Supporting Information

for

Effect of Distal Metal Species on Lewis Basicity of a μ3-Oxo Ligand

in Doubly Oxo-bridged (μ3-O)[Rh(cod)]3(μ4-O)M Core

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1. General procedure

General. All manipulations involving air- and moisture-sensitive compounds were carried out under an argon atmosphere by using standard vacuum line and Schlenk tube techniques or Ar-filled glovebox. C_6D_6, and THF-d_8 were distilled under an argon atmosphere over CaH_2. Toluene, THF, and hexane were dried and deoxygenated by using Grubbs column (Glass Counter Solvent Dispending System, Nikko Hansen & Co, Ltd.). [Rh(OH)(cod)]$_2$, and AuCl(PPh$_3$) were synthesized according to the literature procedure.[1] All other reagents were purchased at the highest commercial quality and used without further purification. ^{1}H NMR (400 MHz), ^{13}C{^{1}H} NMR (100 MHz), and ^{31}P{^{1}H} NMR (162 MHz) spectra were measured on a Bruker Advance III-400 spectrometer in 5 mm NMR tubes. All ^{1}H NMR chemical shifts were reported in ppm relative to the residual solvent protons in C_6D_6 at δ 7.16 and THF-d_8 at δ 1.76. All ^{13}C{^{1}H} NMR chemical shifts were reported in ppm relative to carbon resonance of the solvent itself in C_6D_6 at δ 128.06 and THF-d_8 at δ 25.31. All melting points were recorded on BUCHI melting point M-565. Elemental analyses were recorded by using Perkin-Elmer 2400 at the Faculty of Engineering Science, Osaka University.

Computational Details. Geometry optimizations were performed using Gaussian16 program revision C.01,[2] without any symmetry constraints. Calculations were running using the unrestricted B3LYP functional,[3] corrected for dispersion a proposed by Grimme (D3 correction with Becke-Johnson damping),[4] at the 6-31+G(d) basis set[5] for C, H, O, P, N, and Li, and SDD[6] for Rh and Au with a frequency calculation, and the SMD solvation model (THF)[7] is used for complexes **1-3** and ($μ_3$-O){Rh(cod)}$_3$($μ_4$-O)Li(THF)$_3$. Thermodynamic corrections were calculated with frequency analysis to be either minima (with no imaginary frequencies) or transition states (with one imaginary frequency) at 298.15 K. The electronic energies, free energies, and cartesian coordinates are listed in the following section.

X-ray Diffraction Study. All crystals were mounted on the CryoLoop (Hampton Research Corp.) with a layer of light mineral oil and placed in a nitrogen stream at 113(1) K. Measurements were made on a Rigaku XtaLAB P200 diffractometer using multi-layer mirror monochromated Mo-Ka (0.71075 Å) radiation. Crystal data and structure refinement parameters were listed in Table S1. The structure was solved by SHELXT Version 2014/5[8] and refined on F^2 by full matrix least-squares method using SHELXL-2016/4[9] in the CrystalStructure 4.2.4 program.[10] Non-hydrogen atoms were anisotropically refined. H-atoms were included in the refinement on calculated positions riding on their carrier atoms. The function minimized was [$Σw(Fo^2- Fc^2)^2$] (w = 1 / [$σ^2$(Fo^2) + (aP)^2 + bP]), where P = (Max(Fo^2,0) + 2Fc^2) / 3 with $σ^2$(Fo^2) from counting

statistics. The function $R1$ and $wR2$ were $(\Sigma||Fo| - |Fc||) / \Sigma|Fo|$ and $[\Sigma w(Fo^2 - Fc^2)^2 / \Sigma(wFo^4)]^{1/2}$, respectively. The Mercury 2020.3.0 program was used to draw the molecule.[11]

2. Synthesis of multi-metallic complexes

Synthesis of Rh$_3$Au complex 1.

To a solution of Au[N(SiMe$_3$)$_2$](PPh$_3$) (2.10 g, 3.39 mmol) in THF (25 mL) was added a suspension of [Rh(OH)(cod)]$_2$ (1.54 g, 3.38 mmol) in THF (25 mL). After stirring at room temperature for 2 h under dark, the reaction mixture was concentrated to ca. 15 mL. Hexane (55 mL) was added and yellow powder was precipitated. The supernatant was removed and the yellow solid was washed with hexane (50 mL x 3). All volatiles were removed under reduced pressure to give yellow solid of **1** in 97% yield (2.46 g, 2.19 mmol). Mp. 153-160 °C (dec.). ^{1}H NMR (400 MHz, THF-d_8, 303 K) δ 7.48 (overlapping m, 9H, Ar), 7.33 (m, 6H, Ar), 3.71 (br s, 12H, =CH of cod), 2.57 (m, 12H, CH$_2$ of cod), 1.91 (m, 12H, CH$_2$ of cod). ^{1}H NMR (400 MHz, C$_6$D$_6$, 303 K) δ 7.23 (m, 6H, Ar), 6.87 (overlapping m, 9H, Ar), 34.26 (br s, 12H, =CH of cod), 2.79 (m, 12H, CH$_2$ of cod), 2.07 (m, 12H, CH$_2$ of cod). ^{13}C{^{1}H} NMR (100 MHz, THF-d_8, 303 K) δ 134.6 (d, J_{PC} = 13.4 Hz, Ar), 132.4. (Ar), 129.8 (d, J_{PC} = 11.7 Hz, Ar), 72.1 (d, J_{RhC} = 14.7 Hz, cod), 32.5(s, cod). ^{13}C{^{1}H} NMR (100 MHz, C$_6$D$_6$, 303 K) δ 134.1 (d, J_{PC} = 14.2 Hz, Ar), 131.8. (br s, Ar), 130.0 (s, Ar), 129.2 (s, Ar) 72.3 (d, J_{RhC} = 13.3 Hz, cod), 32.5(s, cod). ^{31}P{^{1}H} NMR (162 MHz, THF-d_8, 303 K) δ 22.6 (s). ^{31}P{^{1}H} NMR (162 MHz, C$_6$D$_6$, 303 K) δ 22.6 (s). Anal. calcd. for C$_{42}$H$_{51}$O$_2$PAuRh$_3$(OC$_4$H$_8$): C, 46.17; H, 4.97. Found: C, 46.19 H, 4.80 N, 0.05.

Synthesis of Rh$_3$Au$_2$ complex 2.

To a solution of AuCl(PPh$_3$) (220.0 mg, 0.444 mmol) in THF (9 mL) was added a solution of AgBF$_4$ (86.6 mg, 0.444 mmol) in THF (2 mL). White precipitate was removed by filtration through glass filter, and the filtrate containing [Au(PPh$_3$)][BF$_4$] was added to a suspension of **1** (500 mg, 0.444 mmol) in THF (2 mL). The reaction mixture was stirred at room temperature for 1 h under dark, and then resulting yellow suspension was centrifuged to give yellow solid. The yellow solid was washed with THF (1 mL) and hexane (2 mL x 3), and dried under reduced pressure to give yellow powder of **2** in 84% yield (619 mg, 0.371 mmol). Mp. 126-133 °C (dec.). ^{1}H NMR (400 MHz, THF-d_8, 303 K) δ 7.60 (m, 6H, Ar), 7.53 (m, 12H, Ar), 7.34 (m, 12H, Ar), 4.18 (br, 12H, =CH of cod), 2.75 (m, 12H, CH$_2$ of cod), 2.06 (m, 12H, CH$_2$ of cod). ^{13}C{^{1}H} NMR (400 MHz, THF-d_8, 303 K) δ 134.5 (d, J_{PC} = 13.5 Hz, Ar), 131.2 (d, J_{PC} = 357.2 Hz, Ar), 130.1 (d, J_{PC} = 12.9 Hz, Ar), 129.0 (d, J_{PC}= 73.7 Hz, Ar), 75.6 (d, J_{RhC} = 14.0 Hz, cod), 32.1 (s, cod).

$^{31}P\{^1H\}$ NMR (162 MHz, THF-d_8, 303 K) δ 23.1 (s). Anal. calcd. for $C_{60}H_{66}O_2P_2BF_4Au_2Rh_3$: C, 43.14; H, 3.98. Found: C, 42.83 H, 3.83 N, 0.05.

**Elimination of AuCl(PPh₃) from a mixture of 2 and Et₄NCl.**

To a brown THF suspension (5 mL) of Rh₃Au₂ (99.9 mg, 59.8 µmol) was added a THF suspension (15 mL) of Et₄NCl (29.7 mg, 179.5 µmol, 3.0 equiv.), giving a yellow-brown suspension. Excess amounts of Et₄NCl were necessary for the quantitative conversion. After stirring for 2 hours, the yellow suspension was centrifuged. The yellow supernatant was concentrated to ca. 5 mL, resulted in a yellow suspension. Further addition of acetonitrile (12 mL) afforded yellow precipitates, and the precipitates were washed with hexane (5 mL x 2) and dried to give Rh₃Au complex **1** in 62% yield (41.6 mg) as a yellow powder. The ^1H NMR data was superimposed to the above-isolated sample.

