru(CO)_3$ (C_{2v}, $^3A_1$)	167.2	165.8	156.9
$BOs(CO)_3^- \rightarrow B^- + Os(CO)_3$ (C_{2v}, $^3A_1$)	175.5	174.2	165.4
$GaNi(GaCp)_4^+ \rightarrow Ga + Ni(GaCp)_4^+$ (C_s, $^2A'$)	62.4	62.1	53.9
$GaPd(GaCp)_4^+ \rightarrow Ga + Pd(GaCp)_4^+$ (C_s, $^2A'$)	79.3	78.8	70.7
$GaPt(GaCp)_4^+ \rightarrow Ga + Pt(GaCp)_4^+$ (C_s, $^2A'$)	79.6	79.2	72.1
$GaNi(GaCp)_4^+ \rightarrow Ga^+ + Ni(GaCp)_4$ (C_s, $^1A'$)	72.1	70.5	62.4
$GaPd(GaCp)_4^+ \rightarrow Ga^+ + Pd(GaCp)_4$ (C_s, $^1A'$)	65.7	64.1	55.5
$GaPt(GaCp)_4^+ \rightarrow Ga^+ + Pt(GaCp)_4$ (C_s, $^1A'$)	71.3	69.6	62.6
$GaPt(PMe_3)_3^+ \rightarrow Ga + Pt(PMe_3)_3^+$ (C_s, $^2A'$)	67.0	66.9	59.2
$InPt(PMe_3)_3^+ \rightarrow In + Pt(PMe_3)_3^+$ (C_s, $^2A'$)	62.5	62.5	54.7
$GaPt(PMe_3)_3^+ \rightarrow Ga^+ + Pt(PMe_3)_3$ (C_s, $^1A'$)	81.4	80.1	72.0
$InPt(PMe_3)_3^+ \rightarrow In^+ + Pt(PMe_3)_3$ (C_s, $^1A'$)	69.8	68.7	60.4

Table S2. The Cartesian coordinates of the studied complexes at the M06-D3 level in combination with either def2-TZVPPD basis set or def2-TZVPP basis set.

$BFe(CO)_3^-$ (C_{3v}, $^1A_1$) E = -1628.491922 au -1 1 Fe 0.00000000 0.00000000 0.08810000 C 0.00000000 1.76811700 -0.18044800 C -1.53123500 -0.88405900 -0.18044800 C 1.53123500 -0.88405900 -0.18044800 O -2.52457200 -1.45756200 -0.32790600 O 0.00000000 2.91512500 -0.32790600 O 2.52457200 -1.45756200 -0.32790600 B 0.00000000 0.00000000 1.76544400
$AlFe(CO)_3^-$ (C_{3v}, $^1A_1$) E = -1846.144958 au -1 1 Fe 0.00000000 0.00000000 0.25754000 C 0.00000000 1.77225000 0.36440100 C 1.53481400 -0.88612500 0.36440100 C -1.53481400 -0.88612500 0.36440100 O 2.53750400 -1.46502900 0.47212000 O 0.00000000 2.93005700 0.47212000 O -2.53750400 -1.46502900 0.47212000 Al 0.00000000 0.00000000 -1.89124000
$GaFe(CO)_3^-$ (C_{3v}, $^1A_1$) E = -3528.560869 au -1 1 Fe 0.00000000 0.00000000 -0.50876000 C 0.00000000 1.75753300 -0.77040500 C -1.52206900 -0.87876700 -0.77040500 C 1.52206900 -0.87876700 -0.77040500 O -2.50501600 -1.44627100 -1.01689800 O 0.00000000 2.89254300 -1.01689800 O 2.50501600 -1.44627100 -1.01689800 Ga 0.00000000 0.00000000 1.66131000
$InFe(CO)_3^-$ (C_{3v}, $^1A_1$) E = -1793.955974 au -1 1 Fe 0.00000000 0.00000000 -0.84148000 C 0.00000000 1.75617700 -1.10996000 C -1.52089400 -0.87808800 -1.10996000 C 1.52089400 -0.87808800 -1.10996000

O -2.49880800 -1.44268700 -1.38385500
O 0.00000000 2.88537400 -1.38385500
O 2.49880800 -1.44268700 -1.38385500
In 0.00000000 0.00000000 1.53204600

$TlFe(CO)_3^-$ (C_{3v}, $^1A_1$)

E = -1776.299418 au

-1 1
Fe 0.00000000 0.00000000 -1.18457100
C 0.00000000 1.74854600 -1.49622500
C -1.51428500 -0.87427300 -1.49622500
C 1.51428500 -0.87427300 -1.49622500
O -2.48261400 -1.43333800 -1.81190200
O 0.00000000 2.86667600 -1.81190200
O 2.48261400 -1.43333800 -1.81190200
Tl 0.00000000 0.00000000 1.24958700

$BRu(CO)_3^-$ (C_{3v}, $^1A_1$)

E = -459.791421 au

-1 1
Ru 0.00000000 0.00000000 0.07776900
C 0.00000000 1.92413800 -0.22245600
C -1.66635300 -0.96206900 -0.22245600
C 1.66635300 -0.96206900 -0.22245600
O -2.65770500 -1.53442600 -0.36450300
O 0.00000000 3.06885300 -0.36450300
O 2.65770500 -1.53442600 -0.36450300
B 0.00000000 0.00000000 1.86608500

$BOs(CO)_3^-$ (C_{3v}, $^1A_1$)

E = -455.582598 au

-1 1
Os 0.00000000 0.00000000 0.05590100
C 0.00000000 1.92257600 -0.23101700
C -1.66500000 -0.96128800 -0.23101700
C 1.66500000 -0.96128800 -0.23101700
O -2.65622100 -1.53357000 -0.39816600
O 0.00000000 3.06714000 -0.39816600
O 2.65622100 -1.53357000 -0.39816600
B 0.00000000 0.00000000 1.89317100

