An Approach to Bimetallic Catalysts by Ligand Design

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MOLECULAR MECHANICS CALCULATIONS

Molecular Mechanic calculations were performed on CAChe™ software (CAChe Worksystem Pro, version 6.1.1, from Fujitsu). Geometry optimization procedure made use of standard MM2 Force Field, augmented for the non-MM2 defined atoms and interactions, using the routine implemented in CAChe™. Energy minimization was conducted until rms < 0.001 kcal·mol^{-1}.

To achieve meaningful energy comparisons, after calculating the most stable conformation of the free ligand (L), the monometallic chelate (ML), the bimetallic complex (M2L2), and dimeric structures around a M2Cl2 core the energy of **only the ligand fragment** is evaluated. It is worth mentioning that to evaluate the energy of the ligands, standard MM2 parameters suffice for the calculation. Calculations were performed on the new designs, but also on known ligands, to validate the methodology. The results obtained are presented in tables.

When the calculations involve metals, CAChe automatically augments the Force Field with the parameters involving metals. These augmented parameters are highlighted in the following table:

Energy term	**parameters**
Stretching P–Rh	k_s = 4.400 mdyn·Å; r_0 = 2.310 Å
Stretching Cl–Rh	k_s = 4.400 mdyn·Å; r_0 = 2.240 Å
Bending Cl–Rh–P	k_θ = 0.450 mdyn·Å·rad^{-2}; θ_0 = 109.47º
Bending Cl–Rh–P	k_θ = 0.450 mdyn·Å·rad^{-2}; θ_0 = 90.00º; 180.00º
Bending Cl–Rh–Cl	k_Φ = 0.480 mdyn·Å·rad^{-2}; 93.20º

Atom types definition: P is atom type 25 configured sp3, Csp2 is atom type 50 (identified as aromatic), Rh is atom type 451050. Force constants of non specified augmented terms are assumed to be set to cero.

The term corresponding to the P-Rh-P bending is defined differently depending on the rhodium definition:

Rh unconfigured (type 451150)	k_θ = 0.0 mdyn·Å·rad^{-2}
Rh dsp3-cis (type 451050)	k_θ = 0.450 mdyn·Å·rad^{-2}; θ_0 = 90.00º
Rh dsp3-trans (type 451050)	k_θ = 0.450 mdyn·Å·rad^{-2}; θ_0 = 180.00º

Phosphorus atoms have been treated as in original MM2 for free phosphines.

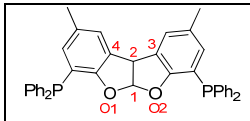
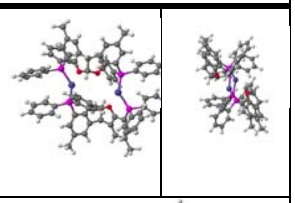
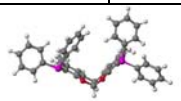
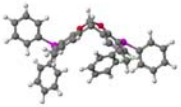
Files definition as appear in tables:

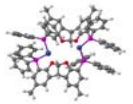
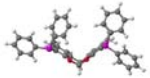
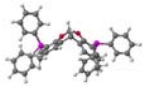
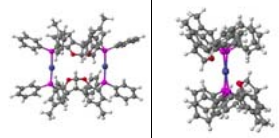
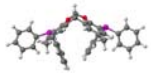
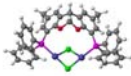
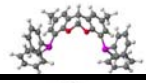
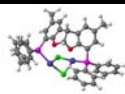
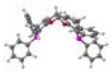
XXX-L-energy: conformational energy of the ligand L in its most stable conformation
XXX-ML: conformational energy of the monometallic fragment ML in its most stable conformation. M defined as rhodium unconfigured.
XXX-ML-energy: conformational energy of the ligand L, in the most stable conformation of the monometallic fragment ML in its most stable conformation. M defined as rhodium unconfigured.
XXX-M2L2-Rh-unc: conformational energy of the bimetallic fragment M2L2 in its most stable conformation. M defined as rhodium unconfigured.
XXX-M2L2-energy-LA and **XXX-M2L2-energy-LB:** conformational energy of each ligand LA and LB, in the most stable conformation of the bimetallic fragment M2L2 in its most stable conformation. M defined as rhodium unconfigured.
XXX-M2L2-Rh-sq-cis: conformational energy of the bimetallic fragment M2L2 in its most stable conformation. M defined as rhodium square planar in cis.

XXX-M2L2-sq-cisA-energy-LA and **XXX-M2L2- sq-cis-energy-LB:** conformational energy of each ligand LA and LB, in the most stable conformation of the bimetallic fragment M2L2 in its most stable conformation. M defined as rhodium square planar in cis.
XXX-M2L2-Rh-sq-trans: conformational energy of the bimetallic fragment M2L2 in its most stable conformation. M defined as rhodium square planar in trans.
XXX-M2L2-Rh-sq-trans-energy-LA and **XXX-M2L2-sq-trans-energy-LB:** conformational energy of each ligand LA and LB, in the most stable conformation of the bimetallic fragment M2L2 in its most stable conformation. M defined as rhodium square planar in trans.
XXX-M2L-Rh-sq-syn and XXX-M2L-sq-anti: conformational energy of the bimetallic fragment (M2Cl2)L in its most stable conformation. M defined as rhodium square planar, and Cl defined as unconfigured
XXX-M2L-Rh-sq-syn-energy and XXX-M2L-sq-anti-energy: conformational energy of the ligand in bimetallic fragment (M2Cl2)L in its most stable conformation. M defined as rhodium square planar, and Cl defined as unconfigured

In the tables it is presented the conformational energy U and its components (stretching, bending, combined stretching-bending, dihedral, improper torsions, van der Waals, electrostatic and hydrogen bonds) in $Kcal \cdot mol^{-1}$, as well as some structural parameters as P-P distance (Å), bending angle of the backbone (º) or P-M-P angle (º), when appropriate.

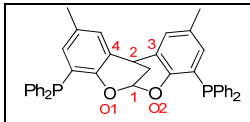
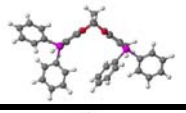
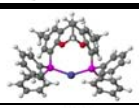
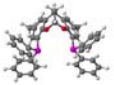
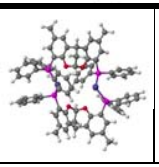
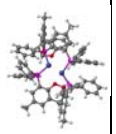
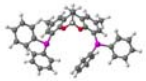
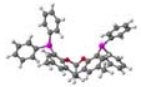
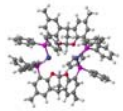
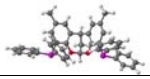
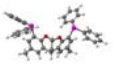
Ligand 10 BFBF2H-PPh2

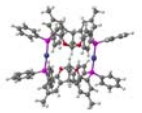
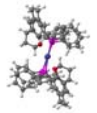
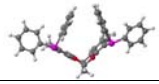
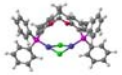
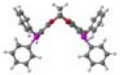
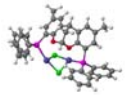
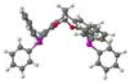
		stretch	angle	Stretch bend	dihedral	improper torsion	Van der Waals	electrostatics	H bond	U	PP distance	Ligand bending[a]	P-M-P angle	Minimizad conformations
L	**BFBFH2-L-energy**	1.448	16.865	0.123	-59.622	0.011	10.163	3.263	0	-27.7	7.31	118.0 107.8	-	
ML	**BFBFH2-ML**	1.316	25.678	0.118	-46.553	0.361	7.262	3.914	0	-7.9	4.28	103.9 98.5	135.0	
	BFBFH2-ML-energy	1.243	23.159	0.118	-47.158	0.361	9.921	3.914	0	-8.4	4.28	103.9 98.5	-	
M2L2-Rh-unconfigured	**BFBFH2-M2L2 Rh-unc**	2.432	44.358	0.220	-117.724	0.073	-1.849	7.993	0	-64.5	7.02 6.95	107.8 114.8 100.8 120.8	127.9 129.6	
	BFBFH2-M2L2-Rh-unc-energy-LA	1.195	19.724	0.112	-59.394	0.026	9.283	3.301	0	-25.7	7.02	107.8 114.8	-	
	BFBFH2- M2L2-Rh-unc-energy-LB	1.235	20.058	0.109	-59.475	0.047	9.311	3.300	0	-25.41	6.95	100.8 120.8	-	

M2L2-cis	**BFBFH2-M2L2 Rh-sq-cis**	2.543	48.809	0.209	-118.166	0.108	-2.381	-7.305	0	-76.18	7.18 7.24	112.5 111.4 97.5 127.1	99.7 96.6	
	BFBFH2-M2L2 Rh-sq-cis-energy-LA	1.260	19.332	0.107	-59.467	0.035	10.026	3.317	0	-25.39	7.18	112.5 111.4	-	
	BFBFH2-M2L2 Rh-sq-cis-energy-LB	1.275	21.503	0.102	-59.824	0.073	11.211	3.334	0	-22.33	7.24	97.5 127.1	-	
M2L2-trans	**BFBFH2-M2L2 Rh-sq-trans**	2.520	44.271	0.248	-117.958	0.032	4.284	-4.615	0	-71.22	7.43 7.43	102.9 122.9 110.2 115.2	176.1 177.6	
	BFBFH2-M2L2 Rh-sq-trans-energy-LA	1.243	19.869	0.121	-59.572	0.021	8.721	3.243	0	-26.35	7.43	102.9 122.9	-	
	BFBFH2-M2L2 Rh-sq-trans-en ergy-LB	1.241	19.733	0.127	-59.558	0.011	8.583	3.236	0	-26.63	7.43	110.2 115.2	-	
M2L-syn	**BFBFH2-M2L-Rh-sq-syn**	1.109	49.033	0.124	-56.623	0.048	4.665	3.425	0	1.78	6.63	110.6 106.2	-	
	BFBFH2-M2L-Rh-sq-syn-energy	1.042	29.258	0.124	-58.538	0.048	9.936	3.425	0	-14.70	6.63	110.6 106.2	-	
M2L-anti	**BFBFH2-M2L-Rh-sq-anti**	1.299	54.593	0.096	-56.486	0.115	6.873	3.417	0	9.90	6.53	95.7 123.9	-	
	BFBFH2-M2L-Rh-sq-anti-energy	1.239	35.104	0.096	-58.409	0.115	10.917	3.417	0	-7.52	6.53	95.7 123.9		

a) calculated as dihedrals O1-C1-C2-C3 and O2-C1-C2-C4.