Elimination of Au[N(SiMe₃)₂](PPh₃) from a mixture of 1 and Li[N(SiMe₃)₂].

To a yellow powder of Rh₃Au complex **1** (10.0 mg, 8.89 µmol) was added a solution of LiN(SiMe₃)₂ (1.5 mg, 8.96 µmol, 1.0 equiv.) in THF-d_8 (0.5 mL) to form a yellow suspension. $^{31}P\{^1H\}$ NMR measurements showed a peak at 33.2 ppm assignable to Au[N(SiMe₃)₂](PPh₃).

3. NMR spectra of a mixture of 1 and LiBF₄

Upon addition of LiBF₄ to **1** in THF-d_8, resonances for the COD ligands of **1** shifted to the lower magnetic field due to the interaction of Li⁺ to the μ₃-oxo ligand of **1** to form Li-interacted species **3**. Gradual downfield shift of the COD ligands by increasing the amount of LiBF₄ is reasonable to the equilibrium between **1** and **3**. In this reaction, **2** was also formed after dissociation of [Au(PPh₃)][BF₄] from **3** and subsequent complexation with remaining **1** (Scheme S1).
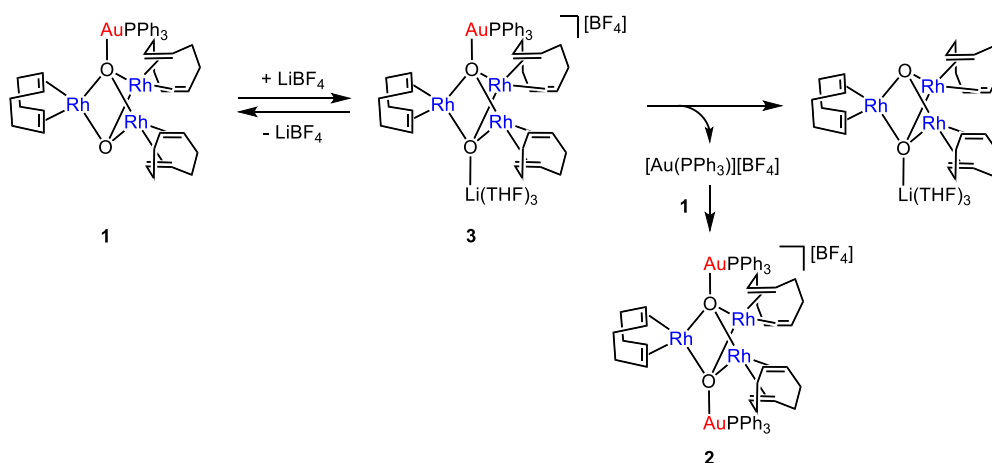
Scheme S1. Overall Description for the Reactivity of **1** with LiBF₄

Experimental details: To a yellow powder of **1** (10.0 mg, 8.89 µmol) was added a THF-d_8 suspension of LiBF$_4$ (1 equiv. = 0.8 mg, 8.5 µmol; 2 equiv. = 1.7 mg, 18.1 µmol; 5 equiv. = 4.1 mg, 44 µmol; 10 equiv. = 8.3 mg, 89 µmol). The addition of 1-5 equiv. of LiBF$_4$ resulted in suspension with a large amount of undissolved yellow powder of **1**, while the addition of 10 equiv. of LiBF$_4$ resulted in disappearance of **1**. $^{31}P\{^1H\}$ and ^1H NMR spectra were measured after 1 hour, showing signals for the COD ligand shifted to lower magnetic fields with increasing the amount of LiBF$_4$ (Figure S1).
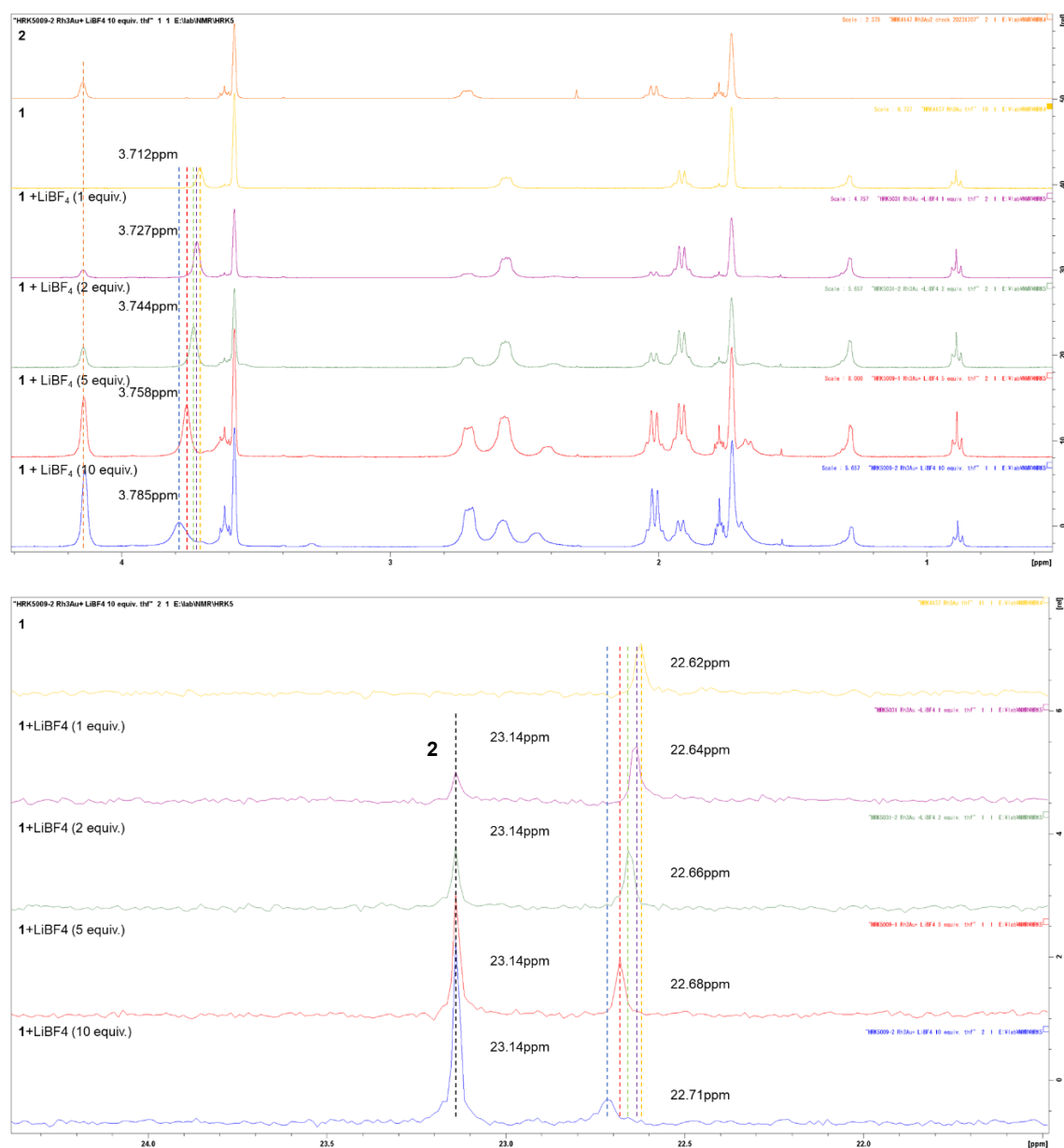
Figure S1. ^1H NMR spectra of a mixture of complex **1** and LiBF$_4$ in THF-d_8.

4. X-Ray crystallographic analysis

Table S1. Crystal data and data collection parameters of Rh_3Au complex **1**

empirical formula	$C_{42}H_{51}O_2PAuRh_3(C_6H_6)$
formula weight	1202.63
crystal system	Monoclinic
space group	$P2_1/n$ (#14)
a, Å	9.4939(5)
b, Å	23.9667(15)
c, Å	18.8664(11)
α, deg.	-
β, deg.	97.2108(13)
γ, deg.	-
V, Å^3	4258.9(4)
Z	4
D_{calcd}, g/cm^3	1.875
μ [Mo-$K\alpha$], mm^{-1}	4.662
T, K	113
crystal size, mm	0.240 x 0.200 x 0.200
θ range for data collection (deg.)	
no. of reflections measured	28557
unique data (Rint)	9613 (0.0170)
data / restraints / parameters	9613/0/496
$R1$ (I > 2.0σ(I))	0.0145
$wR2$ (I > 2.0σ(I))	0.0350
$R1$ (all data)	0.0160
$wR2$ (all data)	0.0350
GOF on F^2	1.067
$\Delta\rho$, e Å $^{-3}$	0.80, -0.80

a) $R1 = (\Sigma||Fo| - |Fc||)/\Sigma|Fo|$ b) $wR2 = [\Sigma w(Fo^2 - Fc^2)^2/\Sigma(wFo^4)]^{1/2}$

