

**Supplementary information for Group 9 Bimetallic Carbonyl
Permethylpentalene Complexes**

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Crystal Data

	(1)	(2)	(3)
Chemical formula	C ₁₈ H ₁₈ O ₄ Rh ₂	C ₁₈ H ₁₈ Ir ₂ O ₄	C ₁₇ H ₁₈ O ₃ Rh ₂
<i>M_r</i>	504.15	682.78	476.14
Crystal system, space group	Monoclinic, <i>P2₁/n</i>	Monoclinic, <i>P2₁/n</i>	Monoclinic, <i>P2₁/n</i>
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.3626 (3), 10.7476 (3), 14.5062 (5)	12.2542 (3), 10.8292 (3), 14.3587 (3)	10.5875 (2), 9.7143 (2), 15.3682 (3)
α, β, γ (°)	90, 107.6252 (12), 90	90, 106.9133 (11), 90	90, 94.8887 (7), 90
<i>V</i> (Å ³)	1836.94 (9)	1823.03 (8)	1574.87 (5)
<i>Z</i>	4	4	4
Radiation Type	Mo K _α	Mo K _α	Mo K _α
μ (mm ⁻¹)	1.81	14.60	2.10
Crystal size (mm)	0.14 × 0.14 × 0.04	0.06 × 0.04 × 0.02	0.04 × 0.04 × 0.02
<i>T_{min}</i> , <i>T_{max}</i>	0.83, 0.93	0.56, 0.75	0.86, 0.96
No. of measured, independent and observed reflections	28297, 8089, 3346 [<i>I</i> > 2.0σ(<i>I</i>)]	7721, 4147, 3453 [<i>I</i> > 2.0σ(<i>I</i>)]	31745, 7197, 3131 [<i>I</i> > 2.0σ(<i>I</i>)]
<i>R_{int}</i>	0.028	0.033	0.023
(sin θ/λ) _{max} (Å ⁻¹)	0.647	0.650	0.650
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.041, 0.101, 1.03	0.035, 0.077, 1.00	0.036, 0.082, 0.99
No. of reflections	3175	3255	3044
No. of parameters	217	218	199
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.96, -1.03	1.77, -1.91	0.95, -0.95
CCDC number	1417859	1417860	1417861

Calculated Cartesian Coordinates

A

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C	1.38271047	-1.17443976	0.26763692
C	2.22285034	0.00000000	0.40629130
C	1.38271047	1.17443976	0.26763692
C	0.00000000	0.71560533	0.26022714
C	0.00000000	-0.71560533	0.26022714
C	-1.38271047	-1.17443976	0.26763692
C	-2.22285034	0.00000000	0.40629130
C	-1.38271047	1.17443976	0.26763692
C	3.68577466	0.00000000	0.75115162
H	4.19316332	0.88473939	0.34655880
H	3.83363769	0.00000000	1.84466772
H	4.19316332	-0.88473939	0.34655880
C	-3.68577466	0.00000000	0.75115162
H	-4.19316332	-0.88473939	0.34655880
H	-3.83363769	0.00000000	1.84466772
H	-4.19316332	0.88473939	0.34655880
C	-1.83743823	2.59909317	0.42330379
H	-1.23430667	3.28630278	-0.18322943
H	-2.88536699	2.72124878	0.12240964
H	-1.75166058	2.91845409	1.47465272
C	-1.83743823	-2.59909317	0.42330379
H	-2.88536699	-2.72124878	0.12240964
H	-1.23430667	-3.28630278	-0.18322943
H	-1.75166058	-2.91845409	1.47465272
C	1.83743823	2.59909317	0.42330379
H	2.88536699	2.72124878	0.12240964
H	1.23430667	3.28630278	-0.18322943
H	1.75166058	2.91845409	1.47465272
C	1.83743823	-2.59909317	0.42330379
H	1.23430667	-3.28630278	-0.18322943
H	2.88536699	-2.72124878	0.12240964
H	1.75166058	-2.91845409	1.47465272
Co	-1.40013268	0.00000000	-1.45635060
Co	1.40013268	0.00000000	-1.45635060
C	1.73593139	-1.27718354	-2.58163303
O	2.01007511	-2.13970499	-3.31728246
C	-1.73593139	-1.27718354	-2.58163303
C	-1.73593139	1.27718354	-2.58163303
C	1.73593139	1.27718354	-2.58163303
O	-2.01007511	-2.13970499	-3.31728246
O	-2.01007511	2.13970499	-3.31728246
O	2.01007511	2.13970499	-3.31728246