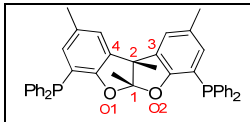
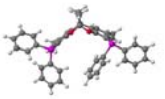
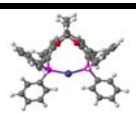
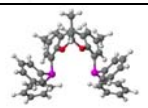
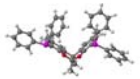
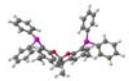
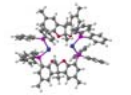
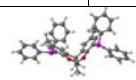
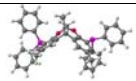
Ligand 13 DBDOC-PPh2

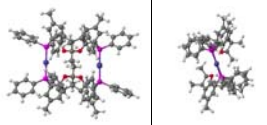
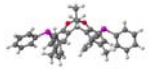
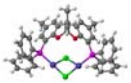
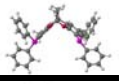
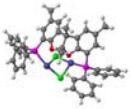
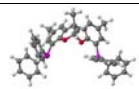
		stretch	angle	Stretch bend	dihedral	improper torsion	Van der Waals	electrostatics	H bond	U	PP distance	Ligand bending [a]	P-M-P angle	Minimizad conformations
L	DBDOC-L-energy	1.449	9.676	0.057	-61.849	0.012	16.000	1.580	0	-33.1	6.95	107.9 103.3	-	
ML	DBDOC-ML	1.244	16.522	-0.001	-51.476	0.245	12.929	2.199	0	-18.3	4.31	96.9 99.4	136.9	
	DBDOC-ML-energy	1.183	14.243	-0.001	-52.066	0.245	15.759	2.199	0	-18.4	4.31	96.9 99.4	-	
M2L2-Rh-unconfigured	DBDOC-M2L2 Rh-unc	2.386	30.225	0.078	-121.966	0.090	7.342	4.927	0	-76.9	6.64 6.98	109.1 99.3 114.4 96.6	112.5 115.0	 
	DBDOC-M2L2-Rh-unc-energy-LA	1.144	12.558	0.026	-61.670	0.035	14.763	1.644	0	-31.5	6.64	109.1 99.3	-	
	DBDOC- M2L2-Rh-unc-energy-LB	1.235	12.542	0.051	-61.437	0.054	16.322	1.669	0	-29.6	6.98	114.4 96.6	-	
M2L2-cis	DBDOC-M2L2 Rh-sq-cis	2.625	33.350	0.066	-121.884	0.087	8.142	-10.477	0	-88.1	6.69 6.85	100.4 108.4 94.5 115.5	97.6 101.5	
	DBDOC-M2L2 Rh-sq-cis-energy-LA	1.271	11.964	0.023	-61.757	0.024	15.543	1.651	0	-31.3	6.69	100.4 108.4	-	
	DBDOC-M2L2 Rh-sq-cis-energy-LB	1.337	12.818	0.044	-61.270	0.063	16.542	1.669	0	-28.8	6.85	94.5 115.5	-	

M2L2-trans	**DBDOC-M2L2 Rh-sq-trans**	2.437	30.145	0.117	-121.74	0.048	12.657	-8.033	0	-84.4	7.12 7.13	99.9 111.4 104.6 106.5	175.2 178.1		
	DBDOC-M2L2 Rh-sq-trans-energy-LA	1.216	12.619	0.060	-61.290	0.028	14.472	1.558	0	-31.3	7.12	99.9 111.4	-		
	DBDOC-M2L2 Rh-sq-trans-en ergy-LB	1.180	12.960	0.057	-61.626	0.021	14.249	1.554	0	-31.6	7.13	104.6 106.5	-		
M2L-syn	**DBDOC-M2L-Rh-sq-syn**	1.042	41.454	0.047	-59.836	0.034	9.787	1.745	0	-5.7	6.54	105.7 101.3	-		
	DBDOC-M2L Rh-sq-syn-energy	0.994	22.414	0.047	-61.746	0.034	15.121	1.745	0	-21.4	6.54	105.7 101.3	-		
ML2-anti	**DBDOC-M2L-Rh-sq-anti**	1.458	46.316	0.042	-58.499	0.081	12.914	1.739	0	4.0	6.43	116.7 92.0			
	DBDOC-M2L Rh-sq-anti-energy	1.402	26.790	0.042	-60.422	0.081	16.526	1.739	0	-13.8	6.43	116.7 92.0			

a) calculated as dihedrals O1-C1-C2-C3 and O2-C1-C2-C4.

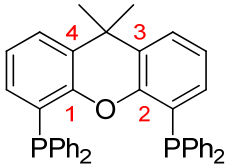
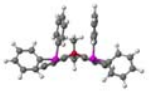
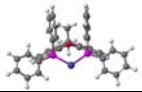
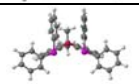
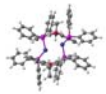
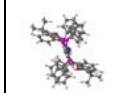
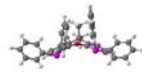
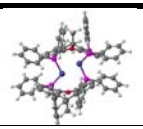
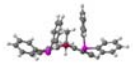
Ligand 4 BFBF-PPh2

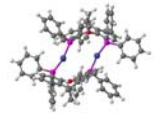
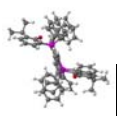
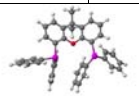
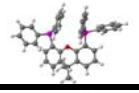
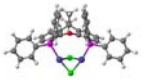
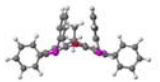
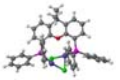
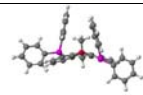
			stretch	angle	Stretch bend	dihedral	improper torsion	Van der Waals	electrostatics	H bond	U	PP distance	Ligand bending [a]	P-M-P angle	Minimizad conformations
L	BFBF-L-energy		1.615	17.102	0.235	-59.606	0.009	9.460	3.264	0	-27.9	7.26	116.2 107.0		
ML	BFBF-ML		1.470	26.490	0.197	-47.327	0.358	6.227	3.868	0	-8.7	4.36	100.8 102.6	140.1	
	BFBF-ML-energy		1.389	24.018	0.197	-47.916	0.358	9.160	3.868	0	-8.9	4.36	100.8 102.6	-	
M2L2-Rh-unconfigured	BFBF-M2L2 Rh-unc		2.657	46.089	0.432	-117.906	0.085	-6.014	8.287	0	-66.4	6.94 7.37	101.2 119.2 102.9 121.1	113.0 115.8	
	BFBF-M2L2-Rh-unc-energy-LA		1.285	20.800	0.209	-59.493	0.040	8.167	0.040	0	-25.7	6.94	101.2 119.2	-	
	BFBF- M2L2-Rh-unc-energy-LB		1.370	20.566	0.223	-59.556	0.045	9.588	3.360	0	-24.4	7.37	102.9 121.1	-	
M2L2-cis	BFBF-M2L2 Rh-sq-cis		2.837	49.598	0.419	-117.924	0.098	-5.878	-7.193	0	-78.0	6.98 7.23	103.7 116.9 98.7 124.3	96.8 100.9	
	BFBF-M2L2 Rh-sq-cis-energy-LA		1.404	19.945	0.208	-59.468	0.034	9.009	3.338	0	-25.5	6.98	103.7 116.9	-	
	BFBF-M2L2 Rh-sq-cis-energy-LB		1.423	21.295	0.211	-59.590	0.063	9.594	3.361	0	-23.6	7.23	98.7 124.3	-	

M2L2-trans	**BFBF-M2L2 Rh-sq-trans**	2.834	44.318	0.479	-117.558	0.030	-2.273	-4.651	0	-76.8	7.53 7.55	120.0 104.8 112.8 112.0	179.2 178.3		
	BFBF-M2L2 Rh-sq-trans-energy-LA	1.382	20.188	0.235	-59.408	0.016	8.139	3.234	0	-26.2	7.53	120.0 104.8	-		
	BFBF-M2L2 Rh-sq-trans-en ergy-LB	1.414	19.878	0.244	-59.326	0.014	8.051	3.232	0	-26.5	7.55	112.8 112.0	-		
M2L-syn	**BFBF-M2L-Rh-sq-syn**	1.308	49.618	0.230	-56.826	0.042	3.252	3.426	0	1.0	6.64	110.3 105.7			
	BFBF-M2L Rh-sq-syn-energy	1.238	30.010	0.230	-58.741	0.042	8.723	3.426	0	-15.1	6.64	110.3 105.7			
ML2-anti	**BFBF-M2L-Rh-sq-anti**	1.449	55.306	0.190	-56.517	0.103	5.054	3.420	0	9.0	6.53	124.4 94.5	-		
	BFBF-M2L Rh-sq-anti-energy	1.388	35.589	0.190	-58.442	0.103	9.330	3.42	0	-8.4215	6.53	124.4 94.5	-		

a) calculated as average of dihedrals O1-C1-C2-C3 and O2-C1-C2-C4.