Table S2. Crystal data and data collection parameters of Rh_3Au_2 complex **2**

	2
empirical formula	$C_{60}H_{66}O_2P_2BF_4Au_2Rh_3(C_6H_6)_{0.5}$
formula weight	1709.64
crystal system	Triclinic
space group	$P\bar{1}$ (#2)
a, Å	12.8050(13)
b, Å	15.7979(17)
c, Å	16.7992(17)
α, deg.	106.2944(10)
β, deg.	101.4607(11)
γ, deg.	107.842(2)
V, Å^3	2950.4(5)
Z	2
D_{calcd}, g/cm^3	1.924
μ [Mo-$K\alpha$], mm^{-1}	5.902
T, K	113
crystal size, mm	0.140 x 0.130 x 0.100
θ range for data collection (deg.)	
no. of reflections measured	42648
unique data (Rint)	13368(0.0523)
data / restraints / parameters	13368/0/694
$R1$ (I > 2.0σ(I))	0.0298
$wR2$ (I > 2.0σ(I))	0.0761
$R1$ (all data)	0.0352
$wR2$ (all data)	0.0782
GOF on F^2	1.045
$\Delta\rho$, e Å^{-3}	2.23, -2.65

a) $R1 = (\Sigma||Fo| - |Fc||)/\Sigma|Fo|$ b) $wR2 = [\Sigma w(Fo^2 - Fc^2)^2/\Sigma(wFo^4)]^{1/2}$

5. DFT calculation
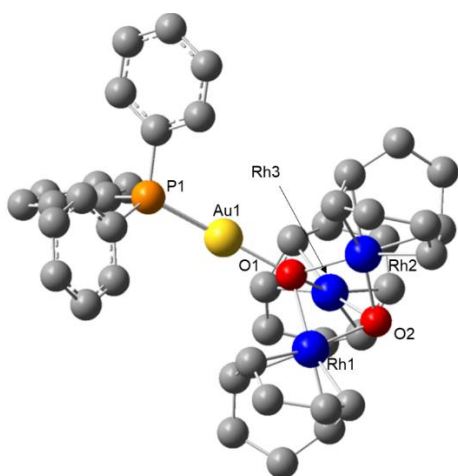
Figure S2. Optimized structure of **1**.
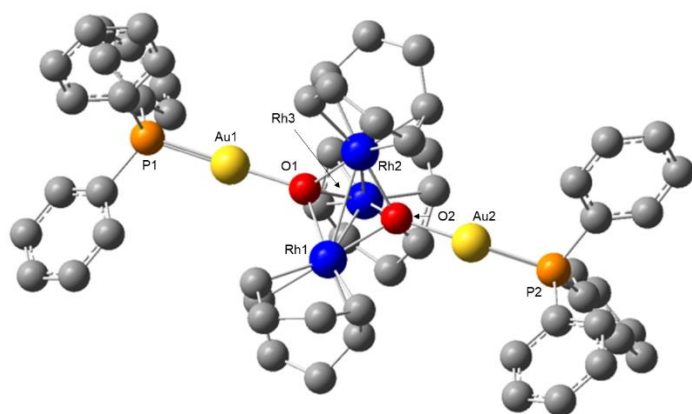
Figure S3. Optimized structure of **2**.
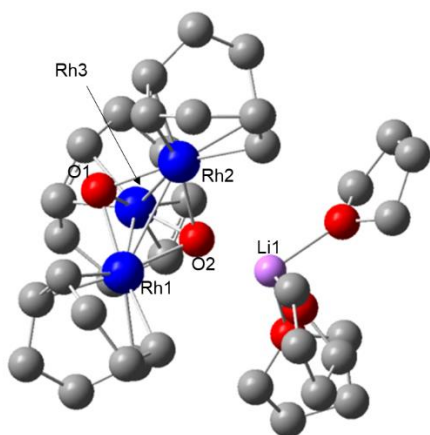
Figure S4. Optimized structure of $(\mu_3\text{-O})\{Rh(cod)\}_3(\mu_4\text{-O})Li(THF)_3$.
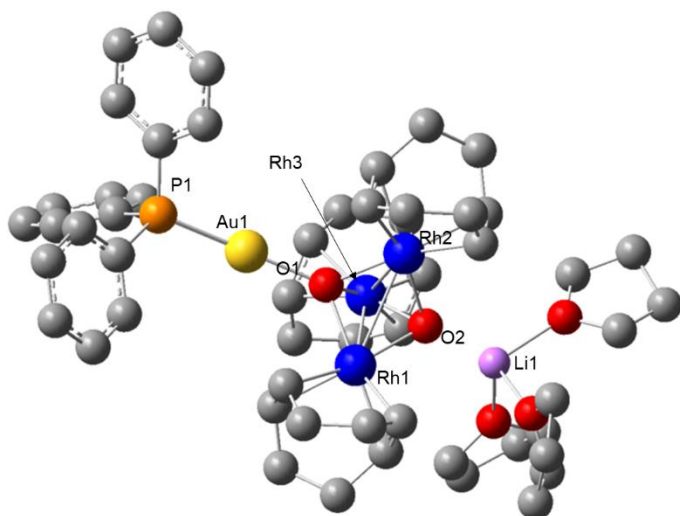
Figure S5. Optimized structure of **3**.

Table S3. Selected geometries for the optimized molecular structures.

	1 M^1 = AuPPh$_3$	2 M^1 = M^2 = AuPPh$_3$	3 M^1 = AuPPh$_3$ M^2 = Li(THF)$_3$	M^2 = Li(THF)$_3$
Rh1 – O1	2.09596	2.09666	2.07637	2.03803
Rh2 – O1	2.09754	2.09573	2.09068	2.04122
Rh3 – O1	2.09260	2.09393	2.07123	2.05932
Rh1 – O2	2.06166	2.09543	2.10704	2.11493
Rh2 – O2	2.06100	2.09103	2.08427	2.10597
Rh3 – O2	2.06018	2.09959	2.11479	2.08109
Rh1 – Rh2	2.84212	2.91073	2.85745	2.85213
Rh1 – Rh3	2.85230	2.88597	2.89564	2.81594
Rh2 – Rh3	2.85235	2.89891	2.86592	2.80991
M^1 – O1	2.03853	2.04940	2.05130	—
M^2 – O2	—	2.04900	1.85819	1.84184
O1 – O2	2.53998	2.52193	2.54518	2.55789
M^1 – O1 – O2	178.39620	178.90168	179.54337	171.52276
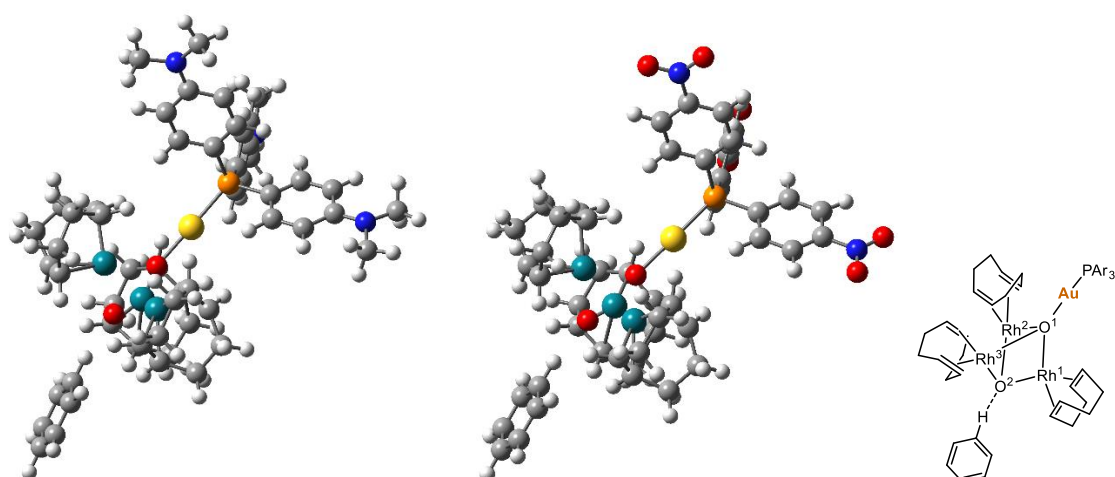
Figure S6. Molecular structures of **1-C₆H₆** with P(4-MeOC₆H₄)₃ (left) and P(4-NO₂C₆H₄)₃ (right) ligands on the gold(I) center.

Table S4 Selected parameters for the C-H···O interaction.