$BCo(CO)_3$ (C_{3v}, $^1A_1$)

E = -1747.495652 au

0 1
C 0.00000000 1.79718800 -0.18835600
C -1.55641100 -0.89859400 -0.18835600

C 1.55641100 -0.89859400 -0.18835600 O -2.52867200 -1.45992900 -0.34664700 O 0.00000000 2.91985900 -0.34664700 O 2.52867200 -1.45992900 -0.34664700 B 0.00000000 0.00000000 1.78279600 Co 0.00000000 0.00000000 0.10355400
$BRh(CO)_3$ (C_{3v}, $^1A_1$) E = -475.376457 au 0 1 C 0.00000000 1.98696000 -0.24340400 C -1.72075800 -0.99348000 -0.24340400 C 1.72075800 -0.99348000 -0.24340400 O -2.69437300 -1.55559700 -0.36858300 O 0.00000000 3.11119400 -0.36858300 O 2.69437300 -1.55559700 -0.36858300 B 0.00000000 0.00000000 1.86717600 Rh 0.00000000 0.00000000 0.08647500
$BIr(CO)_3$ (C_{3v}, $^1A_1$) E = -469.172466 au 0 1 C 0.00000000 1.95497600 -0.23969000 C -1.69305900 -0.97748800 -0.23969000 C 1.69305900 -0.97748800 -0.23969000 O -2.66755800 -1.54011500 -0.38574300 O 0.00000000 3.08023100 -0.38574300 O 2.66755800 -1.54011500 -0.38574300 B 0.00000000 0.00000000 1.88099900 Ir 0.00000000 0.00000000 0.05412000
$BNi(CO)_3^+$ (C_{3v}, $^1A_1$) E = -1872.768898 au 1 1 C 0.00000000 1.88186300 -0.20885000 C -1.62974100 -0.94093100 -0.20885000 C 1.62974100 -0.94093100 -0.20885000 O -2.57896700 -1.48896700 -0.42447900 O 0.00000000 2.97793400 -0.42447900 O 2.57896700 -1.48896700 -0.42447900 B 0.00000000 0.00000000 1.89653900 Ni 0.00000000 0.00000000 0.15943200
$BPd(CO)_3^+$ (C_{3v}, $^1A_1$) E = -492.416312 au

1 1
C 0.00000000 2.11473400 -0.30869700
C -1.83141300 -1.05736700 -0.30869700
C 1.83141300 -1.05736700 -0.30869700
O -2.78048600 -1.60531500 -0.51775600
O 0.00000000 3.21062900 -0.51775600
O 2.78048600 -1.60531500 -0.51775600
B 0.00000000 0.00000000 1.99378200
Pd 0.00000000 0.00000000 0.17421300

$BPt(CO)_3^+$ (C_{3v}, $^1A_1$)

E = -483.857199 au

1 1
C 0.00000000 2.05701200 -0.29032800
C -1.78142400 -1.02850600 -0.29032800
C 1.78142400 -1.02850600 -0.29032800
O -2.73782000 -1.58068100 -0.46041400
O 0.00000000 3.16136200 -0.46041400
O 2.73782000 -1.58068100 -0.46041400
B 0.00000000 0.00000000 1.93853100
Pt 0.00000000 0.00000000 0.08440000

$GaNi(GaCp)_4^+$ (C_s, $^1A'$)

E = -11906.190808 au

1 1
C 0.65427300 4.31514400 1.14504400
C 1.47186500 4.47169900 0.00000000
C -0.66668100 4.06317600 0.70713700
C 0.65427300 4.31514400 -1.14504400
C -0.66668100 4.06317600 -0.70713700
H 0.98150300 4.37835000 2.17063600
H 2.53013000 4.67969900 0.00000000
H -1.52258500 3.89198100 1.34119000
H 0.98150300 4.37835000 -2.17063600
H -1.52258500 3.89198100 -1.34119000
Ga 0.66407800 2.32522800 0.00000000
Ga 2.86829900 0.02595300 0.00000000
Ga 0.66989500 -1.14349900 1.98211300
Ga -1.92087200 0.02016400 0.00000000
Ga 0.66989500 -1.14349900 -1.98211300
C 0.79231100 -1.25271200 4.27017400
C -0.56627000 -1.39212400 3.90133000
C 1.50355000 -2.35770500 3.74393200
C -0.69498600 -2.58248100 3.14784500
C 0.58331200 -3.17887400 3.04975300

H 1.21215700 -0.44753600 4.85186400
H -1.36213700 -0.70652600 4.14694100
H 2.55991600 -2.54366100 3.85675000
H -1.60674600 -2.96369500 2.71451700
H 0.81665100 -4.09792200 2.53612900
C 0.79231100 -1.25271200 -4.27017400
C -0.56627000 -1.39212400 -3.90133000
C 1.50355000 -2.35770500 -3.74393200
C -0.69498600 -2.58248100 -3.14784500
C 0.58331200 -3.17887400 -3.04975300
H 1.21215700 -0.44753600 -4.85186400
H -1.36213700 -0.70652600 -4.14694100
H 2.55991600 -2.54366100 -3.85675000
H -1.60674600 -2.96369500 -2.71451700
H 0.81665100 -4.09792200 -2.53612900
C -3.96803300 0.93791500 0.70637600
C -3.93325400 -0.40530200 1.14264000
C -3.96803300 0.93791500 -0.70637600
C -3.91066200 -1.23567100 0.00000000
C -3.93325400 -0.40530200 -1.14264000
H -4.00053700 1.80964400 1.34105700
H -3.93543800 -0.73818700 2.16889100
H -4.00053700 1.80964400 -1.34105700
H -3.88925500 -2.31448200 0.00000000
H -3.93543800 -0.73818700 -2.16889100
Ni 0.49162500 0.02409000 0.00000000

$GaPd(GaCp)_4^+$ (C_s, $^1A'$)