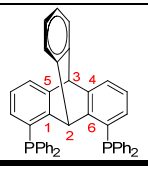
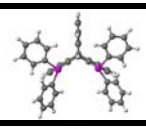
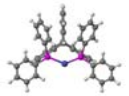
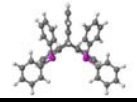
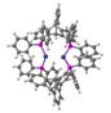
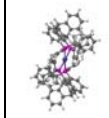
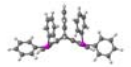
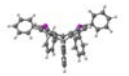
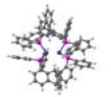
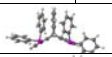
XANTPHOS-PPh2

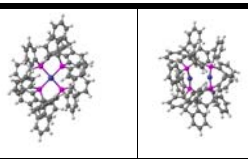
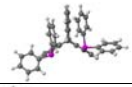
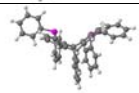
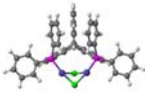
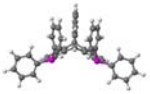
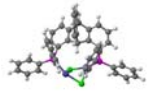
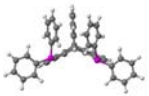
		stretch	angle	Stretch bend	dihedral	improper torsion	Van der Waals	electrostatics	H bond	U	PP distance	Ligand bending[a]	P-M-P angle	Minimized conformations
L	XANT-L-energy	1.802	6.896	0.024	-62.241	0.008	14.777	1.334	0	-37.4	4.15	137.0 136.6		
ML	XANT-ML	1.634	12.637	0.025	-61.417	0.008	10.932	1.483	0	-34.7	3.80	135.1 134.8	110.4	
	XANT-ML-energy	1.623	10.270	0.025	-62.015	0.008	13.453	1.483	0	-35.1	3.80	135.1 134.8	-	
M2L2-Rh-unconfigured	XANT-M2L2 Rh-unc	3.846	28.375	0.040	-119.741	0.194	11.086	3.487	0	-72.7	4.78 4.80	135.8 138.9 136.9 135.6	130.7 130.3	 
	XANT-M2L2-Rh-unc-energy-LA	1.916	10.555	0.021	-60.242	0.098	14.178	1.065	0	-32.4	4.78	135.8 138.9	-	
	XANT- M2L2-Rh-unc-energy-LB	1.922	10.857	0.019	-60.616	0.096	14.387	1.062	0	-32.3	4.80	136.9 135.6	-	
M2L2-cis	XANT-M2L2 Rh-sq-cis	4.420	38.389	0.043	-118.133	0.279	13.436	-11.150	0	-72.7	4.89 4.90	137.8 141.9 138.2 136.0	106.9 108.3	 
	XANT-M2L2 Rh-sq-cis-energy-LA	2.230	10.704	0.023	-59.327	0.141	14.928	1.050	0	-30.2	4.89	137.8 141.9	-	
	XANT-M2L2 Rh-sq-cis-energy-LB	2.174	10937	0.020	-59.913	0.138	15.375	1.043	0	-30.2	4.90	138.2 136.0	-	

M2L2-trans	**XANT-M2L2 Rh-sq-trans**	4.063	38.086	0.040	-119.006	0.194	16.357	-9.067	0	-69.3	4.93 4.94	136.3 135.5 135.1 138.1	168.2 166.0		
	XANT-M2L2 Rh-sq-trans-energy-LA	2.002	12.828	0.020	-60.401	0.090	15.562	0.983	0	-28.9	4.93	136.3 135.5	-		
	XANT-M2L2 Rh-sq-trans-en ergy-LB	2.029	12.500	0.020	-59.793	0.105	15.675	0.986	0	-28.5	4.94	135.1 138.1	-		
4.93M2L-syn	**XANT-M2L-Rh-sq-syn**	2.144	45.091	0.020	-59.131	0.071	8.926	1.047	0	-1.8	5.03	137.2 137.3			
	XANT-M2L Rh-sq-syn-energy	2.102	18.926	0.020	-61.020	0.071	14.231	1.047	0	-24.6	5.03	137.2 137.3			
ML2-anti	**XANT-M2L-Rh-sq-anti**	2.411	54.593	0.028	-57.273	0.077	6.939	1.009	0	7.8	5.15	147.8 142.4	-		
	XANT-M2L Rh-sq-anti-energy	2.256	23.184	0.028	-59.199	0.077	14.223	1.009	0	-18.4	5.15	147.8 142.4			

a) calculated as dihedrals C1-O-CMe_2-C3 and C2-O-CMe_2-C4.

TRIPTYCENE-PPh2

		stretch	angle	Stretch bend	dihedral	improper torsion	Van der Waals	electrostatics	H bond	U	PP distance	Ligand bending[a]	P-M-P angle	Minimizad conformations
L	**TRIPT-L-energy**	1.560	12.155	0.000	-68.328	0.039	19.458	-0.659	0	-35.8	4.53	119.9 120.1		
ML	**TRIPT-ML**	1.402	17.125	0.000	-67.349	0.009	14.047	-0.439	0	-35.2	4.08	117.7 117.4	123.6	
ML	**TRIPT-ML-energy**	1.382	14.778	0.000	-67.948	0.009	16.446	-0.439	0	-35.8	4.08	117.7 117.4		
M2L2-Rh-unconfigured	**TRIPT-M2L2 Rh-unc**	3.933	37.704	0.000	-133.447	0.073	11.163	0.093	0	-80.5	5.26 5.24	122.1 122.3 121.9 122.4	137.7 117.4	 
M2L2-Rh-unconfigured	**TRIPT-M2L2-Rh-unc-energy-LA**	1.984	15.976	0.000	-67.313	0.032	15.220	-0.559	0	-34.7	5.26	122.1 122.3	-	
M2L2-Rh-unconfigured	**TRIPT- M2L2-Rh-unc-energy-LB**	1.919	15.900	0.000	-67.313	0.041	14.981	-0.567	0	-35.0	5.24	121.9 122.4	-	
M2L2-cis	**TRIPT-M2L2 Rh-sq-cis**	4.086	41.107	0.000	-131.903	0.174	8.554	-15.390	0	-93.4	5.30 5.20	124.9 121.7 120.6 123.4	97.7 100.1	
M2L2-cis	**TRIPT-M2L2 Rh-sq-cis-energy-LA**	2.091	16.989	0.000	-66.178	0.075	15.608	-0.548	0	-32.0	5.30	124.9 121.7	-	
M2L2-cis	**TRIPT-M2L2 Rh-sq-cis-energy-LB**	1.970	15.593	0.000	-66.85	0.099	18.122	-0.661	0	-31.7	5.20	120.6 123.4	-	

M2L2-trans	**TRIPT-M2L2 Rh-sq-trans**	3.486	44.936	0.000	-127.434	0.327	6.211	-12.088	0	-84.6	4.74 4.74	117.7 123.2 117.6 123.1	168.2 172.3	
	TRIPT-M2L2 Rh-sq-trans-energy-LA	1.732	15.625	0.000	-64.288	0.163	14.697	-0.554	0	-32.6	4.74	117.7 123.2		
	TRIPT-M2L2 Rh-sq-trans-en ergy-LB	1.731	15.599	0.000	-64.284	0.164	14.674	-0.554	0	-32.7	4.74	117.6 123.1		
M2L-syn	**TRIPT-M2L-Rh-sq-syn**	1.970	46.524	0.000	-65.549	0.032	12.572	-0.551	0	-5.0	5.39	121.8 121.8	-	
	TRIPT-M2L Rh-sq-syn-energy	1.928	25.526	0.000	-67.483	0.032	13.584	-0.551	0	-27.0	5.39	121.8 121.8		
ML2-anti	**TRIPT-M2L-Rh-sq-anti**	2.281	56.316	0.000	-64.233	0.072	13.366	-0.595	0	7.2	5.49	126.1 123.0		
	TRIPT-M2L Rh-sq-anti-energy	2.133	27.898	0.000	-66.166	0.072	12.617	-0.595	0	-24.0	5.49	126.1 123.0		

a) calculated as dihedrals C1-C2-C3-C4 and C6-C2-C3-C5.

Crystallographic details: compound 17.

Table 1. Crystal data and structure refinement for JM045p21c.

Identification code	JM045p21c	
Empirical formula	C90 H76 Cl14 O6 P4 Rh2	
Formula weight	2079.51	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 16.6357(4) Å	α= 90.00 °.
	b = 18.7449(5) Å	β = 100.5780(10) °.
	c = 14.8117(4) Å	γ = 90.00 °.
Volume	4540.3(2) Å^3	
Z	2	
Density (calculated)	1.521 Mg/m^3	
Absorption coefficient	0.898 mm^{-1}	
F(000)	2104	
Crystal size	0.10 x 0.10 x 0.05 mm^3	
Theta range for data collection	2.50 to 39.65 °.	
Index ranges	-18 <=h<=29 ,-29 <=k<=33 ,-26 <=l<=20	
Reflections collected	90973	
Independent reflections	26435 [R(int) = 0.0223]	
Completeness to theta =39.65 °	0.960 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9565 and 0.9155	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	26435 / 0 / 527	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0349 , wR2 = 0.0955	
R indices (all data)	R1 = 0.0435 , wR2 = 0.1021	
Largest diff. peak and hole	2.153 and -1.885 e.Å^{-3}	

Table 2. Bond lengths [Å] and angles [°] for JM045p21c.