	L = PPh₃	L = P(4-NMe₂OC₆H₄)₃	L = P(4-NO₂C₆H₄)₃
Rh1 – O1	2.10435	2.09963	2.10829
Rh2 – O1	2.10006	2.09542	2.10414
Rh3 – O1	2.10387	2.10007	2.10958
Rh1 – O2	2.05110	2.05216	2.05096
Rh2 – O2	2.05307	2.05409	2.05263
Rh3 – O2	2.04989	2.05079	2.04860
Rh1 – Rh2	2.86391	2.86197	2.86828
Rh1 – Rh3	2.84261	2.83924	2.84604
Rh2 – Rh3	2.84376	2.84118	2.84745
Au – O1	2.01442	2.02556	1.99892
Au – P1	2.26293	2.26772	2.25534
O1 – O2	2.53400	2.53253	2.53453
H – O2	2.04682	2.03931	2.05938
C – H	1.09086	1.09117	1.09035
C – H – O2	172.63881	173.06935	171.97504
donor-acceptor interaction	6.09	6.27	5.75

6. Cartesian Coordinates of Optimized Structures

Function: B3LYP(GD3BJ)
Basis set: SDD for Rh, Au and 6-31G(d) for H, C, O, P
Solvent: THF (SMD)

Rh₃Au complex 1

Energy	-2590.1307		
Enthalpy	-2590.1298		
Free energy	-2590.268		
Au	3.78875259	3.10072870	3.64646001
Rh	4.13160966	-0.49243653	4.63502371
Rh	6.35872929	0.47459618	3.13813320
Rh	6.06623382	1.20075769	5.87030356
P	2.68592639	4.98418561	3.04144118
O	4.82379589	1.43349648	4.19840785
O	6.17361732	-0.60609304	4.88329036
C	2.11955091	0.04873441	5.06062002
H	2.10697599	1.13086304	5.20749446
C	2.18545085	-0.40987062	3.72797617
H	2.23692133	0.35176430	2.94868429
C	1.70377818	-1.78477264	3.27334015
H	1.29481903	-1.70680687	2.25875960
H	0.87574455	-2.11715032	3.90930969
C	2.84186431	-2.83072668	3.28174122
H	2.42744740	-3.84869474	3.37296360
H	3.36201206	-2.79449153	2.31680739
C	3.87984961	-2.56910372	4.35957649
H	4.86813076	-2.97645578	4.14386181
C	3.60265336	-2.25369657	5.70966784
H	4.40112988	-2.43509822	6.42884385
C	2.19394398	-2.18382413	6.29564586
H	2.21917756	-2.52830125	7.33637495
H	1.53493172	-2.87805332	5.76225319
C	1.61680630	-0.75122291	6.24962988
H	0.51444533	-0.78026510	6.27031595
H	1.92891509	-0.21534755	7.15455277
C	6.87252235	2.11745406	1.89007773
H	6.42018471	3.00544062	2.33721764
C	6.01400265	1.26239949	1.16737386
H	4.96235449	1.54836523	1.12044431
C	6.48615338	0.30798499	0.07412127
H	7.36913890	0.72317300	-0.42469059

H	5.71042996	0.22999926	-0.69710439
C	6.79445686	-1.10197061	0.62763143
H	5.87191215	-1.69521992	0.61726570
H	7.50754357	-1.62581492	-0.03074760
C	7.29632740	-1.07963052	2.06139754
H	7.11540852	-2.00017781	2.61743057
C	8.29172811	-0.21400203	2.57073040
H	8.79437659	-0.52953020	3.48479600
C	9.05207094	0.80087824	1.71981487
H	9.13566062	0.43363951	0.69082557
H	10.07843260	0.88959452	2.09546186
C	8.38193500	2.19285236	1.74097716
H	8.76388233	2.75625041	2.60126319
H	8.66319170	2.76820190	0.84297280
C	5.23121854	2.76587819	7.04259966
H	4.26759912	3.01690605	6.59404987
C	6.38179565	3.26012628	6.39257452
H	6.22084750	3.84234171	5.48423325
C	7.72396421	3.47956054	7.08461496
H	7.56170645	3.72635713	8.13988218
H	8.22024801	4.35139666	6.64163428
C	8.65053071	2.24901911	6.95613061
H	9.21962782	2.33139245	6.02200301
H	9.39226814	2.23936874	7.77223565
C	7.88846525	0.93594761	6.90020325
H	8.41708771	0.12865779	6.39241481
C	6.82669714	0.56242570	7.75598885
H	6.61326434	-0.50328259	7.83601273
C	6.32682419	1.42225037	8.91479680
H	7.15162081	2.02395345	9.31268570
H	6.00316007	0.76999228	9.73467747
C	5.15079491	2.33252763	8.49589792
H	4.21282315	1.77641486	8.61635983
H	5.08282444	3.20531655	9.16688504
C	0.91604439	4.94965806	3.48591956
C	0.25809838	6.06886367	4.01277196
H	0.80179066	6.99268422	4.18457239
C	-1.10314766	5.99554812	4.32342043
H	-1.60800534	6.86526580	4.73526424
C	-1.81023619	4.80945226	4.10707022
H	-2.86769619	4.75451578	4.35133194
C	-1.15390182	3.68935232	3.58371732
H	-1.69753553	2.76255415	3.42183169

C	0.20597772	3.75569821	3.27926648
H	0.71809620	2.88095630	2.88690286
C	2.74459066	5.29342945	1.24373305
C	3.89760865	4.91249810	0.53908243
H	4.71225894	4.41738427	1.06067071
C	3.99328038	5.15924656	-0.83125500
H	4.88762524	4.85994988	-1.37096176
C	2.93582262	5.77810686	-1.50693859
H	3.00790118	5.96347400	-2.57529690
C	1.78248360	6.15009174	-0.80919207
H	0.95720956	6.62567683	-1.33222634
C	1.68465061	5.90988306	0.56397724
H	0.78531952	6.19778755	1.10008149
C	3.38242942	6.47106960	3.83852810
C	3.86152019	6.35615929	5.15367635
H	3.83400076	5.39409949	5.65822001
C	4.38233964	7.47276742	5.80881719
H	4.75343603	7.37588808	6.82546897
C	4.43720871	8.70740070	5.15246999
H	4.85052517	9.57479540	5.66012282
C	3.96920460	8.82248649	3.84000725
H	4.01636938	9.77828236	3.32518208
C	3.44136212	7.70801370	3.18200913
H	3.08253361	7.80414388	2.16189406

Rh$_3$Au$_2$ complex 2

Energy	-3762.012002		
Enthalpy	-3762.011057		
Free energy	-3762.198906		
Au	0.73346984	2.91588218	11.41461108
Au	-2.48702766	0.94067047	5.97839870
Rh	-2.16448013	1.39791437	9.63723736
Rh	-0.85899721	3.49972652	8.12668561
Rh	0.36307314	0.86736259	8.34929270
P	1.86836230	3.62094499	13.24376515
P	-3.59479219	0.23904028	4.13142287
O	-1.48842495	1.56196388	7.65624979
O	-0.27681867	2.29807443	9.74198784
C	2.82124303	5.14179559	12.91767920
C	4.08173165	5.36059416	13.49015347
H	4.52809026	4.60862057	14.13380298
C	4.76918620	6.54892840	13.22747877
H	5.74748411	6.71324741	13.67097148

C	4.20224242	7.51966353	12.39622720
H	4.74066202	8.44097906	12.19098591
C	2.94489498	7.30155598	11.82162464
H	2.50441154	8.04983971	11.16837194
C	2.25714542	6.11452796	12.07655133
H	1.28743130	5.93923213	11.61826378
C	3.07509035	2.38451951	13.82905673
C	3.80558345	1.66702716	12.86762856
H	3.62429750	1.83802532	11.80966269
C	4.75768172	0.72971847	13.26910788
H	5.31947598	0.17787513	12.52037250
C	4.97807283	0.49503605	14.63124277
H	5.71438831	-0.24030988	14.94384878
C	4.24517177	1.20093370	15.58955117
H	4.41038063	1.01703200	16.64770083
C	3.29496606	2.14631848	15.19207699
H	2.72831002	2.68988976	15.94179547
C	0.77914717	3.99225719	14.65814386
C	-0.36345663	3.19833205	14.84652382
H	-0.59306613	2.40431684	14.14088739
C	-1.20694848	3.43382322	15.93305674
H	-2.09041224	2.81703742	16.07338513
C	-0.92016276	4.46847505	16.83047145
H	-1.58154248	4.65667991	17.67184867
C	0.21236977	5.26599830	16.63987816
H	0.43436282	6.07362362	17.33207221
C	1.06321756	5.03031470	15.55658602
H	1.93962732	5.65480734	15.41233484
C	-0.85923940	5.33322596	9.18185875
H	-0.84807212	5.07761637	10.24322151
C	-2.04773224	6.17372962	8.75305113
H	-1.88067412	7.23649306	8.99187618
H	-2.90590613	5.85183522	9.35502899
C	-2.39364098	6.00414937	7.25722215
H	-3.46139035	6.20198525	7.10933335
H	-1.85876013	6.74591506	6.65456097
C	-2.06974314	4.60151658	6.75262021
H	-2.93067354	3.97028947	6.52894619
C	-0.84735389	4.24440445	6.14515198
H	-0.86398404	3.37359672	5.48660926
C	0.34689823	5.15935704	5.94497195
H	0.18566498	5.82982965	5.08539014
H	1.20191702	4.52349560	5.68609140