E = -10525.868240 au

1 1
C 0.40504100 4.50160600 -1.14493400
C 1.20128600 4.74480800 0.00000000
C -0.88031400 4.10890600 -0.70674700
C 0.40504100 4.50160600 1.14493400
C -0.88031400 4.10890600 0.70674700
H 0.72320600 4.60071000 -2.17058200
H 2.23026200 5.06786000 0.00000000
H -1.71261500 3.84547600 -1.34067300
H 0.72320600 4.60071000 2.17058200
H -1.71261500 3.84547600 1.34067300
Ga 0.63969800 2.51709200 0.00000000
Ga 3.02592900 0.12022100 0.00000000
Ga 0.76246000 -1.20353500 -2.13372000
Ga -2.07192100 -0.05599400 0.00000000
Ga 0.76246000 -1.20353500 2.13372000

C 0.68913700 -1.27953400 -4.43369600
C -0.63111400 -1.45042500 -3.95755400
C 1.46097200 -2.37773700 -3.98435400
C -0.67652800 -2.65271000 -3.21495300
C 0.61528600 -3.22629300 -3.23077700
H 1.04530400 -0.45859300 -5.03555100
H -1.45632000 -0.77596100 -4.12493600
H 2.50708300 -2.54316000 -4.18795600
H -1.54270100 -3.05682400 -2.71410200
H 0.90587200 -4.14877500 -2.75372800
C 0.68913700 -1.27953400 4.43369600
C -0.63111400 -1.45042500 3.95755400
C 1.46097200 -2.37773700 3.98435400
C -0.67652800 -2.65271000 3.21495300
C 0.61528600 -3.22629300 3.23077700
H 1.04530400 -0.45859300 5.03555100
H -1.45632000 -0.77596100 4.12493600
H 2.50708300 -2.54316000 4.18795600
H -1.54270100 -3.05682400 2.71410200
H 0.90587200 -4.14877500 2.75372800
C -4.16771900 0.76538200 -0.70624100
C -4.07059700 -0.57441500 -1.14247900
C -4.16771900 0.76538200 0.70624100
C -4.00977200 -1.40257700 0.00000000
C -4.07059700 -0.57441500 1.14247900
H -4.24160800 1.63468600 -1.34079500
H -4.05834900 -0.90721500 -2.16868300
H -4.24160800 1.63468600 1.34079500
H -3.93938500 -2.47928200 0.00000000
H -4.05834900 -0.90721500 2.16868300
Pd 0.53506300 0.03909300 0.00000000

$GaPt(GaCp)_4^+$ (C_s, $^1A'$)

E = -10517.298973 au

1 1

C -0.31836700 4.46908800 1.14576500
C -1.12237300 4.68981100 0.00000000
C 0.97717700 4.11150700 0.70680200
C -0.31836700 4.46908800 -1.14576500
C 0.97717700 4.11150700 -0.70680200
H -0.63970000 4.55774800 2.17130500
H -2.15962000 4.98509500 0.00000000
H 1.81552500 3.86771700 1.34056500
H -0.63970000 4.55774800 -2.17130500

H 1.81552500 3.86771700 -1.34056500
Ga -0.50969600 2.49804900 0.00000000
Ga -3.03536000 0.13992900 0.00000000
Ga -0.65993700 -1.19377100 2.11967400
Pt -0.54059200 0.04142100 0.00000000
Ga 2.09587400 -0.06990600 0.00000000
Ga -0.65993700 -1.19377100 -2.11967400
C -0.65494900 -1.26072600 4.40463000
C 0.67721600 -1.45920500 3.97360900
C -1.43415500 -2.34407900 3.92816400
C 0.72370600 -2.66295700 3.23314500
C -0.57901700 -3.21110800 3.20460200
H -1.01536000 -0.43167500 4.99254800
H 1.50899900 -0.79990900 4.16653900
H -2.48964500 -2.48837600 4.09613200
H 1.59759900 -3.08326100 2.75989800
H -0.87211900 -4.12678800 2.71628100
C -0.65494900 -1.26072600 -4.40463000
C 0.67721600 -1.45920500 -3.97360900
C -1.43415500 -2.34407900 -3.92816400
C 0.72370600 -2.66295700 -3.23314500
C -0.57901700 -3.21110800 -3.20460200
H -1.01536000 -0.43167500 -4.99254800
H 1.50899900 -0.79990900 -4.16653900
H -2.48964500 -2.48837600 -4.09613200
H 1.59759900 -3.08326100 -2.75989800
H -0.87211900 -4.12678800 -2.71628100
C 4.20812900 0.72133000 0.70622300
C 4.09199700 -0.61695600 1.14241800
C 4.20812900 0.72133000 -0.70622300
C 4.01941700 -1.44417100 0.00000000
C 4.09199700 -0.61695600 -1.14241800
H 4.29432600 1.58945100 1.34087900
H 4.07527900 -0.94946100 2.16866100
H 4.29432600 1.58945100 -1.34087900
H 3.93359600 -2.51977900 0.00000000
H 4.07527900 -0.94946100 -2.16866100

$GaPt(PMe_3)_3^+$ (C_s, $^1A'$)

E = -3427.297897 au

1 1
Pt 0.00153500 0.05129800 0.00000000
Ga -0.03793000 -2.31867700 0.00000000
P 2.34789900 0.37639700 0.00000000