Bond lengths----	
Rh1-C1	1.8114(11)
Rh1-P1	2.3161(3)
Rh1-P2	2.3349(3)
Rh1-Cl1	2.3792(3)
P1-C2	1.8192(11)
P1-C14	1.8227(10)
P1-C8	1.8251(11)
C1-O1	1.1519(14)
P2-C34	1.8183(11)
P2-C28	1.8269(11)
P2-C40	1.8268(11)
C2-C7	1.3939(16)
C2-C3	1.4046(16)
O2-C23	1.3687(13)
O2-C22	1.4665(13)
C3-C4	1.3909(18)
O3-C21	1.3825(13)
O3-C22	1.4142(13)
C4-C5	1.397(2)
C5-C6	1.394(2)
C6-C7	1.3958(18)
C8-C9	1.3942(16)
C8-C13	1.4013(15)
C9-C10	1.3953(18)
C10-C11	1.388(2)
C11-C12	1.391(2)
C12-C13	1.3947(18)
C14-C23	1.3920(15)
C14-C15	1.4093(14)
C15-C16	1.4003(15)
C16-C17	1.4041(17)
C16-C24	1.5099(16)
C17-C18	1.3853(15)
C18-C23	1.3886(14)
C18-C19	1.5086(15)

C19-C20	1.5221(15)
C19-C25	1.5267(15)
C19-C22	1.5704(15)
C20-C27	1.3835(16)
C20-C21	1.3908(15)
C21-C40#1	1.3958(14)
C22-C26	1.5051(16)
C27-C42#1	1.4030(17)
C28-C33	1.3954(16)
C28-C29	1.3960(16)
C29-C30	1.3888(17)
C30-C31	1.392(2)
C31-C32	1.392(2)
C32-C33	1.3920(19)
C34-C39	1.3966(17)
C34-C35	1.3991(17)
C35-C36	1.3916(19)
C36-C37	1.389(2)
C37-C38	1.390(2)
C38-C39	1.394(2)
C40-C21#1	1.3958(14)
C40-C41	1.4101(16)
C41-C42	1.3968(17)
C42-C27#1	1.4030(17)
C42-C43	1.5086(19)
C1S-Cl3S	1.7375(16)
C1S-Cl2S	1.7540(17)
C1S-Cl1S	1.7637(16)
C2S-Cl4S	1.750(2)
C2S-Cl6S	1.7551(19)
C2S-Cl5S	1.767(2)

Angles----------

C1-Rh1-P1	90.27(3)
C1-Rh1-P2	89.58(3)
P1-Rh1-P2	167.857(10)
C1-Rh1-Cl1	176.46(3)
P1-Rh1-Cl1	87.899(10)

P2-Rh1-Cl1	92.847(10)
C2-P1-C14	103.16(5)
C2-P1-C8	108.17(5)
C14-P1-C8	101.43(5)
C2-P1-Rh1	107.07(3)
C14-P1-Rh1	116.09(3)
C8-P1-Rh1	119.58(3)
O1-C1-Rh1	178.16(10)
C34-P2-C28	103.09(5)
C34-P2-C40	105.23(5)
C28-P2-C40	104.27(5)
C34-P2-Rh1	111.03(4)
C28-P2-Rh1	113.06(3)
C40-P2-Rh1	118.71(4)
C7-C2-C3	119.58(10)
C7-C2-P1	123.37(9)
C3-C2-P1	117.03(8)
C23-O2-C22	107.23(8)
C4-C3-C2	120.32(12)
C21-O3-C22	106.64(8)
C3-C4-C5	119.74(13)
C6-C5-C4	120.20(12)
C5-C6-C7	120.03(13)
C2-C7-C6	120.13(12)
C9-C8-C13	119.44(10)
C9-C8-P1	119.91(8)
C13-C8-P1	120.42(8)
C8-C9-C10	119.91(11)
C11-C10-C9	120.60(12)
C10-C11-C12	119.72(12)
C11-C12-C13	120.11(12)
C12-C13-C8	120.19(11)
C23-C14-C15	116.12(9)
C23-C14-P1	118.61(7)
C15-C14-P1	125.24(8)
C16-C15-C14	122.27(10)
C15-C16-C17	119.29(10)
C15-C16-C24	120.47(11)

C17-C16-C24	120.21(10)
C18-C17-C16	119.23(10)
C17-C18-C23	120.26(10)
C17-C18-C19	132.02(10)
C23-C18-C19	107.72(9)
C18-C19-C20	112.02(9)
C18-C19-C25	114.58(9)
C20-C19-C25	113.13(9)
C18-C19-C22	101.17(8)
C20-C19-C22	98.74(8)
C25-C19-C22	115.61(10)
C27-C20-C21	120.37(10)
C27-C20-C19	130.84(10)
C21-C20-C19	108.77(9)
O3-C21-C20	112.18(9)
O3-C21-C40#1	125.10(9)
C20-C21-C40#1	122.72(10)
O3-C22-O2	107.47(8)
O3-C22-C26	109.08(9)
O2-C22-C26	107.73(9)
O3-C22-C19	107.46(8)
O2-C22-C19	104.39(8)
C26-C22-C19	120.04(9)
O2-C23-C18	113.45(9)
O2-C23-C14	123.80(9)
C18-C23-C14	122.75(9)
C20-C27-C42#1	119.21(10)
C33-C28-C29	119.26(10)
C33-C28-P2	122.19(9)
C29-C28-P2	118.44(8)
C30-C29-C28	120.78(11)
C29-C30-C31	119.67(12)
C30-C31-C32	119.98(12)
C33-C32-C31	120.24(13)
C32-C33-C28	120.07(12)
C39-C34-C35	119.34(11)
C39-C34-P2	118.99(9)
C35-C34-P2	121.57(9)

C36-C35-C34	120.32(12)
C37-C36-C35	120.03(13)
C36-C37-C38	119.95(14)
C37-C38-C39	120.26(14)
C38-C39-C34	120.01(12)
C21-C40-C41#1	115.71(9)
C21-C40-P2#1	125.27(8)
C41-C40-P2	119.02(8)
C42-C41-C40	122.70(10)
C41-C42-C27#1	119.28(11)
C41-C42-C43	120.44(12)
C27-C42-C43#1	120.28(11)
Cl3S-C1S-Cl2S	110.90(10)
Cl3S-C1S-Cl1S	109.82(9)
Cl2S-C1S-Cl1S	110.42(9)
Cl4S-C2S-Cl6S	109.02(10)
Cl4S-C2S-Cl5S	110.86(11)
Cl6S-C2S-Cl5S	110.16(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2, -y+2, -z

Table 3. Torsion angles [°] for JM045p21c.

C1-Rh1-P1-C2	124.04(5)
P2-Rh1-P1-C2	34.79(6)
Cl1-Rh1-P1-C2	-58.98(4)
C1-Rh1-P1-C14	9.48(5)
P2-Rh1-P1-C14	-79.77(6)
Cl1-Rh1-P1-C14	-173.54(4)
C1-Rh1-P1-C8	-112.63(5)
P2-Rh1-P1-C8	158.12(6)
Cl1-Rh1-P1-C8	64.35(4)
P1-Rh1-C1-O1	82(3)
P2-Rh1-C1-O1	-111(3)
Cl1-Rh1-C1-O1	23(3)
C1-Rh1-P2-C34	-125.13(5)
P1-Rh1-P2-C34	-35.81(7)
Cl1-Rh1-P2-C34	57.44(4)
C1-Rh1-P2-C28	-9.83(5)
P1-Rh1-P2-C28	79.50(6)
Cl1-Rh1-P2-C28	172.74(4)
C1-Rh1-P2-C40	112.77(5)
P1-Rh1-P2-C40	-157.91(5)
Cl1-Rh1-P2-C40	-64.66(4)
C14-P1-C2-C7	-107.93(10)
C8-P1-C2-C7	-1.02(11)
Rh1-P1-C2-C7	129.09(9)
C14-P1-C2-C3	74.08(10)
C8-P1-C2-C3	-179.01(9)
Rh1-P1-C2-C3	-48.89(9)
C7-C2-C3-C4	0.65(18)
P1-C2-C3-C4	178.71(10)
C2-C3-C4-C5	-0.5(2)
C3-C4-C5-C6	-0.1(2)
C4-C5-C6-C7	0.4(2)
C3-C2-C7-C6	-0.30(18)
P1-C2-C7-C6	-178.23(10)
C5-C6-C7-C2	-0.2(2)
C2-P1-C8-C9	107.93(10)

C14-P1-C8-C9	-143.96(10)
Rh1-P1-C8-C9	-14.86(11)
C2-P1-C8-C13	-77.58(10)
C14-P1-C8-C13	30.53(10)
Rh1-P1-C8-C13	159.62(8)
C13-C8-C9-C10	-1.39(19)
P1-C8-C9-C10	173.15(11)
C8-C9-C10-C11	-0.1(2)
C9-C10-C11-C12	1.4(2)
C10-C11-C12-C13	-1.1(2)
C11-C12-C13-C8	-0.3(2)
C9-C8-C13-C12	1.60(18)
P1-C8-C13-C12	-172.92(10)
C2-P1-C14-C23	175.72(8)
C8-P1-C14-C23	63.76(9)
Rh1-P1-C14-C23	-67.52(9)
C2-P1-C14-C15	-5.90(10)
C8-P1-C14-C15	-117.86(9)
Rh1-P1-C14-C15	110.86(9)
C23-C14-C15-C16	0.71(15)
P1-C14-C15-C16	-177.71(8)
C14-C15-C16-C17	1.55(16)
C14-C15-C16-C24	-176.81(11)
C15-C16-C17-C18	-1.88(16)
C24-C16-C17-C18	176.49(11)
C16-C17-C18-C23	-0.04(16)
C16-C17-C18-C19	179.18(11)
C17-C18-C19-C20	-91.54(14)
C23-C18-C19-C20	87.76(11)
C17-C18-C19-C25	39.08(17)
C23-C18-C19-C25	-141.63(10)
C17-C18-C19-C22	164.17(11)
C23-C18-C19-C22	-16.53(11)
C18-C19-C20-C27	59.63(15)
C25-C19-C20-C27	-71.72(16)
C22-C19-C20-C27	165.51(12)
C18-C19-C20-C21	-118.58(10)
C25-C19-C20-C21	110.07(11)

C22-C19-C20-C21	-12.70(11)
C22-O3-C21-C20	17.23(12)
C22-O3-C21-C40#1	-162.48(10)
C27-C20-C21-O3	179.97(10)
C19-C20-C21-O3	-1.60(12)
C27-C20-C21-C40#1	-0.31(17)
C19-C20-C21-C40#1	178.12(10)
C21-O3-C22-O2	86.62(10)
C21-O3-C22-C26	-156.84(9)
C21-O3-C22-C19	-25.23(10)
C23-O2-C22-O3	-136.90(9)
C23-O2-C22-C26	105.69(10)
C23-O2-C22-C19	-22.97(10)
C18-C19-C22-O3	137.48(8)
C20-C19-C22-O3	22.84(10)
C25-C19-C22-O3	-98.12(10)
C18-C19-C22-O2	23.55(10)
C20-C19-C22-O2	-91.09(9)
C25-C19-C22-O2	147.95(9)
C18-C19-C22-C26	-97.22(11)
C20-C19-C22-C26	148.14(10)
C25-C19-C22-C26	27.18(14)
C22-O2-C23-C18	13.22(12)
C22-O2-C23-C14	-166.75(9)
C17-C18-C23-O2	-177.51(10)
C19-C18-C23-O2	3.09(12)
C17-C18-C23-C14	2.46(16)
C19-C18-C23-C14	-176.93(9)
C15-C14-C23-O2	177.24(9)
P1-C14-C23-O2	-4.23(14)
C15-C14-C23-C18	-2.73(15)
P1-C14-C23-C18	175.80(8)
C21-C20-C27-C42#1	-0.06(18)
C19-C20-C27-C42#1	-178.10(12)
C34-P2-C28-C33	19.44(11)
C40-P2-C28-C33	129.15(10)
Rh1-P2-C28-C33	-100.53(10)
C34-P2-C28-C29	-164.42(9)