C	0.69582840	5.97584643	7.20906406
H	1.76540552	6.21474487	7.19966507
H	0.16793868	6.93552228	7.20311632
C	0.36422951	5.21483918	8.48893839
H	1.22202757	4.86596545	9.06501382
C	2.43487310	0.75951380	8.86132275
H	2.68812537	1.71827511	9.31580732
C	3.30653318	0.33846074	7.68215492
H	3.69498382	-0.67124493	7.85260439
H	4.18069412	0.99733261	7.62791732
C	2.53863345	0.40221539	6.34329266
H	2.62691372	1.41408381	5.92994184
H	2.99538525	-0.27612845	5.60461499
C	1.05799949	0.10787225	6.49911647
H	0.42677799	0.54651946	5.72407760
C	0.50163803	-0.95471002	7.24249425
H	-0.52096554	-1.24187914	6.99462365
C	1.32561941	-2.01544807	7.96572339
H	0.79312140	-2.97260960	7.92660708
H	2.27319097	-2.17086991	7.43867978
C	1.58291915	-1.63771466	9.44084561
H	0.74211561	-1.99097002	10.04978929
H	2.48053265	-2.15216647	9.82021902
C	1.69080672	-0.13952755	9.65477255
H	1.44127220	0.19018563	10.66523968
C	-3.51483833	-1.15041300	10.43344290
H	-2.70354532	-1.85629281	10.21875394
H	-4.44261035	-1.74390308	10.46982140
C	-3.55738321	-0.15596306	9.28800033
H	-3.31125101	-0.58070625	8.31279143
C	-4.24763172	1.07499505	9.28654562
H	-4.46617979	1.51314755	8.31181901
C	-5.11701163	1.56831076	10.43906144
H	-5.55106680	0.71244947	10.96698967
H	-5.96114567	2.13835006	10.03449141
C	-4.32394440	2.46169968	11.41821874
H	-4.35865314	3.49808919	11.06154306
H	-4.79777399	2.45892213	12.41309716
C	-2.86117982	2.07017746	11.51834029
H	-2.19681753	2.88129512	11.82270432
C	-2.36518820	0.75677862	11.66415366
H	-1.35245345	0.65762549	12.05663797
C	-3.24729193	-0.48060853	11.79945179

H	-4.19098900	-0.21036817	12.28513766
H	-2.75674737	-1.20108452	12.46387664
C	-4.87570656	-0.99972744	4.52226455
C	-5.17417106	-2.05820375	3.65306500
H	-4.62603293	-2.17487329	2.72323728
C	-6.17950516	-2.97045675	3.98545136
H	-6.40566467	-3.79101347	3.31001803
C	-6.88948730	-2.82932094	5.18162536
H	-7.66895581	-3.54159280	5.43813133
C	-6.59116246	-1.77509928	6.05207013
H	-7.13453600	-1.66599615	6.98667414
C	-5.58438883	-0.86514772	5.72712016
H	-5.34291218	-0.05534641	6.41023385
C	-2.48941712	-0.52938660	2.90133807
C	-1.38767312	-1.26698020	3.36342643
H	-1.19555296	-1.34036952	4.43061527
C	-0.53514448	-1.89367004	2.45353636
H	0.31723291	-2.46154912	2.81634904
C	-0.77243615	-1.77952013	1.07918525
H	-0.10398321	-2.26132469	0.37082962
C	-1.86404385	-1.03809467	0.61661699
H	-2.04732073	-0.94353835	-0.45026241
C	-2.72343246	-0.41299135	1.52410368
H	-3.56775480	0.16450357	1.15991959
C	-4.44523654	1.60308907	3.26947292
C	-3.77088149	2.82880282	3.14547598
H	-2.77934595	2.94741275	3.57452011
C	-4.37497650	3.89465182	2.47842465
H	-3.84857179	4.84062167	2.38547888
C	-5.65901266	3.74694329	1.94099364
H	-6.13244352	4.57977597	1.42818158
C	-6.33529023	2.53065489	2.07087350
H	-7.33407731	2.41441009	1.65896003
C	-5.73105967	1.45741971	2.73263750
H	-6.26222149	0.51582192	2.83086184

Rh₃AuLi complex 3

Energy	-3294.754505
Enthalpy	-3294.753561
Free energy	-3294.938105

Symbol	X	Y	Z
Au	3.92808522	3.11524133	3.67479952
Rh	4.39259973	-0.41855326	4.61045724

Rh	6.50787801	0.55157988	2.93774588
Rh	6.44835292	1.31028533	5.69199162
P	2.64456016	4.91246556	3.16968765
O	5.07505445	1.48055661	4.14396847
C	2.46443930	0.21538758	5.22641781
H	2.54480326	1.28294529	5.44066080
C	2.39978336	-0.15167142	3.86594012
H	2.45623716	0.65967046	3.13891940
C	1.77731976	-1.44611307	3.35680077
H	1.29241532	-1.25984088	2.39137292
H	0.98516284	-1.77243561	4.03905408
C	2.83734764	-2.55479708	3.19128580
H	2.36595523	-3.55086900	3.22490175
H	3.29653918	-2.46207908	2.19932730
C	3.95086014	-2.45199731	4.21605604
H	4.88358329	-2.91530811	3.90900382
C	3.79200278	-2.22707033	5.59824671
H	4.62311262	-2.53537648	6.22050894
C	2.44570726	-2.09450007	6.30255147
H	2.52960709	-2.50828152	7.31436012
H	1.69310091	-2.70177313	5.78745213
C	1.98248701	-0.62406471	6.39431408
H	0.88576658	-0.56918654	6.49028678
H	2.39516052	-0.17763169	7.30736900
C	6.83885012	2.22708784	1.67730399
H	6.42120041	3.09263150	2.19626971
C	5.92019085	1.36577262	1.04193196
H	4.86430690	1.62420968	1.13108128
C	6.27517353	0.44781204	-0.12338000
H	7.08537136	0.89189355	-0.71200511
H	5.41459649	0.37255340	-0.79827400
C	6.67059408	-0.96593622	0.35727697
H	5.76359677	-1.57606379	0.44919007
H	7.30515412	-1.46492160	-0.39376604
C	7.34803537	-0.95750719	1.71488564
H	7.27069495	-1.88941622	2.26946440
C	8.37625920	-0.07879783	2.11767589
H	8.99121285	-0.40917699	2.95101968
C	9.01013136	0.97431965	1.21379345
H	8.98213069	0.63342528	0.17294442
H	10.07075693	1.07886672	1.47146943
C	8.31614313	2.34705503	1.35126106
H	8.78500603	2.90060879	2.17390940

H	8.47130605	2.95036844	0.44178870
C	5.56822315	2.75630764	6.96352878
H	4.52826034	2.85205905	6.64488861
C	6.53819997	3.40375893	6.16959171
H	6.17487343	3.93391104	5.28831277
C	7.90526409	3.83948321	6.68176517
H	7.84854190	4.06472160	7.75222952
H	8.19658791	4.77361362	6.18750685
C	8.97531367	2.76159847	6.41285296
H	9.38592579	2.91026407	5.40650743
H	9.82009107	2.86883480	7.11332155
C	8.41390577	1.35367855	6.46579349
H	8.98160681	0.62503989	5.89763202
C	7.55842132	0.83476422	7.46030667
H	7.55889091	-0.24521738	7.57191592
C	7.08174983	1.62072686	8.67812143
H	7.85129050	2.33976638	8.98116198
H	6.95803269	0.93389518	9.52394009
C	5.74158098	2.34343026	8.41415909
H	4.91785605	1.66084685	8.65598277
H	5.63269880	3.21178484	9.08448844
C	0.90956518	4.68468544	3.68693494
C	0.14289324	5.73498077	4.20993136
H	0.57896473	6.72106479	4.33714494
C	-1.18795625	5.51150218	4.57471075
H	-1.77779771	6.32788376	4.98255348
C	-1.75644889	4.24398740	4.41793935
H	-2.79043743	4.07295613	4.70505923
C	-0.99157708	3.19337851	3.89850551
H	-1.42660538	2.20439722	3.78268832
C	0.33877975	3.41022612	3.53833340
H	0.93733233	2.59052641	3.14977049
C	2.59859274	5.26926164	1.38146150
C	3.75444075	5.02290759	0.62358854
H	4.63528798	4.60195605	1.10091219
C	3.76888099	5.30760436	-0.74254486
H	4.66583932	5.11210276	-1.32386787
C	2.62761980	5.83016187	-1.36080055
H	2.63675431	6.04451813	-2.42607019
C	1.47225385	6.06784051	-0.60987112
H	0.58272595	6.46805514	-1.08873723
C	1.45473652	5.78896722	0.75940506
H	0.55309967	5.97195094	1.33600960