C 2.69258900 2.16399500 0.00000000
C 3.33372900 -0.20624000 1.41499400
C 3.33372900 -0.20624000 -1.41499400
P -1.16671000 0.40049700 2.03402600
C -1.17041700 2.18397600 2.39911500
C -2.93563400 -0.01896000 2.13098700
C -0.52869600 -0.31340100 3.58242200
P -1.16671000 0.40049700 -2.03402600
C -1.17041700 2.18397600 -2.39911500
C -0.52869600 -0.31340100 -3.58242200
C -2.93563400 -0.01896000 -2.13098700
H 2.25235500 2.62578300 0.88367200
H 3.76877200 2.34869400 0.00000000
H 2.25235500 2.62578300 -0.88367200
H 3.28617900 -1.29390100 1.47717600
H 4.37770100 0.09992800 1.32126900
H 2.92163900 0.20532900 2.33655800
H 2.92163900 0.20532900 -2.33655800
H 4.37770100 0.09992800 -1.32126900
H 3.28617900 -1.29390100 -1.47717600
H -1.62204900 2.72995300 1.57050600
H -1.73199100 2.39149500 3.31223600
H -0.14593800 2.53492300 2.52393900
H -3.06819800 -1.09379600 2.00290200
H -3.36045600 0.28108900 3.09114900
H -3.47329800 0.48711700 1.32917800
H 0.51570600 -0.03042900 3.71276300
H -1.10534000 0.03406000 4.44216600
H -0.58291300 -1.40170900 3.53670200
H -1.73199100 2.39149500 -3.31223600
H -1.62204900 2.72995300 -1.57050600
H -0.14593800 2.53492300 -2.52393900
H -1.10534000 0.03406000 -4.44216600
H 0.51570600 -0.03042900 -3.71276300
H -0.58291300 -1.40170900 -3.53670200
H -3.47329800 0.48711700 -1.32917800
H -3.36045600 0.28108900 -3.09114900
H -3.06819800 -1.09379600 -2.00290200

$InPt(PMe_3)_3^+$ (C_s, $^1A'$)

E = -1692.698391 au

1 1

Pt -0.00197800 0.26413000 0.00000000
In 0.00526400 -2.32342700 0.00000000

P 2.34043500 0.59190100 0.00000000
C 2.65354000 2.38617500 0.00000000
C 3.34604400 0.02935700 1.41144000
C 3.34604400 0.02935700 -1.41144000
P -1.17129300 0.58654900 2.02949100
C -1.35163400 2.37959100 2.29403000
C -2.88788800 0.00128600 2.20431000
C -0.43721600 0.04152700 3.60554000
P -1.17129300 0.58654900 -2.02949100
C -1.35163400 2.37959100 -2.29403000
C -0.43721600 0.04152700 -3.60554000
C -2.88788800 0.00128600 -2.20431000
H 2.20383700 2.83894400 0.88374300
H 3.72602300 2.59159100 0.00000000
H 2.20383700 2.83894400 -0.88374300
H 3.32994700 -1.05976400 1.46719100
H 4.38111700 0.36448100 1.31681000
H 2.92613300 0.42264700 2.33718500
H 2.92613300 0.42264700 -2.33718500
H 4.38111700 0.36448100 -1.31681000
H 3.32994700 -1.05976400 -1.46719100
H -1.90728300 2.82045100 1.46639300
H -1.88174000 2.58100300 3.22721900
H -0.36800800 2.84757800 2.33458700
H -2.91346600 -1.08851000 2.16938100
H -3.32452400 0.33617000 3.14762500
H -3.48779700 0.38154800 1.37754100
H 0.56735600 0.45378300 3.70028200
H -1.03992900 0.36848300 4.45552400
H -0.36081300 -1.04630600 3.62255600
H -1.88174000 2.58100300 -3.22721900
H -1.90728300 2.82045100 -1.46639300
H -0.36800800 2.84757800 -2.33458700
H -1.03992900 0.36848300 -4.45552400
H 0.56735600 0.45378300 -3.70028200
H -0.36081300 -1.04630600 -3.62255600
H -3.48779700 0.38154800 -1.37754100
H -3.32452400 0.33617000 -3.14762500
H -2.91346600 -1.08851000 -2.16938100

$Fe(CO)_3^-$

E = -1603.697270 au

-1 2
Fe 0.00000000 0.00000000 0.00000000
C 0.00000000 1.79802700 0.00000000
C -1.55713700 -0.89901300 0.00000000
C 1.55713700 -0.89901300 0.00000000
O -2.56647400 -1.48175500 0.00000000
O 0.00000000 2.96350900 0.00000000
O 2.56647400 -1.48175500 0.00000000

$Ru(CO)_3^-$

E = -434.972230 au

-1 2
C -1.49252000 0.38463100 0.00000000
C 0.54660000 -0.30978800 1.82419900
C 0.54660000 -0.30978800 -1.82419900
O 0.54660000 -0.79170100 2.88042500
O -2.65485400 0.42159000 0.00000000
O 0.54660000 -0.79170100 -2.88042500
Ru 0.33839000 0.24327700 0.00000000

$Os(CO)_3^-$

E = -430.757827 au

-1 2
C 1.54686500 0.51807800 0.00000000
C -0.41127500 -0.40331800 1.83988300
C -0.41127500 -0.40331800 -1.83988300
O -0.41127500 -0.88042500 2.90100800
O 2.69598100 0.71441900 0.00000000
O -0.41127500 -0.88042500 -2.90100800
Os -0.25438600 0.13293100 0.00000000

$Fe(CO)_3$

E = -1603.640680 au

0 3
Fe 0.00000000 0.00000000 0.27315300
C 0.00000000 1.81973800 0.71495900
C 0.00000000 -1.81973800 0.71495900
C 0.00000000 0.00000000 -1.57186600

O 0.00000000 -2.92850400 0.96606200
O 0.00000000 2.92850400 0.96606200
O 0.00000000 0.00000000 -2.71341000

$Ru(CO)_3$

E = -434.885449 au

0 3
C 0.00000000 1.95578200 0.60442600
C 0.00000000 -1.95578200 0.60442600
C 0.00000000 0.00000000 -1.60306700
O 0.00000000 -3.09002400 0.69388800
O 0.00000000 3.09002400 0.69388800
O 0.00000000 0.00000000 -2.74397000
Ru 0.00000000 0.00000000 0.30033700