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C	-1.17421134	-1.38322131	0.53863564
C	0.00000000	-2.21977681	0.70314125
C	1.17421134	-1.38322131	0.53863564
C	0.71325396	0.00000000	0.53261593

C	-0.71325396	0.00000000	0.53261593
C	-1.17421134	1.38322131	0.53863564
C	0.00000000	2.21977681	0.70314125
C	1.17421134	1.38322131	0.53863564
C	0.00000000	-3.65856282	1.13385589
H	0.88460579	-4.19104308	0.76238931
H	0.00000000	-3.73775614	2.23471734
H	-0.88460579	-4.19104308	0.76238931
C	0.00000000	3.65856282	1.13385589
H	-0.88460579	4.19104308	0.76238931
H	0.00000000	3.73775614	2.23471734
H	0.88460579	4.19104308	0.76238931
C	2.59737778	1.83191923	0.73983345
H	3.29848071	1.23906386	0.13909867
H	2.72952801	2.88499970	0.46193129
H	2.89147099	1.72476124	1.79639483
C	-2.59737778	1.83191923	0.73983345
H	-2.72952801	2.88499970	0.46193129
H	-3.29848071	1.23906386	0.13909867
H	-2.89147099	1.72476124	1.79639483
C	2.59737778	-1.83191923	0.73983345
H	2.72952801	-2.88499970	0.46193129
H	3.29848071	-1.23906386	0.13909867
H	2.89147099	-1.72476124	1.79639483
C	-2.59737778	-1.83191923	0.73983345
H	-3.29848071	-1.23906386	0.13909867
H	-2.72952801	-2.88499970	0.46193129
H	-2.89147099	-1.72476124	1.79639483
Rh	0.00000000	1.49901947	-1.39485430
Rh	0.00000000	-1.49901947	-1.39485430
C	-1.33937088	-1.91223658	-2.64503359
O	-2.14977324	-2.24704445	-3.41102056
C	-1.33937088	1.91223658	-2.64503359
C	1.33937088	1.91223658	-2.64503359
C	1.33937088	-1.91223658	-2.64503359
O	-2.14977324	2.24704445	-3.41102056
O	2.14977324	2.24704445	-3.41102056
O	2.14977324	-2.24704445	-3.41102056

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C	1.37909280	-1.17784951	0.28714579
C	2.22929956	0.00000000	0.43188635
C	1.37909280	1.17784951	0.28714579
C	0.00000000	0.71635491	0.31724591
C	0.00000000	-0.71635491	0.31724591
C	-1.37909280	-1.17784951	0.28714579
C	-2.22929956	0.00000000	0.43188635
C	-1.37909280	1.17784951	0.28714579
C	3.65911339	0.00000000	0.89010151
H	4.19742360	0.88424905	0.52556090
H	3.71849676	0.00000000	1.99304362
H	4.19742360	-0.88424905	0.52556090
C	-3.65911339	0.00000000	0.89010151
H	-4.19742360	-0.88424905	0.52556090

H	-3.71849676	0.00000000	1.99304362
H	-4.19742360	0.88424905	0.52556090
C	-1.83337143	2.59704850	0.50243299
H	-1.23529367	3.30948145	-0.07941130
H	-2.88267066	2.72966621	0.21034456
H	-1.74243417	2.87371223	1.56547497
C	-1.83337143	-2.59704850	0.50243299
H	-2.88267066	-2.72966621	0.21034456
H	-1.23529367	-3.30948145	-0.07941130
H	-1.74243417	-2.87371223	1.56547497
C	1.83337143	2.59704850	0.50243299
H	2.88267066	2.72966621	0.21034456
H	1.23529367	3.30948145	-0.07941130
H	1.74243417	2.87371223	1.56547497
C	1.83337143	-2.59704850	0.50243299
H	1.23529367	-3.30948145	-0.07941130
H	2.88267066	-2.72966621	0.21034456
H	1.74243417	-2.87371223	1.56547497
Ir	-1.52418658	0.00000000	-1.65625697
Ir	1.52418658	0.00000000	-1.65625697
C	1.89838510	-1.34383720	-2.90206138
O	2.18952688	-2.19797304	-3.64208622
C	-1.89838510	-1.34383720	-2.90206138
C	-1.89838510	1.34383720	-2.90206138
C	1.89838510	1.34383720	-2.90206138
O	-2.18952688	-2.19797304	-3.64208622
O	-2.18952688	2.19797304	-3.64208622
O	2.18952688	2.19797304	-3.64208622