C40-P2-C28-C29	-54.70(10)
Rh1-P2-C28-C29	75.62(9)
C33-C28-C29-C30	-0.99(17)
P2-C28-C29-C30	-177.25(10)
C28-C29-C30-C31	0.6(2)
C29-C30-C31-C32	0.2(2)
C30-C31-C32-C33	-0.4(3)
C31-C32-C33-C28	0.0(2)
C29-C28-C33-C32	0.70(19)
P2-C28-C33-C32	176.82(11)
C28-P2-C34-C39	-113.18(12)
C40-P2-C34-C39	137.81(11)
Rh1-P2-C34-C39	8.16(12)
C28-P2-C34-C35	63.32(12)
C40-P2-C34-C35	-45.68(13)
Rh1-P2-C34-C35	-175.33(11)
C39-C34-C35-C36	2.6(2)
P2-C34-C35-C36	-173.92(14)
C34-C35-C36-C37	-1.8(3)
C35-C36-C37-C38	-0.9(4)
C36-C37-C38-C39	2.7(4)
C37-C38-C39-C34	-1.9(3)
C35-C34-C39-C38	-0.8(3)
P2-C34-C39-C38	175.81(16)
C34-P2-C40-C21#1	80.33(10)
C28-P2-C40-C21#1	-27.82(11)
Rh1-P2-C40-C21#1	-154.70(8)
C34-P2-C40-C41	-99.84(10)
C28-P2-C40-C41	152.01(9)
Rh1-P2-C40-C41	25.13(10)
C21#1-C40-C41-C42	-0.60(18)
P2-C40-C41-C42	179.56(10)
C40-C41-C42-C27#1	1.0(2)
C40-C41-C42-C43	-179.56(14)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2, -y+2, -z

Crystallographic details: compound 19.

Table 1. Crystal data and structure refinement for JM233-5.

Identification code	JM233-5	
Empirical formula	C82 H76 Cl2 O12 P4 Rh2	
Formula weight	1654.03	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 18.1626(9) Å	α= 90.00 °.
	b = 17.4391(9) Å	β = 108.713(2) °.
	c = 13.3646(6) Å	γ = 90.00 °.
Volume	4009.3(3) $Å^3$	
Z	2	
Density (calculated)	1.370 Mg/m^3	
Absorption coefficient	0.616 mm^{-1}	
F(000)	1696	
Crystal size	0.2 x 0.2 x 0.3 mm^3	
Theta range for data collection	2.62 to 36.54°.	
Index ranges	0 <=h<=30 ,-26 <=k<=0 ,-21 <=l<=21	
Reflections collected	49393	
Independent reflections	17840 [R(int) = 0.0674]	
Completeness to theta =36.54 °	90.2 %	
Absorption correction	Empirical	
Max. and min. transmission	0.98 and 0.81	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17840 / 124 / 546	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0728 , wR2 = 0.1971	
R indices (all data)	R1 = 0.0999 , wR2 = 0.2213	
Largest diff. peak and hole	3.597 and -1.773 $e.Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for JM233-5.

Bond lengths----	
Rh1-C1	1.819(3)
Rh1-P1	2.3056(9)
Rh1-P2	2.3228(8)
Rh1-Cl1	2.3764(8)
P1-C8'	1.785(10)
P1-C40	1.800(3)
P1-C2	1.831(3)
P1-C8	1.842(2)
C1-O1	1.137(4)
C2-C3	1.384(4)
C2-C7	1.392(5)
P2-C14	1.807(3)
P2-C26	1.823(3)
P2-C20	1.833(3)
C7-C6	1.387(5)
O2-C31	1.380(3)
O2-C34	1.422(3)
C6-C5	1.389(6)
O3-C35	1.369(4)
O3-C34	1.455(3)
C5-C4	1.367(5)
C4-C3	1.402(5)
C8-C9	1.3900
C8-C13	1.3900
C9-C10	1.3900
C10-C11	1.3900
C11-C12	1.3900
C12-C13	1.3900
C8'-C9'	1.369(17)
C8'-C13'	1.443(16)
C9'-C10'	1.451(19)
C10'-C11'	1.371(19)
C11'-C12'	1.45(2)
C12'-C13'	1.34(2)
C14-C19	1.386(5)

C14-C15	1.406(5)
C15-C16	1.388(6)
C16-C17	1.380(7)
C17-C18	1.365(6)
C18-C19	1.391(5)
C20-C21	1.393(4)
C20-C25	1.396(5)
C21-C22	1.388(5)
C22-C23	1.396(6)
C23-C24	1.394(5)
C24-C25	1.392(4)
C26-C31	1.384(4)
C26-C27	1.412(4)
C27-C28	1.405(5)
C28-C29	1.402(4)
C28-C32	1.500(4)
C29-C30	1.372(4)
C30-C31	1.393(4)
C30-C33	1.502(4)
C33-C36	1.503(4)
C33-C34	1.547(4)
C35-C36	1.387(4)
C35-C40#1	1.400(4)
C36-C37	1.382(4)
C37-C38	1.402(4)
C38-C39	1.391(4)
C38-C41	1.509(5)
C39-C40#1	1.411(4)
C40-C35#1	1.400(4)
C40-C39#1	1.411(4)

Angles----------

C1-Rh1-P1	89.21(11)
C1-Rh1-P2	92.93(11)
P1-Rh1-P2	162.88(3)
C1-Rh1-Cl1	177.23(10)
P1-Rh1-Cl1	89.28(3)
P2-Rh1-Cl1	89.20(3)

C8'-P1-C40	113.0(4)
C8'-P1-C2	98.4(4)
C40-P1-C2	103.50(14)
C8'-P1-C8	8.5(4)
C40-P1-C8	104.58(14)
C2-P1-C8	100.30(14)
C8'-P1-Rh1	117.1(4)
C40-P1-Rh1	103.91(10)
C2-P1-Rh1	120.49(11)
C8-P1-Rh1	121.80(10)
O1-C1-Rh1	177.0(3)
C3-C2-C7	119.3(3)
C3-C2-P1	122.4(3)
C7-C2-P1	117.9(2)
C14-P2-C26	104.32(14)
C14-P2-C20	104.70(14)
C26-P2-C20	104.72(13)
C14-P2-Rh1	117.02(11)
C26-P2-Rh1	115.65(10)
C20-P2-Rh1	109.23(11)
C6-C7-C2	120.5(3)
C31-O2-C34	107.4(2)
C7-C6-C5	119.8(4)
C35-O3-C34	107.3(2)
C4-C5-C6	119.9(3)
C5-C4-C3	120.6(3)
C2-C3-C4	119.8(3)
C9-C8-C13	120.0
C9-C8-P1	121.84(15)
C13-C8-P1	117.87(15)
C10-C9-C8	120.0
C9-C10-C11	120.0
C10-C11-C12	120.0
C11-C12-C13	120.0
C12-C13-C8	120.0
C9'-C8'-C13'	118.2(10)
C9'-C8'-P1	120.5(8)
C13'-C8'-P1	121.2(9)

C8'-C9'-C10'	118.6(11)
C11'-C10'-C9'	123.4(14)
C10'-C11'-C12'	116.1(13)
C13'-C12'-C11'	120.9(14)
C12'-C13'-C8'	122.5(14)
C19-C14-C15	118.5(3)
C19-C14-P2	122.4(2)
C15-C14-P2	119.1(3)
C16-C15-C14	120.0(4)
C17-C16-C15	120.2(4)
C18-C17-C16	120.5(4)
C17-C18-C19	120.0(4)
C14-C19-C18	120.9(3)
C21-C20-C25	119.0(3)
C21-C20-P2	122.9(3)
C25-C20-P2	118.0(2)
C22-C21-C20	120.8(3)
C21-C22-C23	120.1(3)
C24-C23-C22	119.3(3)
C25-C24-C23	120.3(3)
C24-C25-C20	120.4(3)
C31-C26-C27	115.9(3)
C31-C26-P2	120.3(2)
C27-C26-P2	123.1(2)
C28-C27-C26	122.2(3)
C29-C28-C27	118.7(3)
C29-C28-C32	119.9(3)
C27-C28-C32	121.4(3)
C30-C29-C28	120.2(3)
C29-C30-C31	119.6(2)
C29-C30-C33	132.0(3)
C31-C30-C33	108.3(2)
O2-C31-C26	123.6(3)
O2-C31-C30	113.0(2)
C26-C31-C30	123.1(3)
C30-C33-C36	115.7(2)
C30-C33-C34	101.1(2)
C36-C33-C34	102.2(2)

O2-C34-O3	108.2(2)
O2-C34-C33	108.6(2)
O3-C34-C33	106.2(2)
O3-C35-C36	113.5(2)
O3-C35-C40#1	123.6(3)
C36-C35-C40#1	122.9(3)
C37-C36-C35	120.6(3)
C37-C36-C33	131.5(3)
C35-C36-C33	107.9(2)
C36-C37-C38	118.8(3)
C39-C38-C37	119.7(3)
C39-C38-C41	120.5(3)
C37-C38-C41	119.8(3)
C38-C39-C40#1	122.8(3)
C35#1-C40-C39#1	115.2(3)
C35-C40-P1#1	119.0(2)
C39-C40-P1#1	125.4(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, -z+2

Table 3. Torsion angles [°] for JM233-5.