$Os(CO)_3$

E = -430.663389 au

0 3
C 0.00000000 1.94836500 0.51768700
C 0.00000000 -1.94836500 0.51768700
C 0.00000000 0.00000000 -1.68093800
O 0.00000000 -3.07973500 0.66473900
O 0.00000000 3.07973500 0.66473900
O 0.00000000 0.00000000 -2.82544100
Os 0.00000000 0.00000000 0.20843500

$Co(CO)_3$

E = -1722.724964 au

0 2
C 0.00000000 1.83896900 0.00000000
C 1.59259400 -0.91948400 0.00000000
C -1.59259400 -0.91948400 0.00000000
O 2.57650000 -1.48754300 0.00000000
O 0.00000000 2.97508600 0.00000000
O -2.57650000 -1.48754300 0.00000000
Co 0.00000000 0.00000000 0.00000000

$Rh(CO)_3$ E = -450.585516 au 0 2 C 0.00000000 0.00000000 1.59641000 C 0.00000000 1.94682000 -0.59383600 C 0.00000000 -1.94682000 -0.59383600 O 0.00000000 3.07870000 -0.65356300 O 0.00000000 0.00000000 2.73212300 O 0.00000000 -3.07870000 -0.65356300 Rh 0.00000000 0.00000000 -0.30783100
$Ir(CO)_3$ E = -444.374972 au 0 2 C 0.00000000 0.00000000 -1.65668700 C 0.00000000 1.92656600 0.50821000 C 0.00000000 -1.92656600 0.50821000 O 0.00000000 3.05742300 0.62223600 O 0.00000000 0.00000000 -2.79642100 O 0.00000000 -3.05742300 0.62223600 Ir 0.00000000 0.00000000 0.21113300
$Ni(CO)_3^+$ E = -1848.021361 au 1 2 C 0.00000000 0.00000000 -1.67181300 C 0.00000000 1.89809300 0.72035200 C 0.00000000 -1.89809300 0.72035200 O 0.00000000 2.98253400 0.97687500 O 0.00000000 0.00000000 -2.78728300 O 0.00000000 -2.98253400 0.97687500 Ni 0.00000000 0.00000000 0.28767500
$Pd(CO)_3^+$ E = -467.640097 au 1 2 C 0.00000000 0.00000000 -1.76969300

C 0.00000000 -2.04732100 0.59161700
C 0.00000000 2.04732100 0.59161700
O 0.00000000 -3.15741500 0.69620900
O 0.00000000 0.00000000 -2.88506100
O 0.00000000 3.15741500 0.69620900
Pd 0.00000000 0.00000000 0.33608500

$Pt(CO)_3^+$

E = -459.077242 au

1 2
C 0.00000000 0.00000000 -1.79520800
C 0.00000000 -1.98616500 0.51361300
C 0.00000000 1.98616500 0.51361300
O 0.00000000 -3.09611900 0.63852400
O 0.00000000 0.00000000 -2.91250700
O 0.00000000 3.09611900 0.63852400
Pt 0.00000000 0.00000000 0.22681500

$Ni(CO)_3$

E = -1848.311358 au

0 1
C 0.00000000 1.81833200 0.00000000
C -1.57472100 -0.90916600 0.00000000
C 1.57472100 -0.90916600 0.00000000
O -2.55603200 -1.47572600 0.00000000
O 0.00000000 2.95145200 0.00000000
O 2.55603200 -1.47572600 0.00000000
Ni 0.00000000 0.00000000 0.00000000

$Pd(CO)_3$

E = -467.951358 au

0 1
C 0.00000000 2.01392300 0.00000000
C 1.74410900 -1.00696200 0.00000000
C -1.74410900 -1.00696200 0.00000000
O 2.72356400 -1.57245100 0.00000000
O 0.00000000 3.14490100 0.00000000
O -2.72356400 -1.57245100 0.00000000
Pd 0.00000000 0.00000000 0.00000000

$Pt(CO)_3$ E = -459.389146 au 0 1 C 1.70548900 0.98466400 0.00000000 C -1.70548900 0.98466400 0.00000000 C 0.00000000 -1.96932900 0.00000000 O -2.68696600 1.55132100 0.00000000 O 2.68696600 1.55132100 0.00000000 O 0.00000000 -3.10264200 0.00000000 Pt 0.00000000 0.00000000 0.00000000
$Ni(GaCp)_4^+$ E = -9981.321977 au 1 2 C -0.97265100 4.40943100 -1.14533200 C -1.79554200 4.54503000 0.00000000 C 0.35213500 4.18998400 -0.70602100 C -0.97265100 4.40943100 1.14533200 C 0.35213500 4.18998400 0.70602100 H -1.30153800 4.46718600 -2.17073800 H -2.85752700 4.73273600 0.00000000 H 1.21156600 4.04043000 -1.34092800 H -1.30153800 4.46718600 2.17073800 H 1.21156600 4.04043000 1.34092800 Ga -0.99189200 2.41898900 0.00000000 Ga -1.00117500 -1.17769100 -2.04900200 Ga 1.67879900 0.02014200 0.00000000 Ga -1.00117500 -1.17769100 2.04900200 C -1.08869200 -1.29391800 -4.33743500 C 0.26763100 -1.46781100 -3.98060100 C -1.82425800 -2.37821800 -3.79804400 C 0.37321600 -2.65546300 -3.22375900 C -0.91661300 -3.21989600 -3.10984900 H -1.49381000 -0.48276100 -4.92128100 H 1.07765800 -0.80313300 -4.23750000 H -2.88501300 -2.54085600 -3.90483000 H 1.27901100 -3.05847400 -2.79745700 H -1.16836100 -4.13165900 -2.59189000 C -1.08869200 -1.29391800 4.33743500 C 0.26763100 -1.46781100 3.98060100