C	3.22887988	6.43635568	3.98498549
C	3.76491381	6.33258704	5.27893634
H	3.84928049	5.35878273	5.75394569
C	4.19841634	7.47665650	5.94991251
H	4.61293892	7.38954620	6.95056102
C	4.10947230	8.72808799	5.32987807
H	4.45361682	9.61781158	5.85026452
C	3.58598795	8.83244470	4.03767947
H	3.52142204	9.80189922	3.55120940
C	3.14517135	7.68996293	3.36383397
H	2.74328745	7.77711885	2.35905340
Li	7.53575708	-1.97881064	5.29311078
O	7.88556536	-3.54681772	4.06489008
C	9.21551828	-4.12379848	3.98539774
C	6.95508496	-4.35916507	3.30545398
C	9.02712753	-5.52168921	3.40375988
H	9.82479773	-3.49133131	3.32866795
H	9.64744736	-4.11749807	4.98781085
C	7.81177144	-5.32316805	2.48897759
H	6.30241975	-4.89007700	4.01005666
H	6.34442076	-3.69776598	2.68733791
H	8.79478924	-6.24057497	4.19889274
H	9.91836436	-5.86968718	2.87278626
H	7.28113789	-6.25211844	2.25969015
H	8.11643815	-4.85463584	1.54545136
O	9.46605889	-1.72063804	5.94269675
C	9.92095601	-2.15066718	7.23814621
C	10.63344740	-1.22612891	5.25605191
C	10.92379479	-1.08122606	7.67345080
H	9.04917142	-2.23664986	7.88412833
H	10.39920249	-3.13734912	7.14267554
C	11.53616785	-0.59470607	6.33616761
H	11.13521232	-2.06541635	4.75767398
H	10.29425177	-0.51837817	4.49867640
H	11.67320343	-1.48331770	8.36198427
H	10.39938638	-0.26300868	8.17574352
H	12.57073197	-0.92951704	6.21451484
H	11.52721020	0.49697072	6.27299755
O	6.84919479	-2.92202224	6.92876167
C	7.04597189	-4.33351837	7.12700761
C	6.23250247	-2.42382829	8.13581736
C	5.76247073	-4.79780853	7.81278301
H	7.22793288	-4.77933553	6.14946022

H	7.92609552	-4.49173063	7.76808860
C	5.37301781	-3.58180690	8.68947249
H	7.02089656	-2.14213055	8.84642334
H	5.66575036	-1.53179314	7.86570582
H	5.91364043	-5.71138184	8.39563402
H	4.99084849	-4.99320335	7.06103376
H	5.60272101	-3.75651031	9.74497129
H	4.30500008	-3.36095366	8.61142023
O	6.50104606	-0.55124599	4.70633204

Rh₃Li complex

Energy	-2122.871666		
Enthalpy	-2122.870721		
Free energy	-2123.007195		
Rh	4.37502372	-0.60590344	4.73432806
Rh	6.31377256	0.55198015	3.05204540
Rh	6.33663641	1.17390472	5.79216578
O	4.90656590	1.32232015	4.34321725
C	2.48154601	-0.08189557	5.51204559
H	2.55093157	0.96314503	5.81651089
C	2.34338164	-0.33275260	4.12731922
H	2.33720383	0.53771817	3.47196850
C	1.71501422	-1.59692147	3.54904729
H	1.17783802	-1.34559627	2.62639062
H	0.96208330	-1.99207820	4.24036150
C	2.78045083	-2.67153469	3.24246236
H	2.32421926	-3.67635975	3.23177390
H	3.17447856	-2.50047114	2.23284401
C	3.95773520	-2.61962386	4.20048052
H	4.87645445	-3.03307793	3.79423854
C	3.87713053	-2.52151335	5.60487370
H	4.74552785	-2.86517721	6.15606404
C	2.56390262	-2.48088956	6.38041794
H	2.69668900	-2.98413745	7.34604402
H	1.79560684	-3.05272165	5.84713015
C	2.08143055	-1.03367925	6.62605900
H	0.99074751	-1.01327600	6.79152394
H	2.54052886	-0.66102657	7.55051922
C	6.40991947	2.31288288	1.87923229
H	5.94451824	3.10447368	2.46745058
C	5.54014712	1.39565652	1.24698017
H	4.47194287	1.54424850	1.40403310
C	5.91310860	0.58173186	0.00979534

H	6.63805709	1.13637613	-0.59676147
H	5.02462129	0.45511408	-0.62079540
C	6.47625596	-0.80920102	0.37931542
H	5.64007987	-1.51204430	0.48371779
H	7.10701064	-1.19752209	-0.43884508
C	7.22891789	-0.80704943	1.69817243
H	7.27668280	-1.77386642	2.19624470
C	8.18940449	0.14927980	2.09269895
H	8.88845335	-0.15823439	2.86784963
C	8.65853827	1.30626545	1.21411331
H	8.59764564	1.01986201	0.15783245
H	9.71921242	1.50404597	1.41309272
C	7.84499260	2.59497305	1.46917505
H	8.31307692	3.15153402	2.29074546
H	7.88366456	3.25510627	0.58596246
C	5.37711005	2.49167487	7.13386638
H	4.32287708	2.50687356	6.85418948
C	6.26107180	3.24604160	6.32868055
H	5.82315747	3.76964337	5.47954770
C	7.60034962	3.78751506	6.81904333
H	7.55670832	3.97667223	7.89771707
H	7.79502859	4.75874012	6.34791788
C	8.75516149	2.81840145	6.49001748
H	9.12065157	3.03335310	5.47786185
H	9.60803053	2.98559429	7.17043883
C	8.32183824	1.36398608	6.51280608
H	8.93850400	0.70627938	5.90839416
C	7.55112259	0.74485152	7.51923220
H	7.65407048	-0.33260352	7.60300863
C	7.04541388	1.45541506	8.77151989
H	7.75604061	2.23393928	9.07362290
H	7.00989650	0.74087459	9.60358767
C	5.63803465	2.06275197	8.56826662
H	4.88706240	1.30308609	8.81893174
H	5.47579642	2.90123828	9.26689859
Li	7.59497635	-2.01165573	5.29807441
O	8.01318291	-3.54678619	4.06005532
C	9.32234234	-4.16905174	4.03307475
C	7.07377672	-4.34887877	3.30307035
C	9.09892493	-5.58072200	3.49768421
H	9.96862652	-3.58399029	3.36757566
H	9.73365462	-4.13934037	5.04415436
C	7.91472885	-5.37270179	2.54420548

H	6.38342917	-4.83085818	4.00658518
H	6.50545099	-3.68483343	2.64861384
H	8.81996469	-6.26107043	4.31170368
H	9.99012884	-5.98006868	3.00381920
H	7.35651919	-6.29015792	2.33441508
H	8.26044611	-4.95140008	1.59257496
O	9.51466218	-1.68147392	5.89800207
C	10.04917375	-2.05324277	7.17839400
C	10.61551337	-1.14236220	5.14306586
C	11.02103465	-0.92715259	7.53910815
H	9.21278736	-2.16173265	7.86780496
H	10.56902907	-3.01941620	7.08643998
C	11.53056101	-0.43149994	6.16167940
H	11.14196239	-1.96576064	4.64258159
H	10.19679775	-0.47904927	4.38501590
H	11.82872476	-1.28051838	8.18753861
H	10.48618663	-0.12778649	8.05991106
H	12.57747581	-0.70037824	5.99077754
H	11.44571432	0.65562506	6.07972403
O	7.00590418	-3.01522756	6.93889886
C	7.28085648	-4.40823291	7.15567155
C	6.34693970	-2.53165275	8.12895800
C	6.02489158	-4.93543943	7.84744444
H	7.48814759	-4.85791964	6.18448996
H	8.16792879	-4.51082676	7.79933207
C	5.57814840	-3.73554315	8.71759139
H	7.10809201	-2.16794394	8.83182043
H	5.71427533	-1.69578583	7.82805697
H	6.22351329	-5.83698661	8.43512737
H	5.26254877	-5.17358123	7.09844347
H	5.84658631	-3.88238577	9.76844559
H	4.49673371	-3.58388680	8.66706179
O	6.48953699	-0.64646570	4.74431891

Function: B3LYP(GD3BJ)
Basis set: SDD for Rh, Au and 6-31G(d) for H, C, O, P

1-C$_6$H$_6$

Energy	-2822.263483		
Enthalpy	-2822.262538		
Free energy	-2822.420591		
Au	3.84558228	3.13108522	3.63728926
Rh	4.16186330	-0.43265003	4.63056233