C1-Rh1-P1-C8'	121.5(4)
P2-Rh1-P1-C8'	-141.2(4)
Cl1-Rh1-P1-C8'	-56.2(4)
C1-Rh1-P1-C40	-113.12(13)
P2-Rh1-P1-C40	-15.74(14)
Cl1-Rh1-P1-C40	69.19(9)
C1-Rh1-P1-C2	2.03(14)
P2-Rh1-P1-C2	99.41(14)
Cl1-Rh1-P1-C2	-175.65(11)
C1-Rh1-P1-C8	129.57(15)
P2-Rh1-P1-C8	-133.05(14)
Cl1-Rh1-P1-C8	-48.12(12)
P1-Rh1-C1-O1	-18(6)
P2-Rh1-C1-O1	179(100)
Cl1-Rh1-C1-O1	39(7)
C8'-P1-C2-C3	105.4(5)
C40-P1-C2-C3	-10.8(3)
C8-P1-C2-C3	97.0(3)
Rh1-P1-C2-C3	-126.2(3)
C8'-P1-C2-C7	-67.3(5)
C40-P1-C2-C7	176.5(3)
C8-P1-C2-C7	-75.7(3)
Rh1-P1-C2-C7	61.1(3)
C1-Rh1-P2-C14	-138.76(16)
P1-Rh1-P2-C14	124.41(15)
Cl1-Rh1-P2-C14	39.47(13)
C1-Rh1-P2-C26	-15.19(13)
P1-Rh1-P2-C26	-112.02(13)
Cl1-Rh1-P2-C26	163.04(10)
C1-Rh1-P2-C20	102.58(14)
P1-Rh1-P2-C20	5.76(15)
Cl1-Rh1-P2-C20	-79.19(10)
C3-C2-C7-C6	-1.2(6)
P1-C2-C7-C6	171.8(3)
C2-C7-C6-C5	0.0(6)
C7-C6-C5-C4	1.2(6)

C6-C5-C4-C3	-1.3(6)
C7-C2-C3-C4	1.1(5)
P1-C2-C3-C4	-171.5(3)
C5-C4-C3-C2	0.2(6)
C8'-P1-C8-C9	-121(3)
C40-P1-C8-C9	63.7(2)
C2-P1-C8-C9	-43.3(2)
Rh1-P1-C8-C9	-179.35(17)
C8'-P1-C8-C13	53(3)
C40-P1-C8-C13	-122.5(2)
C2-P1-C8-C13	130.5(2)
Rh1-P1-C8-C13	-5.5(2)
C13-C8-C9-C10	0.0
P1-C8-C9-C10	173.68(19)
C8-C9-C10-C11	0.0
C9-C10-C11-C12	0.0
C10-C11-C12-C13	0.0
C11-C12-C13-C8	0.0
C9-C8-C13-C12	0.0
P1-C8-C13-C12	-173.93(19)
C40-P1-C8'-C9'	60.9(11)
C2-P1-C8'-C9'	-47.7(11)
C8-P1-C8'-C9'	56(2)
Rh1-P1-C8'-C9'	-178.3(9)
C40-P1-C8'-C13'	-122.0(10)
C2-P1-C8'-C13'	129.4(10)
C8-P1-C8'-C13'	-127(3)
Rh1-P1-C8'-C13'	-1.3(12)
C13'-C8'-C9'-C10'	-1(2)
P1-C8'-C9'-C10'	175.9(11)
C8'-C9'-C10'-C11'	5(2)
C9'-C10'-C11'-C12'	-6(2)
C10'-C11'-C12'-C13'	5(2)
C11'-C12'-C13'-C8'	-2(3)
C9'-C8'-C13'-C12'	0(2)
P1-C8'-C13'-C12'	-176.8(13)
C26-P2-C14-C19	90.9(3)
C20-P2-C14-C19	-18.8(3)

Rh1-P2-C14-C19	-139.9(3)
C26-P2-C14-C15	-88.7(3)
C20-P2-C14-C15	161.6(3)
Rh1-P2-C14-C15	40.5(4)
C19-C14-C15-C16	-0.5(6)
P2-C14-C15-C16	179.2(4)
C14-C15-C16-C17	1.0(7)
C15-C16-C17-C18	-0.2(7)
C16-C17-C18-C19	-1.2(7)
C15-C14-C19-C18	-0.9(6)
P2-C14-C19-C18	179.4(3)
C17-C18-C19-C14	1.8(6)
C14-P2-C20-C21	100.6(3)
C26-P2-C20-C21	-8.8(3)
Rh1-P2-C20-C21	-133.3(3)
C14-P2-C20-C25	-82.3(3)
C26-P2-C20-C25	168.3(2)
Rh1-P2-C20-C25	43.8(3)
C25-C20-C21-C22	-3.0(5)
P2-C20-C21-C22	174.1(3)
C20-C21-C22-C23	1.5(5)
C21-C22-C23-C24	1.6(5)
C22-C23-C24-C25	-3.2(5)
C23-C24-C25-C20	1.7(5)
C21-C20-C25-C24	1.4(5)
P2-C20-C25-C24	-175.8(2)
C14-P2-C26-C31	-169.8(2)
C20-P2-C26-C31	-60.0(3)
Rh1-P2-C26-C31	60.2(3)
C14-P2-C26-C27	20.7(3)
C20-P2-C26-C27	130.4(3)
Rh1-P2-C26-C27	-109.3(3)
C31-C26-C27-C28	-0.9(4)
P2-C26-C27-C28	169.1(2)
C26-C27-C28-C29	-2.3(5)
C26-C27-C28-C32	-179.3(3)
C27-C28-C29-C30	1.3(5)
C32-C28-C29-C30	178.3(3)

C28-C29-C30-C31	2.8(4)
C28-C29-C30-C33	-174.3(3)
C34-O2-C31-C26	-179.6(3)
C34-O2-C31-C30	-4.9(3)
C27-C26-C31-O2	179.4(3)
P2-C26-C31-O2	9.1(4)
C27-C26-C31-C30	5.2(4)
P2-C26-C31-C30	-165.1(2)
C29-C30-C31-O2	178.9(3)
C33-C30-C31-O2	-3.3(3)
C29-C30-C31-C26	-6.4(4)
C33-C30-C31-C26	171.4(3)
C29-C30-C33-C36	-63.9(4)
C31-C30-C33-C36	118.7(3)
C29-C30-C33-C34	-173.4(3)
C31-C30-C33-C34	9.2(3)
C31-O2-C34-O3	-103.9(2)
C31-O2-C34-C33	10.9(3)
C35-O3-C34-O2	133.1(2)
C35-O3-C34-C33	16.7(3)
C30-C33-C34-O2	-12.2(3)
C36-C33-C34-O2	-131.9(2)
C30-C33-C34-O3	103.9(2)
C36-C33-C34-O3	-15.8(3)
C34-O3-C35-C36	-11.0(3)
C34-O3-C35-C40#1	168.9(3)
O3-C35-C36-C37	-178.3(3)
C40#1-C35-C36-C37	1.7(4)
O3-C35-C36-C33	0.3(3)
C40#1-C35-C36-C33	-179.6(3)
C30-C33-C36-C37	79.2(4)
C34-C33-C36-C37	-171.9(3)
C30-C33-C36-C35	-99.2(3)
C34-C33-C36-C35	9.6(3)
C35-C36-C37-C38	-0.7(4)
C33-C36-C37-C38	-179.0(3)
C36-C37-C38-C39	-0.3(4)
C36-C37-C38-C41	-179.5(3)

C37-C38-C39-C40#1	0.5(5)
C41-C38-C39-C40#1	179.6(3)
C8'-P1-C40-C35#1	178.8(4)
C2-P1-C40-C35#1	-75.9(3)
C8-P1-C40-C35#1	179.5(2)
Rh1-P1-C40-C35#1	50.8(2)
C8'-P1-C40-C39#1	5.5(5)
C2-P1-C40-C39#1	110.8(3)
C8-P1-C40-C39#1	6.2(3)
Rh1-P1-C40-C39#1	-122.5(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, -z+2

Crystallographic details: compound 20.

Table 1. Crystal data and structure refinement for JM147_0m.

Identification code	JM147_0m	
Empirical formula	C88 H76 Cl10 O6 P4 Rh2	
Formula weight	1913.69	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 12.7468(5) Å	α= 90.00 °.
	b = 18.3066(7) Å	β = 105.1580(10) °.
	c = 19.1337(8) Å	γ = 90.00 °.
Volume	4309.5(3) Å^3	
Z	2	
Density (calculated)	1.475 Mg/m^3	
Absorption coefficient	0.819 mm^{-1}	
F(000)	1944	
Crystal size	0.20 x 0.10 x 0.05 mm^3	
Theta range for data collection	3.28 to 37.50 °.	
Index ranges	-21 <=h<=10 ,-31 <=k<=31 ,-32 <=l<=29	
Reflections collected	65761	
Independent reflections	21725 [R(int) = 0.0224]	
Completeness to theta =37.50 °	0.957 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9602 and 0.8533	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	21725 / 57 / 538	
Goodness-of-fit on F^2	1.075	
Final R indices [I>2sigma(I)]	R1 = 0.0456 , wR2 = 0.1284	
R indices (all data)	R1 = 0.0558 , wR2 = 0.1385	
Largest diff. peak and hole	1.854 and -2.240 e.Å^{-3}	

Table 2. Bond lengths [Å] and angles [°] for JM147_0m.