C -1.82425800 -2.37821800 3.79804400
C 0.37321600 -2.65546300 3.22375900
C -0.91661300 -3.21989600 3.10984900
H -1.49381000 -0.48276100 4.92128100
H 1.07765800 -0.80313300 4.23750000
H -2.88501300 -2.54085600 3.90483000
H 1.27901100 -3.05847400 2.79745700
H -1.16836100 -4.13165900 2.59189000
C 3.67896000 0.92601200 -0.70731600
C 3.63655700 -0.41844500 -1.14400500
C 3.67896000 0.92601200 0.70731600
C 3.60941900 -1.24939000 0.00000000
C 3.63655700 -0.41844500 1.14400500
H 3.71168500 1.79775500 -1.34173700
H 3.63067300 -0.75138200 -2.17007000
H 3.71168500 1.79775500 1.34173700
H 3.57672500 -2.32773900 0.00000000
H 3.63067300 -0.75138200 2.17007000
Ni -0.75081800 0.03752200 0.00000000

$Pd(GaCp)_4^+$

E = -8600.972544 au

1 2
C -0.93670500 4.52910900 1.14593200
C -1.76211600 4.65432500 0.00000000
C 0.38978900 4.32876200 0.70593600
C -0.93670500 4.52910900 -1.14593200
C 0.38978900 4.32876200 -0.70593600
H -1.26644900 4.58275100 2.17126600
H -2.82624500 4.82950100 0.00000000
H 1.25107800 4.19519200 1.34181100
H -1.26644900 4.58275100 -2.17126600
H 1.25107800 4.19519200 -1.34181100
Ga -0.95143100 2.53320300 0.00000000
Ga -0.87143100 -1.29262600 2.11087200
Ga 1.54966000 0.17622500 0.00000000
Ga -0.87143100 -1.29262600 -2.11087200
C -0.91423700 -1.58732100 4.39277100
C 0.44928600 -1.61214400 4.02571600
C -1.55062900 -2.69641800 3.78035500
C 0.65803100 -2.73078100 3.18974800
C -0.57406600 -3.40161600 3.03681400

H -1.38822600 -0.85978300 5.03231600
H 1.19667300 -0.89707100 4.33239600
H -2.59119800 -2.96301400 3.87651000
H 1.59495400 -3.02312000 2.74094400
H -0.74469200 -4.29493200 2.45727600
C -0.91423700 -1.58732100 -4.39277100
C 0.44928600 -1.61214400 -4.02571600
C -1.55062900 -2.69641800 -3.78035500
C 0.65803100 -2.73078100 -3.18974800
C -0.57406600 -3.40161600 -3.03681400
H -1.38822600 -0.85978300 -5.03231600
H 1.19667300 -0.89707100 -4.33239600
H -2.59119800 -2.96301400 -3.87651000
H 1.59495400 -3.02312000 -2.74094400
H -0.74469200 -4.29493200 -2.45727600
C 3.49249000 1.13636500 0.70846200
C 3.48771500 -0.21062300 1.14549300
C 3.49249000 1.13636500 -0.70846200
C 3.48330600 -1.04297200 0.00000000
C 3.48771500 -0.21062300 -1.14549300
H 3.49849200 2.00827100 1.34318600
H 3.48628400 -0.54313600 2.17149700
H 3.49849200 2.00827100 -1.34318600
H 3.47400100 -2.12179600 0.00000000
H 3.48628400 -0.54313600 -2.17149700
Pd -0.86054700 0.05000800 0.00000000

$Pt(GaCp)_4^+$

E = -8592.402781 au

C 0.89420200 4.47703800 -1.14629000
C 1.72330400 4.57825900 0.00000000
C -0.43733200 4.31266700 -0.70617500
C 0.89420200 4.47703800 1.14629000
C -0.43733200 4.31266700 0.70617500
H 1.22559900 4.51952700 -2.17156100
H 2.79186800 4.72382500 0.00000000
H -1.30184100 4.19964900 -1.34162000
H 1.22559900 4.51952700 2.17156100
H -1.30184100 4.19964900 1.34162000
Ga 0.85497200 2.49145900 0.00000000
Ga 0.82139800 -1.25812300 -2.11207600
Pt 0.70404500 0.02760800 0.00000000

Ga -1.70828200 0.10029300 0.00000000
Ga 0.82139800 -1.25812300 2.11207600
C 0.90546200 -1.43430500 -4.39315500
C -0.45772500 -1.56309900 -4.04689900
C 1.60596200 -2.52674300 -3.81976400
C -0.60365800 -2.72931100 -3.26358000
C 0.66725900 -3.32678900 -3.12261900
H 1.33927400 -0.64893800 -4.99136900
H -1.24582100 -0.88222600 -4.32834100
H 2.66245500 -2.72208900 -3.91307900
H -1.52427700 -3.09772900 -2.83778700
H 0.88877600 -4.23128500 -2.57887800
C 0.90546200 -1.43430500 4.39315500
C -0.45772500 -1.56309900 4.04689900
C 1.60596200 -2.52674300 3.81976400
C -0.60365800 -2.72931100 3.26358000
C 0.66725900 -3.32678900 3.12261900
H 1.33927400 -0.64893800 4.99136900
H -1.24582100 -0.88222600 4.32834100
H 2.66245500 -2.72208900 3.91307900
H -1.52427700 -3.09772900 2.83778700
H 0.88877600 -4.23128500 2.57887800
C -3.65281400 1.04693700 -0.70851400
C -3.63955200 -0.30028500 -1.14562500
C -3.65281400 1.04693700 0.70851400
C -3.63018900 -1.13260200 0.00000000
C -3.63955200 -0.30028500 1.14562500
H -3.66272800 1.91897000 -1.34303400
H -3.63543600 -0.63283200 -2.17163100
H -3.66272800 1.91897000 1.34303400
H -3.61373300 -2.21125900 0.00000000
H -3.63543600 -0.63283200 2.17163100