Rh	6.44241545	0.52782204	3.18884223
Rh	6.07251642	1.23502609	5.91711040
P	2.69393019	4.97608036	3.01237122
O	4.87575235	1.49631211	4.20662930
O	6.19162147	-0.54978004	4.91595135
C	2.16046015	0.11699201	5.05746836
H	2.15177915	1.19994708	5.19951137
C	2.21867316	-0.35204203	3.72733727
H	2.26918517	0.40156703	2.93984921
C	1.73014413	-1.72983812	3.28891724
H	1.31364809	-1.66253312	2.27657716
H	0.90333407	-2.05152915	3.93253828
C	2.86547221	-2.77983620	3.30283624
H	2.44985917	-3.79599027	3.40686424
H	3.38043024	-2.75525220	2.33509717
C	3.91139828	-2.51045718	4.37025232
H	4.89607935	-2.92008821	4.15110130
C	3.64268926	-2.18003016	5.71764243
H	4.44759332	-2.34125017	6.43327846
C	2.23784616	-2.10527215	6.31113144
H	2.26664216	-2.44293118	7.35394152
H	1.57643211	-2.80437420	5.78705340
C	1.66175712	-0.67191605	6.25591444
H	0.55930804	-0.69841405	6.28465146
H	1.98180714	-0.12900201	7.15360152
C	7.02309450	2.16317116	1.97246014
H	6.56013045	3.05488522	2.40168217
C	6.19146843	1.31527310	1.20962409
H	5.14442437	1.60645311	1.11470308
C	6.70789648	0.35668703	0.14021401
H	7.61606957	0.76642506	-0.31670302
H	5.97115845	0.28433602	-0.66899605
C	6.97945648	-1.05589108	0.70836505
H	6.05333242	-1.64081012	0.65685004
H	7.71678555	-1.58757511	0.08401601
C	7.41367256	-1.03825608	2.16342916
H	7.19843251	-1.95479914	2.71050119
C	8.38763863	-0.17801401	2.71916920
H	8.83444462	-0.48736104	3.66301926
C	9.19742767	0.82846206	1.90529414
H	9.32754865	0.45817603	0.88211506
H	10.20642374	0.90772107	2.32714217
C	8.53871461	2.22681116	1.89399013

H	8.88295361	2.78552320	2.77278020
H	8.86839261	2.80061120	1.01138007
C	5.21846438	2.76514620	7.10853953
H	4.26535731	3.03310222	6.64633147
C	6.38792046	3.27208024	6.50100246
H	6.25484545	3.88293728	5.60685039
C	7.71417554	3.45847725	7.23304050
H	7.52646452	3.67164127	8.29158058
H	8.22780958	4.34211531	6.83513048
C	8.63587261	2.22512816	7.08620053
H	9.22465564	2.33307417	6.16724344
H	9.36046470	2.18447716	7.91658557
C	7.86684656	0.92044406	6.97200551
H	8.39470658	0.12526301	6.44598549
C	6.78313548	0.52744704	7.78973157
H	6.55801147	-0.53757004	7.82131758
C	6.26053246	1.35269210	8.96312667
H	7.07949749	1.93386114	9.40198966
H	5.91356544	0.67774405	9.75445970
C	5.10045037	2.28545016	8.54519459
H	4.15761430	1.73026412	8.62191265
H	5.01887636	3.13513922	9.24407364
C	0.93631007	4.91101535	3.50041825
C	0.22184502	6.06185842	3.86104028
H	0.71978605	7.02654950	3.88533328
C	-1.12855908	5.96598045	4.20526030
H	-1.67671012	6.86020851	4.48879032
C	-1.76935313	4.72391234	4.19252830
H	-2.81837520	4.65124134	4.46580832
C	-1.05680708	3.57284725	3.84194228
H	-1.54614711	2.60309219	3.84539328
C	0.29298902	3.66313126	3.50134825
H	0.85156406	2.76478020	3.25233923
C	2.70481320	5.24820938	1.20761208
C	3.85408728	4.88296535	0.48853304
H	4.68998834	4.41524932	1.00189007
C	3.91638828	5.10232637	-0.88772206
H	4.80721134	4.81295235	-1.43782511
C	2.83039420	5.67706343	-1.55553511
H	2.87694920	5.83971040	-2.62875519
C	1.67987712	6.02980542	-0.84471806
H	0.83030306	6.46594748	-1.36287910
C	1.61456512	5.81633140	0.53427604

H	0.71424305	6.08022542	1.08097608
C	3.36056224	6.50622449	3.75207427
C	3.89277328	6.43860945	5.04965936
H	3.93379328	5.48589137	5.57080739
C	4.38728432	7.58960653	5.66322343
H	4.80184334	7.52796055	6.66534650
C	4.36299731	8.81156062	4.98348136
H	4.75603634	9.70572872	5.45929037
C	3.84580228	8.87983464	3.68692726
H	3.83638028	9.82552270	3.15205423
C	3.34567324	7.73056654	3.06987822
H	2.95673021	7.78532855	2.05754815
C	8.84125164	-3.55424826	4.73226934
C	7.57800352	-3.33279724	5.29139338
C	6.90114852	-4.39761032	5.89598342
C	7.47988655	-5.66981243	5.94498841
C	8.74405861	-5.88409344	5.38605537
C	9.42502067	-4.82420335	4.77827334
H	9.36755165	-2.73242820	4.25291331
H	7.12223454	-2.34277817	5.24545038
H	5.91523341	-4.23349230	6.32396944
H	6.94752148	-6.49319646	6.41548144
H	9.19547268	-6.87266047	5.42215340
H	10.40677972	-4.98926136	4.34051931

1(p-NMe$_2$)-C$_6$H$_6$

Energy	-3223.991903		
Enthalpy	-3223.990959		
Free energy	-3224.179982		
Au	3.81581232	3.14718053	3.60783521
Rh	4.14712283	-0.41711118	4.62101203
Rh	6.42365474	0.54250629	3.17623017
Rh	6.04770468	1.26672591	5.89569163
P	2.66502247	5.00105028	2.99025164
O	4.85428867	1.50643595	4.18437508
O	6.17777216	-0.52708031	4.91026372
C	2.14478945	0.13527956	5.04066200
H	2.13528149	1.21898619	5.17417260
C	2.20567158	-0.34291276	3.71403873
H	2.25709046	0.40590915	2.92244571
C	1.71795674	-1.72372905	3.28436740
H	1.30302033	-1.66323860	2.27081679
H	0.89008008	-2.04152175	3.92884972

C	2.85323379	-2.77366121	3.30722086
H	2.43731408	-3.78934156	3.41698392
H	3.36980041	-2.75511421	2.34012122
C	3.89765497	-2.49657984	4.37437094
H	4.88235669	-2.90870030	4.15969946
C	3.62653576	-2.15713215	5.71925674
H	4.42976865	-2.31449985	6.43771339
C	2.22047756	-2.07871297	6.30972722
H	2.24746575	-2.40915900	7.35507221
H	1.56003398	-2.78175890	5.78941093
C	1.64396696	-0.64590616	6.24319545
H	0.54119669	-0.67276009	6.26969295
H	1.96161948	-0.09665056	7.13794269
C	6.99641746	2.17793831	1.95621461
H	6.52879866	3.06769597	2.38359173
C	6.16842308	1.32489897	1.19541435
H	5.12070016	1.61252817	1.10037563
C	6.68898162	0.36637970	0.12799006
H	7.59527973	0.77898805	-0.33051593
H	5.95196270	0.28885485	-0.68069619
C	6.96742521	-1.04381972	0.69893894
H	6.04369769	-1.63278094	0.64905440
H	7.70688094	-1.57357137	0.07503007
C	7.40152312	-1.02115115	2.15416319
H	7.19109039	-1.93818073	2.70242919
C	8.37209706	-0.15536134	2.70780057
H	8.82150433	-0.46113314	3.65163971
C	9.17702508	0.85288785	1.89115531
H	9.30833359	0.48099238	0.86855743
H	10.18608371	0.93769244	2.31220140
C	8.51166402	2.24809448	1.87704483
H	8.85364212	2.81037328	2.75451049
H	8.83850357	2.82171629	0.99297755
C	5.18084079	2.80228304	7.07087148
H	4.22641430	3.05790463	6.60517021
C	6.34621621	3.31224964	6.45823954
H	6.20734788	3.91325807	5.55869875
C	7.67064939	3.51697683	7.18857929
H	7.48137290	3.74071616	8.24488084
H	8.17747403	4.40007431	6.78041080
C	8.60216121	2.28926138	7.05602266
H	9.19057853	2.39208684	6.13617682
H	9.32667953	2.26355181	7.88739499

C	7.84338576	0.97731293	6.95468109
H	8.37863314	0.18095796	6.43786690
C	6.76240152	0.58434848	7.77636609
H	6.54600248	-0.48207962	7.82005724
C	6.23354956	1.41823595	8.94091239
H	7.04799642	2.01082580	9.37326327
H	5.89198152	0.74935152	9.73993087
C	5.06635973	2.33731009	8.51258299
H	4.12779690	1.77566168	8.59523169
H	4.97781210	3.19405798	9.20233394
C	0.91251446	4.90824547	3.45278888
C	0.16762141	6.03767793	3.81846667
H	0.64848739	7.01095766	3.86329515
C	-1.17929809	5.93687538	4.15137925
H	-1.70901862	6.83600018	4.44123565
C	-1.84475335	4.68633285	4.12785429
C	-1.07801548	3.54568557	3.78119130
H	-1.52498338	2.55940490	3.78201343
C	0.26576828	3.66179284	3.45240091
H	0.82712709	2.76284853	3.21055624
C	2.71501123	5.29036417	1.19929509
C	3.86286281	4.92726129	0.47628639
H	4.69181978	4.44315487	0.98632156
C	3.95585990	5.15169999	-0.89058852
H	4.85631641	4.83857408	-1.40411480
C	2.89168951	5.75845258	-1.60379787
C	1.72683470	6.09817861	-0.87258890
H	0.87128793	6.53446609	-1.37330602
C	1.64879897	5.86855241	0.49731343
H	0.73388191	6.12908404	1.02215188
C	3.32522142	6.50079365	3.77200684
C	3.85899103	6.42117179	5.06863477
H	3.90314076	5.46146296	5.57698717
C	4.35948188	7.54389625	5.71352993
H	4.77530525	7.42488921	6.70623851
C	4.34664196	8.81325536	5.08281548
C	3.82998547	8.88136677	3.76555647
H	3.82591422	9.81960073	3.22450175
C	3.33075868	7.74752635	3.13225493
H	2.95709816	7.83532395	2.11583194
C	8.83502577	-3.52077807	4.73882820
C	7.57217284	-3.29704463	5.29796926
C	6.90071522	-4.35705721	5.91689264