Bond lengths----	
Rh1-C1	1.8123(17)
Rh1-P1	2.3245(4)
Rh1-P2	2.3304(4)
Rh1-Cl1	2.3914(4)
P1-C14	1.8211(15)
P1-C8	1.8234(15)
P1-C2	1.8268(15)
O1-C1	1.143(2)
O2-C19	1.3751(18)
O2-C22	1.4395(19)
P2-C31	1.8225(15)
P2-C24	1.8320(16)
P2-C37	1.8368(16)
C2-C7	1.397(2)
C2-C3	1.397(2)
O3-C25#1	1.3780(17)
O3-C22	1.4233(18)
C3-C4	1.393(3)
C4-C5	1.386(3)
C5-C6	1.398(3)
C6-C7	1.387(2)
C8-C13	1.397(2)
C8-C9	1.405(2)
C9-C10	1.392(2)
C10-C11	1.387(3)
C11-C12	1.385(3)
C12-C13	1.394(2)
C14-C15	1.397(2)
C14-C19	1.401(2)
C15-C16	1.399(2)
C16-C17	1.392(2)
C16-C23	1.508(2)
C17-C18	1.390(2)
C18-C19	1.393(2)
C18-C20	1.506(2)

C20-C26#1	1.515(2)
C20-C21	1.534(2)
C21-C22	1.507(2)
C24-C29	1.402(2)
C24-C25	1.406(2)
C25-O3#1	1.3780(17)
C25-C26	1.393(2)
C26-C27	1.395(2)
C26-C20#1	1.515(2)
C27-C28	1.394(2)
C28-C29	1.396(2)
C28-C30	1.505(2)
C31-C36	1.391(3)
C31-C32	1.395(2)
C32-C33	1.394(3)
C33-C34	1.382(4)
C34-C35	1.384(4)
C35-C36	1.394(3)
C37-C38	1.400(2)
C37-C42	1.403(2)
C38-C39	1.394(2)
C39-C40	1.391(3)
C40-C41	1.384(3)
C41-C42	1.395(3)
C1V-Cl1V	1.727(4)
C1V-Cl2V	1.736(4)
C1V'-Cl2'	1.746(5)
C1V'-Cl1'	1.755(5)
Cl1W-C1W	1.711(5)
Cl1W-C1W'	1.757(4)
C1W-Cl2W	1.736(4)
C1W'-Cl3W	1.762(4)

Angles----------

C1-Rh1-P1	92.91(5)
C1-Rh1-P2	93.42(5)
P1-Rh1-P2	172.581(14)
C1-Rh1-Cl1	174.89(6)

P1-Rh1-Cl1	85.496(15)
P2-Rh1-Cl1	88.521(15)
C14-P1-C8	106.01(7)
C14-P1-C2	103.14(7)
C8-P1-C2	101.24(7)
C14-P1-Rh1	108.24(5)
C8-P1-Rh1	113.51(5)
C2-P1-Rh1	123.14(5)
O1-C1-Rh1	177.80(17)
C19-O2-C22	119.12(12)
C31-P2-C24	102.69(7)
C31-P2-C37	103.93(7)
C24-P2-C37	106.75(7)
C31-P2-Rh1	111.59(6)
C24-P2-Rh1	116.37(5)
C37-P2-Rh1	114.19(5)
C7-C2-C3	118.91(14)
C7-C2-P1	118.33(11)
C3-C2-P1	122.53(12)
C25-O3-C22#1	116.23(12)
C4-C3-C2	120.17(16)
C5-C4-C3	120.53(17)
C4-C5-C6	119.68(17)
C7-C6-C5	119.78(17)
C6-C7-C2	120.92(16)
C13-C8-C9	119.29(14)
C13-C8-P1	118.68(12)
C9-C8-P1	121.98(12)
C10-C9-C8	119.89(16)
C11-C10-C9	120.19(17)
C12-C11-C10	120.33(16)
C11-C12-C13	120.00(17)
C12-C13-C8	120.28(16)
C15-C14-C19	118.20(13)
C15-C14-P1	124.88(11)
C19-C14-P1	116.80(11)
C14-C15-C16	121.28(14)
C17-C16-C15	118.73(15)

C17-C16-C23	120.08(15)
C15-C16-C23	121.18(16)
C18-C17-C16	121.39(14)
C17-C18-C19	118.76(14)
C17-C18-C20	124.70(13)
C19-C18-C20	116.45(13)
O2-C19-C18	121.27(13)
O2-C19-C14	117.33(12)
C18-C19-C14	121.40(13)
C18-C20-C26#1	111.35(12)
C18-C20-C21	105.81(12)
C26-C20-C21#1	109.24(12)
C22-C21-C20	105.98(12)
O3-C22-O2	107.77(11)
O3-C22-C21	111.09(12)
O2-C22-C21	112.64(12)
C29-C24-C25	117.89(14)
C29-C24-P2	121.66(11)
C25-C24-P2	120.05(11)
O3-C25-C26#1	122.34(12)
O3-C25-C24#1	116.34(13)
C26-C25-C24	121.31(13)
C25-C26-C27	118.84(13)
C25-C26-C20#1	120.26(12)
C27-C26-C20#1	120.89(13)
C28-C27-C26	121.79(14)
C27-C28-C29	118.08(14)
C27-C28-C30	120.76(15)
C29-C28-C30	121.13(15)
C28-C29-C24	122.07(14)
C36-C31-C32	119.16(15)
C36-C31-P2	118.37(13)
C32-C31-P2	122.36(13)
C33-C32-C31	119.96(19)
C34-C33-C32	120.43(19)
C33-C34-C35	120.00(18)
C34-C35-C36	119.9(2)
C31-C36-C35	120.59(19)

C38-C37-C42	118.75(15)
C38-C37-P2	122.93(13)
C42-C37-P2	118.17(13)
C39-C38-C37	120.29(17)
C40-C39-C38	120.50(18)
C41-C40-C39	119.60(17)
C40-C41-C42	120.44(19)
C41-C42-C37	120.41(18)
Cl1V-C1V-Cl2V	113.4(3)
Cl2'-C1V'-Cl1'	97.2(6)
C1W-Cl1W-C1W'	19.0(4)
Cl1W-C1W-Cl2W	106.6(3)
Cl1W-C1W'-Cl3W	119.3(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x, -y+0, -z

Table 3. Torsion angles [°] for JM147_0m.

C1-Rh1-P1-C14	-135.57(7)
P2-Rh1-P1-C14	12.95(12)
Cl1-Rh1-P1-C14	49.30(5)
C1-Rh1-P1-C8	107.03(8)
P2-Rh1-P1-C8	-104.45(12)
Cl1-Rh1-P1-C8	-68.10(6)
C1-Rh1-P1-C2	-15.50(8)
P2-Rh1-P1-C2	133.02(11)
Cl1-Rh1-P1-C2	169.36(6)
P1-Rh1-C1-O1	-72(4)
P2-Rh1-C1-O1	112(4)
Cl1-Rh1-C1-O1	-1(5)
C1-Rh1-P2-C31	-114.50(8)
P1-Rh1-P2-C31	97.00(12)
Cl1-Rh1-P2-C31	60.77(6)
C1-Rh1-P2-C24	2.89(8)
P1-Rh1-P2-C24	-145.62(11)
Cl1-Rh1-P2-C24	178.15(5)
C1-Rh1-P2-C37	128.02(8)
P1-Rh1-P2-C37	-20.49(13)
Cl1-Rh1-P2-C37	-56.72(6)
C14-P1-C2-C7	-175.01(13)
C8-P1-C2-C7	-65.43(14)
Rh1-P1-C2-C7	62.56(14)
C14-P1-C2-C3	-0.55(15)
C8-P1-C2-C3	109.04(14)
Rh1-P1-C2-C3	-122.98(13)
C7-C2-C3-C4	1.2(3)
P1-C2-C3-C4	-173.27(15)
C2-C3-C4-C5	-0.2(3)
C3-C4-C5-C6	-0.3(3)
C4-C5-C6-C7	-0.1(3)
C5-C6-C7-C2	1.1(3)
C3-C2-C7-C6	-1.6(3)
P1-C2-C7-C6	173.07(15)
C14-P1-C8-C13	-115.43(13)

C2-P1-C8-C13	137.22(13)
Rh1-P1-C8-C13	3.25(14)
C14-P1-C8-C9	67.04(14)
C2-P1-C8-C9	-40.31(14)
Rh1-P1-C8-C9	-174.27(11)
C13-C8-C9-C10	1.2(2)
P1-C8-C9-C10	178.72(12)
C8-C9-C10-C11	-1.8(2)
C9-C10-C11-C12	1.4(3)
C10-C11-C12-C13	-0.3(3)
C11-C12-C13-C8	-0.3(3)
C9-C8-C13-C12	-0.1(2)
P1-C8-C13-C12	-177.72(13)
C8-P1-C14-C15	-11.43(15)
C2-P1-C14-C15	94.55(14)
Rh1-P1-C14-C15	-133.54(12)
C8-P1-C14-C19	164.54(11)
C2-P1-C14-C19	-89.48(12)
Rh1-P1-C14-C19	42.43(12)
C19-C14-C15-C16	0.1(2)
P1-C14-C15-C16	176.03(12)
C14-C15-C16-C17	-2.9(2)
C14-C15-C16-C23	178.06(17)
C15-C16-C17-C18	1.5(2)
C23-C16-C17-C18	-179.47(17)
C16-C17-C18-C19	2.7(2)
C16-C17-C18-C20	-173.58(14)
C22-O2-C19-C18	25.6(2)
C22-O2-C19-C14	-153.88(13)
C17-C18-C19-O2	174.88(13)
C20-C18-C19-O2	-8.5(2)
C17-C18-C19-C14	-5.6(2)
C20-C18-C19-C14	170.95(13)
C15-C14-C19-O2	-176.25(13)
P1-C14-C19-O2	7.50(18)
C15-C14-C19-C18	4.2(2)
P1-C14-C19-C18	-172.01(11)
C17-C18-C20-C26#1	-102.84(16)