$Ni(GaCp)_4$

E = -9981.516818 au

0 1
C 0.96430300 4.37446400 1.14290200
C 1.78360500 4.52483200 0.00000000
C -0.35341700 4.13267500 0.70388000
C 0.96430300 4.37446400 -1.14290200
C -0.35341700 4.13267500 -0.70388000
H 1.29266900 4.43053900 2.16888000

H 2.84293700 4.72837500 0.00000000
H -1.20800700 3.94874100 1.33701100
H 1.29266900 4.43053900 -2.16888000
H -1.20800700 3.94874100 -1.33701100
Ga 1.06614700 2.28544500 0.00000000
Ga 1.06888300 -1.10899000 1.92988800
Ga -1.68011800 0.02187000 0.00000000
Ga 1.06888300 -1.10899000 -1.92988800
C 1.08646500 -1.25772300 4.30727600
C -0.25923800 -1.45205700 3.93321000
C 1.84273500 -2.33364100 3.78787200
C -0.33847200 -2.64256600 3.18540100
C 0.95751600 -3.18980100 3.09330200
H 1.47309800 -0.43257200 4.88454900
H -1.08000900 -0.78828900 4.15784100
H 2.90478800 -2.47971700 3.90748400
H -1.23084300 -3.04943400 2.73427000
H 1.22879400 -4.09820200 2.57868400
C 1.08646500 -1.25772300 -4.30727600
C -0.25923800 -1.45205700 -3.93321000
C 1.84273500 -2.33364100 -3.78787200
C -0.33847200 -2.64256600 -3.18540100
C 0.95751600 -3.18980100 -3.09330200
H 1.47309800 -0.43257200 -4.88454900
H -1.08000900 -0.78828900 -4.15784100
H 2.90478800 -2.47971700 -3.90748400
H -1.23084300 -3.04943400 -2.73427000
H 1.22879400 -4.09820200 -2.57868400
C -3.79738400 0.90216400 0.70573900
C -3.74120200 -0.43889500 1.14174500
C -3.79738400 0.90216400 -0.70573900
C -3.70582100 -1.26753100 0.00000000
C -3.74120200 -0.43889500 -1.14174500
H -3.82824700 1.77473000 1.33968200
H -3.72044200 -0.77206200 2.16793100
H -3.82824700 1.77473000 -1.33968200
H -3.65128900 -2.34528800 0.00000000
H -3.72044200 -0.77206200 -2.16793100
Ni 0.61088500 0.03931500 0.00000000

$Pd(GaCp)_4$

E = -8601.204433 au

0 1
C 0.35112800 5.06348600 -1.14171000
C 1.18064300 5.07398800 0.00000000
C -0.99087500 5.04645700 -0.70561000
C 0.35112800 5.06348600 1.14171000
C -0.99087500 5.04645700 0.70561000
H 0.68460700 5.05940300 -2.16757700
H 2.25934300 5.07929500 0.00000000
H -1.86343400 5.02713900 -1.33955600
H 0.68460700 5.05940300 2.16757700
H -1.86343400 5.02713900 1.33955600
Ga 0.00736200 2.99374500 0.00000000
Ga 1.12647200 -0.60858100 -1.90113900
Ga -2.14736800 -0.63677200 0.00000000
Ga 1.12647200 -0.60858100 1.90113900
C 1.51104900 -1.62486400 -4.03126800
C 0.55553200 -2.43426600 -3.38034000
C 2.71973600 -1.70920900 -3.30435000
C 1.17154800 -3.01752200 -2.25535100
C 2.50691900 -2.57055500 -2.20670900
H 1.34829100 -1.04552400 -4.92657400
H -0.46957600 -2.57356000 -3.68674000
H 3.64244600 -1.20581400 -3.54704200
H 0.69776100 -3.67637500 -1.54381900
H 3.23772000 -2.83387300 -1.45793700
C 1.51104900 -1.62486400 4.03126800
C 0.55553200 -2.43426600 3.38034000
C 2.71973600 -1.70920900 3.30435000
C 1.17154800 -3.01752200 2.25535100
C 2.50691900 -2.57055500 2.20670900
H 1.34829100 -1.04552400 4.92657400
H -0.46957600 -2.57356000 3.68674000
H 3.64244600 -1.20581400 3.54704200
H 0.69776100 -3.67637500 1.54381900
H 3.23772000 -2.83387300 1.45793700
C -4.23009000 -1.57828300 -0.70633700
C -3.22777800 -2.47191100 -1.14079700
C -4.23009000 -1.57828300 0.70633700
C -2.61053300 -3.02290600 0.00000000
C -3.22777800 -2.47191100 1.14079700
H -4.88170100 -0.99802600 -1.34067600
H -2.97411400 -2.68904900 -2.16679500
H -4.88170100 -0.99802600 1.34067600
H -1.79761200 -3.73257800 0.00000000
H -2.97411400 -2.68904900 2.16679500