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C	-0.32959691	-1.82634526	2.99668787
C	0.81580858	-2.41804316	2.33585764
C	1.75643732	-1.36508340	2.00646545
C	1.31226532	-0.16743847	2.71354567
C	0.05871799	-0.46065942	3.36622759
C	-0.33762219	0.67391136	4.13715615
C	0.71872171	1.67573747	3.99018147
C	1.71317775	1.17102905	3.07854463
C	1.07253899	-3.89034658	2.20319255
H	1.78519066	-4.10565021	1.39825082
H	1.49567193	-4.28743205	3.14102954
H	0.15364756	-4.44539811	1.97975291
C	0.86293756	2.91779097	4.82078917
H	-0.11314511	3.30864550	5.13532771
H	1.44992105	2.71512901	5.73297289
H	1.37604525	3.71314646	4.26557623
C	3.01808680	1.85351140	2.77928647
H	3.46344126	1.49500003	1.84541243
H	2.89207801	2.94091419	2.69469281
H	3.74311311	1.66417335	3.58763064
C	-1.48190548	0.75412741	5.10958595
H	-1.84339367	1.78360628	5.22695035
H	-2.32884180	0.13580196	4.78899085
H	-1.16523744	0.39784329	6.10305510

C	3.15826293	-1.59997235	1.51614567
H	3.23215470	-2.51346820	0.91591650
H	3.53075475	-0.77309131	0.90341895
H	3.83963752	-1.71078212	2.37660645
C	-1.45161105	-2.60137204	3.63218828
H	-2.38919452	-2.03071957	3.64044360
H	-1.63818649	-3.54323822	3.10148114
H	-1.20262186	-2.84665038	4.67815702
Rh	-0.33887205	1.47564768	1.99991238
Rh	-0.25899306	-1.25782488	0.79760941
C	-2.10279216	-1.05381596	0.64331704
O	-3.26916105	-1.03063340	0.72483182
C	-2.07072479	2.11985038	1.85798159
C	0.28776370	2.75901354	0.57979786
O	-3.15681461	2.55454533	1.86061402
O	0.64975899	3.89553154	0.55512557
C	0.33762219	-0.67391136	-4.13715615
C	-0.71872171	-1.67573747	-3.99018147
H	-1.44992105	-2.71512901	-5.73297289
H	0.11314511	-3.30864550	-5.13532771
C	-1.07253899	3.89034658	-2.20319255
H	-0.15364756	4.44539811	-1.97975291
H	-1.49567193	4.28743205	-3.14102954
H	-1.78519066	4.10565021	-1.39825082
C	-3.15826293	1.59997235	-1.51614567
H	-3.53075475	0.77309131	-0.90341895
H	-3.23215470	2.51346820	-0.91591650
H	-3.83963752	1.71078212	-2.37660645
C	-1.71317775	-1.17102905	-3.07854463
C	1.45161105	2.60137204	-3.63218828
H	1.63818649	3.54323822	-3.10148114
H	2.38919452	2.03071957	-3.64044360
H	1.20262186	2.84665038	-4.67815702
C	-3.01808680	-1.85351140	-2.77928647
H	-2.89207801	-2.94091419	-2.69469281
H	-3.46344126	-1.49500003	-1.84541243
H	-3.74311311	-1.66417335	-3.58763064
C	1.48190548	-0.75412741	-5.10958595
H	2.32884180	-0.13580196	-4.78899085
C	-1.31226532	0.16743847	-2.71354567
H	1.84339367	-1.78360628	-5.22695035
H	1.16523744	-0.39784329	-6.10305510
Rh	0.25899306	1.25782488	-0.79760941
Rh	0.33887205	-1.47564768	-1.99991238
C	2.07072479	-2.11985038	-1.85798159
O	3.15681461	-2.55454533	-1.86061402
C	2.10279216	1.05381596	-0.64331704
C	-0.28776370	-2.75901354	-0.57979786
O	3.26916105	1.03063340	-0.72483182
O	-0.64975899	-3.89553154	-0.55512557
C	-0.05871799	0.46065942	-3.36622759
C	0.32959691	1.82634526	-2.99668787
C	-0.81580858	2.41804316	-2.33585764
C	-1.75643732	1.36508340	-2.00646545
C	-0.86293756	-2.91779097	-4.82078917
H	-1.37604525	-3.71314646	-4.26557623