C	7.48433423	-5.62641762	5.98030956
C	8.74821376	-5.84286905	5.42143166
C	9.42376181	-4.78788196	4.79916129
H	9.35681956	-2.70282068	4.24806228
H	7.11239406	-2.30908865	5.24151073
H	5.91496527	-4.19109534	6.34456909
H	6.95594921	-6.44602952	6.46189250
H	9.20346633	-6.82927651	5.46868862
H	10.40520907	-4.95459462	4.36117634
N	4.82472341	9.93877674	5.72771411
N	-3.18808179	4.58052805	4.43588349
N	2.98641836	6.00421557	-2.96072693
C	4.99252122	11.17358687	4.97960984
H	5.70827536	11.06785001	4.14859862
H	4.03582975	11.51501918	4.56716066
H	5.35850936	11.95073468	5.65275694
C	5.53843598	9.79189936	6.98652677
H	4.90091664	9.32475873	7.74585733
H	6.45227725	9.18577408	6.88307441
H	5.81964754	10.78063313	7.35310272
C	-3.88765519	5.72919797	4.98696377
H	-3.46073417	6.06036990	5.94717275
H	-3.86209243	6.57517967	4.29002091
H	-4.93417680	5.46502295	5.14815826
C	-3.78155459	3.26339854	4.60421582
H	-3.69205027	2.67316079	3.68499549
H	-3.31696155	2.69531379	5.42552511
H	-4.84480078	3.37780314	4.82203415
C	4.10635160	5.45709185	-3.71018090
H	5.05913713	5.83578152	-3.32269252
H	4.13461464	4.35644919	-3.67962271
H	4.02428297	5.77134974	-4.75206445
C	1.80604409	6.43002926	-3.69418017
H	0.99504453	5.68532987	-3.65402005
H	1.42090866	7.37833378	-3.30110574
H	2.07502349	6.59022794	-4.73963129

1(*p*-NO₂)-C₆H₆

Energy	-3435.774354		
Enthalpy	-3435.773410		
Free energy	-3435.952772		
Au	3.84097877	3.11825767	3.59870377
Rh	4.15425705	-0.43073290	4.62097315

Rh	6.43844635	0.51447603	3.16629016
Rh	6.06203003	1.26256461	5.88632805
P	2.69383128	4.96618371	3.00224954
O	4.86376928	1.49722424	4.16602207
O	6.18375451	-0.53442907	4.91023981
C	2.15015305	0.11369474	5.03942726
H	2.13687524	1.19896165	5.16812329
C	2.21152577	-0.37335180	3.71560751
H	2.26001354	0.36874812	2.91640886
C	1.73038590	-1.75958870	3.29616774
H	1.31431298	-1.70913316	2.28288805
H	0.90492235	-2.07582102	3.94371235
C	2.87145889	-2.80294055	3.32556623
H	2.46148312	-3.81942293	3.44357786
H	3.38733946	-2.78947283	2.35822665
C	3.91446473	-2.51447788	4.39064562
H	4.90203308	-2.92045305	4.17815840
C	3.64325533	-2.16620419	5.73249205
H	4.44920761	-2.31182191	6.45013985
C	2.23789697	-2.08968903	6.32422604
H	2.26795283	-2.41214757	7.37148961
H	1.58046555	-2.79936490	5.80995592
C	1.65439612	-0.66030691	6.24885686
H	0.55247486	-0.69227238	6.27710958
H	1.97110419	-0.10323433	7.13895352
C	7.02200175	2.12923669	1.92516356
H	6.55738249	3.02799013	2.33937836
C	6.19361207	1.26804108	1.17330564
H	5.14548060	1.55481645	1.07085162
C	6.71415543	0.29210375	0.12175585
H	7.62301285	0.69537749	-0.33881808
H	5.98062241	0.20520126	-0.68861198
C	6.98484583	-1.11032705	0.71487894
H	6.05975669	-1.69722858	0.67044719
H	7.72449323	-1.65167635	0.10241273
C	7.41570306	-1.06823179	2.17024058
H	7.19871525	-1.97465656	2.73309849
C	8.38633966	-0.19789491	2.71468675
H	8.82882481	-0.49055873	3.66571661
C	9.19751149	0.79630439	1.88744073
H	9.33118225	0.40957241	0.87109135
H	10.20473382	0.88349311	2.31122762
C	8.53786835	2.19374224	1.85127293

H	8.87837575	2.76688744	2.72214181
H	8.87001550	2.75306467	0.96076701
C	5.20866095	2.80647852	7.05990767
H	4.25326280	3.06613665	6.59602661
C	6.37751900	3.30673395	6.44483659
H	6.24542403	3.90540775	5.54162390
C	7.70430564	3.50326979	7.17320859
H	7.51687403	3.73032124	8.22860002
H	8.21766605	4.38159746	6.76396286
C	8.62599816	2.26824279	7.04128836
H	9.21469483	2.36442344	6.12113426
H	9.35045166	2.23802016	7.87166271
C	7.85783695	0.96179501	6.94507573
H	8.38445949	0.16034130	6.42766130
C	6.77489958	0.57891444	7.76779728
H	6.54894740	-0.48540452	7.81120649
C	6.25270487	1.41855156	8.93094475
H	7.07173833	2.00535124	9.36148871
H	5.90672286	0.75353481	9.73065434
C	5.09172300	2.34547948	8.50284803
H	4.14909593	1.79128236	8.58782601
H	5.01129416	3.20386028	9.19059875
C	0.93045997	4.89976414	3.48349633
C	0.21341823	6.04563946	3.85755127
H	0.70197556	7.01421935	3.88855450
C	-1.13237558	5.94827629	4.20797850
H	-1.70576616	6.81881563	4.50239385
C	-1.73962863	4.69445294	4.17897390
C	-1.04855109	3.53786614	3.82191892
H	-1.55424082	2.57998776	3.82734381
C	0.29669843	3.64623663	3.47728157
H	0.85766701	2.75166683	3.22241216
C	2.70330767	5.28786195	1.20200991
C	3.85166604	4.92434518	0.47920976
H	4.68299054	4.43836309	0.98194309
C	3.92369465	5.16393430	-0.89101477
H	4.79887148	4.88863659	-1.46684591
C	2.83195163	5.75872262	-1.52139472
C	1.67483337	6.11528141	-0.83192514
H	0.84636770	6.56579847	-1.36482632
C	1.61536813	5.87526163	0.54013320
H	0.71564356	6.13802994	1.08705826
C	3.35454117	6.48730984	3.77486212

C	3.90048477	6.38108084	5.06499649
H	3.94935986	5.41626578	5.56142725
C	4.40609686	7.50809386	5.70840220
H	4.83493533	7.44554654	6.70111401
C	4.36496389	8.73093216	5.04055396
C	3.84244278	8.86243217	3.75558952
H	3.84042726	9.83088946	3.27042372
C	3.33545760	7.72850762	3.12232724
H	2.93699480	7.81521029	2.11661844
C	8.83973682	-3.54716802	4.76801598
C	7.57685738	-3.32069866	5.32590241
C	6.89784105	-4.38077588	5.93633372
C	7.47417964	-5.65372941	5.99190855
C	8.73778617	-5.87321102	5.43388960
C	9.42095474	-4.81796886	4.82068397
H	9.36843389	-2.72909187	4.28489715
H	7.12299914	-2.33064601	5.27418559
H	5.91259181	-4.21293842	6.36442081
H	6.94055248	-6.47349884	6.46700981
H	9.18727080	-6.86232357	5.47521416
H	10.40244370	-4.98718848	4.38418537
N	4.90336861	9.93026069	5.71482869
O	5.36258577	9.78736934	6.84664469
O	4.85578161	10.99595504	5.10130391
N	-3.16584402	4.58711057	4.54991222
O	-3.75088529	5.62386783	4.86156401
O	-3.67745479	3.46921655	4.52123707
N	2.89948343	6.01293556	-2.97532449
O	3.92969406	5.68566880	-3.56172388
O	1.92121354	6.53814874	-3.50578973

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