Pd 0.02970600 0.53139100 0.00000000

$Pt(GaCp)_4$

E = -8592.626254 au

0 1
C -0.37913700 4.93718500 1.14214900
C -1.20899400 4.93824700 0.00000000
C 0.96350300 4.93543100 0.70586000
C -0.37913700 4.93718500 -1.14214900
C 0.96350300 4.93543100 -0.70586000
H -0.71232900 4.92642300 2.16794900
H -2.28756200 4.92853700 0.00000000
H 1.83595100 4.92274400 1.33996300
H -0.71232900 4.92642300 -2.16794900
H 1.83595100 4.92274400 -1.33996300
Ga -0.01142900 2.88884400 0.00000000
Ga -1.09644900 -0.66015800 1.89705100
Pt -0.00760300 0.44568700 0.00000000
Ga 2.18787800 -0.64321100 0.00000000
Ga -1.09644900 -0.66015800 -1.89705100
C -1.55837500 -1.58359300 4.02683200
C -0.62640600 -2.46073100 3.43000200
C -2.75500900 -1.64436800 3.27452000
C -1.24365800 -3.06047000 2.31478400
C -2.55609000 -2.55855000 2.21729800
H -1.39040500 -0.97819700 4.90367500
H 0.38520500 -2.63046900 3.76427800
H -3.65974100 -1.09277300 3.47645100
H -0.78225800 -3.76244900 1.63720200
H -3.27985400 -2.81589200 1.45973000
C -1.55837500 -1.58359300 -4.02683200
C -0.62640600 -2.46073100 -3.43000200
C -2.75500900 -1.64436800 -3.27452000
C -1.24365800 -3.06047000 -2.31478400
C -2.55609000 -2.55855000 -2.21729800
H -1.39040500 -0.97819700 -4.90367500
H 0.38520500 -2.63046900 -3.76427800
H -3.65974100 -1.09277300 -3.47645100
H -0.78225800 -3.76244900 -1.63720200
H -3.27985400 -2.81589200 -1.45973000
C 4.25000800 -1.56891400 0.70740700
C 3.26162900 -2.47941300 1.14067100

C 4.25000800 -1.56891400 -0.70740700
C 2.65382800 -3.03924200 0.00000000
C 3.26162900 -2.47941300 -1.14067100
H 4.89455800 -0.98070800 1.34155400
H 3.00827200 -2.69674300 2.16661400
H 4.89455800 -0.98070800 -1.34155400
H 1.84520500 -3.75378400 0.00000000
H 3.00827200 -2.69674300 -2.16661400

$Pt(PMe_3)_3^+$

E = -1502.421668 au

1 2
Pt 0.33799400 0.03845800 0.00000000
P -1.99369400 0.00610100 0.00000000
C -2.62987100 -1.69335900 0.00000000
C -2.84096200 0.77769000 1.40979700
C -2.84096200 0.77769000 -1.40979700
P 0.81001500 -0.00227600 2.29340600
C 0.03829700 -1.33515600 3.25795100
C 2.58035500 -0.24536500 2.62193800
C 0.42106400 1.49259300 3.24745500
P 0.81001500 -0.00227600 -2.29340600
C 0.03829700 -1.33515600 -3.25795100
C 0.42106400 1.49259300 -3.24745500
C 2.58035500 -0.24536500 -2.62193800
H -2.26920000 -2.22184600 0.88230200
H -3.72173600 -1.69652600 0.00000000
H -2.26920000 -2.22184600 -0.88230200
H -2.58409000 1.83570300 1.46075000
H -3.92327000 0.68056500 1.30280100
H -2.53822300 0.29918400 2.34109900
H -2.53822300 0.29918400 -2.34109900
H -3.92327000 0.68056500 -1.30280100
H -2.58409000 1.83570300 -1.46075000
H 0.28820600 -2.29914100 2.81527500
H 0.39239100 -1.31454300 4.29010600
H -1.04653700 -1.22741900 3.25879500
H 3.15000800 0.56566400 2.16921300
H 2.77554300 -0.26641200 3.69642200
H 2.90871700 -1.18477400 2.17831300
H -0.65150100 1.68283700 3.23650900
H 0.75022300 1.37811900 4.28177800

H 0.92639800 2.35038600 2.80523400
H 0.39239100 -1.31454300 -4.29010600
H 0.28820600 -2.29914100 -2.81527500
H -1.04653700 -1.22741900 -3.25879500
H 0.75022300 1.37811900 -4.28177800
H -0.65150100 1.68283700 -3.23650900
H 0.92639800 2.35038600 -2.80523400
H 2.90871700 -1.18477400 -2.17831300
H 2.77554300 -0.26641200 -3.69642200
H 3.15000800 0.56566400 -2.16921300

$Pt(PMe_3)_3$

E = -1502.609123 au

0 1
Pt -0.05921800 -0.06266800 0.00000000
P 2.24851600 -0.01660100 0.00000000
C 2.90327400 1.69401100 0.00000000
C 3.20424100 -0.72151300 1.39971400
C 3.20424100 -0.72151300 -1.39971400
P -1.11991500 0.00532200 2.04866800
C -0.63070600 1.39525900 3.13953100
C -2.94649300 0.14711000 2.17384600
C -0.84328800 -1.40877700 3.18070700
P -1.11991500 0.00532200 -2.04866800
C -0.63070600 1.39525900 -3.13953100
C -0.84328800 -1.40877700 -3.18070700
C -2.94649300 0.14711000 -2.17384600
H 2.53446400 2.21891100 0.88204100
H 3.99645400 1.70835600 0.00000000
H 2.53446400 2.21891100 -0.88204100
H 2.99356300 -1.78813700 1.48264100
H 4.28166700 -0.57657400 1.28023800
H 2.87649900 -0.24235400 2.32368900
H 2.87649900 -0.24235400 -2.32368900
H 4.28166700 -0.57657400 -1.28023800
H 2.99356300 -1.78813700 -1.48264100
H -0.83076400 2.34009700 2.63377900
H -1.16840700 1.37595900 4.09128600
H 0.44213400 1.33607600 3.32885300
H -3.40339600 -0.70823200 1.67478000
H -3.29236300 0.18818300 3.21070600
H -3.26769900 1.04850300 1.65048500

H 0.22701600 -1.51677600 3.35974000
H -1.35935900 -1.27023300 4.13449500
H -1.19958300 -2.32539700 2.71075400
H -1.16840700 1.37595900 -4.09128600
H -0.83076400 2.34009700 -2.63377900
H 0.44213400 1.33607600 -3.32885300
H -1.35935900 -1.27023300 -4.13449500
H 0.22701600 -1.51677600 -3.35974000
H -1.19958300 -2.32539700 -2.71075400
H -3.26769900 1.04850300 -1.65048500
H -3.29236300 0.18818300 -3.21070600
H -3.40339600 -0.70823200 -1.67478000