C19-C18-C20-C26#1	80.80(16)
C17-C18-C20-C21	138.58(15)
C19-C18-C20-C21	-37.77(16)
C18-C20-C21-C22	67.15(14)
C26#1-C20-C21-C22	-52.82(15)
C25#1-O3-C22-O2	78.04(15)
C25#1-O3-C22-C21	-45.79(17)
C19-O2-C22-O3	-114.93(13)
C19-O2-C22-C21	7.96(18)
C20-C21-C22-O3	67.41(15)
C20-C21-C22-O2	-53.60(15)
C31-P2-C24-C29	3.77(14)
C37-P2-C24-C29	112.76(13)
Rh1-P2-C24-C29	-118.42(12)
C31-P2-C24-C25	176.32(12)
C37-P2-C24-C25	-74.68(13)
Rh1-P2-C24-C25	54.14(13)
C29-C24-C25-O3#1	179.70(13)
P2-C24-C25-O3#1	6.86(18)
C29-C24-C25-C26	0.8(2)
P2-C24-C25-C26	-172.03(11)
O3#1-C25-C26-C27	179.42(14)
C24-C25-C26-C27	-1.8(2)
O3#1-C25-C26-C20#1	-1.8(2)
C24-C25-C26-C20#1	177.03(13)
C25-C26-C27-C28	1.6(2)
C20#1-C26-C27-C28	-177.19(15)
C26-C27-C28-C29	-0.5(2)
C26-C27-C28-C30	177.56(16)
C27-C28-C29-C24	-0.5(2)
C30-C28-C29-C24	-178.55(16)
C25-C24-C29-C28	0.4(2)
P2-C24-C29-C28	173.07(13)
C24-P2-C31-C36	-104.26(16)
C37-P2-C31-C36	144.62(15)
Rh1-P2-C31-C36	21.10(17)
C24-P2-C31-C32	71.81(16)
C37-P2-C31-C32	-39.31(17)

Rh1-P2-C31-C32	-162.82(14)
C36-C31-C32-C33	0.2(3)
P2-C31-C32-C33	-175.82(16)
C31-C32-C33-C34	-0.7(3)
C32-C33-C34-C35	1.0(4)
C33-C34-C35-C36	-0.9(4)
C32-C31-C36-C35	-0.1(3)
P2-C31-C36-C35	176.14(19)
C34-C35-C36-C31	0.4(4)
C31-P2-C37-C38	136.59(14)
C24-P2-C37-C38	28.47(15)
Rh1-P2-C37-C38	-101.60(14)
C31-P2-C37-C42	-47.95(15)
C24-P2-C37-C42	-156.07(13)
Rh1-P2-C37-C42	73.85(14)
C42-C37-C38-C39	-1.3(2)
P2-C37-C38-C39	174.15(13)
C37-C38-C39-C40	0.9(3)
C38-C39-C40-C41	0.1(3)
C39-C40-C41-C42	-0.7(3)
C40-C41-C42-C37	0.3(3)
C38-C37-C42-C41	0.7(3)
P2-C37-C42-C41	-174.96(15)
C1W'-Cl1W-C1W-Cl2W	57.8(9)
C1W-Cl1W-C1W'-Cl3W	-168.7(15)

Symmetry transformations used to generate equivalent atoms:

#1 -x, -y+0, -z

Crystallographic details: compound 22.

Table 1. Crystal data and structure refinement for JM-044_0m.

Identification code	JM-044_0m	
Empirical formula	C45 H37 Cl5 O4 P2 Rh2	
Formula weight	1086.76	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.2602(16) Å	α= 87.046(10) °.
	b = 14.114(4) Å	β = 76.892(8) °.
	c = 14.469(2) Å	γ = 79.328(9) °.
Volume	2200.8(8) $Å^3$	
Z	2	
Density (calculated)	1.640 Mg/m^3	
Absorption coefficient	1.169 mm^{-1}	
F(000)	1088	
Crystal size	0.40 x 0.30 x 0.30 mm^3	
Theta range for data collection	2.62 to 32.50 °.	
Index ranges	-17 <=h<=16 ,-19 <=k<=21 ,-21 <=l<=13	
Reflections collected	30226	
Independent reflections	14497 [R(int) = 0.0274]	
Completeness to theta =32.50 °	0.910 %	
Absorption correction	Empirical	
Max. and min. transmission	1.00 and 0.82	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14497 / 0 / 527	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0499 , wR2 = 0.1327	
R indices (all data)	R1 = 0.0609 , wR2 = 0.1473	
Largest diff. peak and hole	2.896 and -2.848 $e.Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for JM-044_0m.

Bond lengths----	
Rh1-C43	1.805(3)
Rh1-P1	2.2391(9)
Rh1-Cl1	2.3977(8)
Rh1-Cl2	2.4145(9)
Cl1-Rh2	2.3920(8)
P1-C3	1.811(3)
P1-C19	1.820(3)
P1-C25	1.825(3)
C1-O1	1.431(3)
C1-O2	1.447(3)
C1-C15	1.503(5)
C1-C8	1.585(4)
O1-C2	1.368(4)
Rh2-C44	1.806(3)
Rh2-P2	2.2402(8)
Rh2-Cl2	2.4173(8)
P2-C31	1.814(3)
P2-C13	1.818(3)
P2-C37	1.824(3)
C2-C7	1.381(4)
C2-C3	1.397(4)
O2-C14	1.368(3)
C3-C4	1.401(4)
O3-C43	1.144(4)
C4-C5	1.404(4)
O4-C44	1.147(4)
C5-C6	1.400(5)
C5-C17	1.504(5)
C6-C7	1.384(4)
C7-C8	1.516(4)
C8-C9	1.518(4)
C8-C16	1.533(4)
C9-C10	1.381(4)
C9-C14	1.381(4)
C10-C11	1.404(4)

C11-C12	1.403(4)
C11-C18	1.508(4)
C12-C13	1.407(4)
C13-C14	1.391(4)
C19-C20	1.395(4)
C19-C24	1.408(4)
C20-C21	1.401(5)
C21-C22	1.389(6)
C22-C23	1.391(6)
C23-C24	1.388(5)
C25-C30	1.393(5)
C25-C26	1.405(4)
C26-C27	1.390(5)
C27-C28	1.380(6)
C28-C29	1.398(5)
C29-C30	1.391(5)
C31-C32	1.393(5)
C31-C36	1.406(5)
C32-C33	1.380(6)
C33-C34	1.395(7)
C34-C35	1.388(7)
C35-C36	1.384(6)
C37-C42	1.382(4)
C37-C38	1.392(5)
C38-C39	1.389(4)
C39-C40	1.386(6)
C40-C41	1.375(6)
C41-C42	1.401(5)
C1S-Cl1S	1.759(4)
C1S-Cl3S	1.764(5)
C1S-Cl2S	1.768(5)

Angles----------

C43-Rh1-P1	88.01(11)
C43-Rh1-Cl1	175.00(12)
P1-Rh1-Cl1	96.39(3)
C43-Rh1-Cl2	92.89(11)
P1-Rh1-Cl2	174.89(3)

Cl1-Rh1-Cl2	82.52(3)
Rh2-Cl1-Rh1	89.61(3)
C3-P1-C19	101.47(14)
C3-P1-C25	106.07(14)
C19-P1-C25	104.09(14)
C3-P1-Rh1	112.58(9)
C19-P1-Rh1	120.84(10)
C25-P1-Rh1	110.46(10)
O1-C1-O2	106.8(2)
O1-C1-C15	108.9(2)
O2-C1-C15	107.7(2)
O1-C1-C8	107.0(2)
O2-C1-C8	106.5(2)
C15-C1-C8	119.3(3)
C2-O1-C1	108.0(2)
C44-Rh2-P2	86.26(11)
C44-Rh2-Cl1	171.68(11)
P2-Rh2-Cl1	98.36(3)
C44-Rh2-Cl2	92.74(11)
P2-Rh2-Cl2	178.90(2)
Cl1-Rh2-Cl2	82.58(3)
Rh1-Cl2-Rh2	88.62(3)
C31-P2-C13	102.28(14)
C31-P2-C37	106.19(14)
C13-P2-C37	104.42(13)
C31-P2-Rh2	116.43(10)
C13-P2-Rh2	117.85(10)
C37-P2-Rh2	108.48(10)
O1-C2-C7	114.0(3)
O1-C2-C3	123.3(2)
C7-C2-C3	122.7(3)
C14-O2-C1	109.0(2)
C2-C3-C4	116.4(3)
C2-C3-P1	117.0(2)
C4-C3-P1	126.5(2)
C3-C4-C5	122.2(3)
C6-C5-C4	118.9(3)
C6-C5-C17	120.8(3)

C4-C5-C17	120.2(3)
C7-C6-C5	119.8(3)
C2-C7-C6	119.9(3)
C2-C7-C8	108.4(2)
C6-C7-C8	131.5(3)
C7-C8-C9	109.0(3)
C7-C8-C16	113.8(2)
C9-C8-C16	114.6(2)
C7-C8-C1	100.9(2)
C9-C8-C1	101.2(2)
C16-C8-C1	115.8(3)
C10-C9-C14	120.5(3)
C10-C9-C8	130.7(3)
C14-C9-C8	108.5(2)
C9-C10-C11	119.4(3)
C12-C11-C10	119.0(3)
C12-C11-C18	120.2(3)
C10-C11-C18	120.8(3)
C11-C12-C13	122.1(3)
C14-C13-C12	116.4(2)
C14-C13-P2	119.3(2)
C12-C13-P2	124.3(2)
O2-C14-C9	113.7(2)
O2-C14-C13	123.8(2)
C9-C14-C13	122.5(3)
C20-C19-C24	118.8(3)
C20-C19-P1	121.7(2)
C24-C19-P1	119.5(2)
C19-C20-C21	120.3(3)
C22-C21-C20	120.2(3)
C21-C22-C23	120.1(3)
C24-C23-C22	119.9(3)
C23-C24-C19	120.8(3)
C30-C25-C26	119.2(3)
C30-C25-P1	118.0(2)
C26-C25-P1	122.7(3)
C27-C26-C25	119.6(3)
C28-C27-C26	120.7(3)

C27-C28-C29	120.3(3)
C30-C29-C28	119.1(3)
C29-C30-C25	121.0(3)
C32-C31-C36	118.5(3)
C32-C31-P2	121.2(3)
C36-C31-P2	120.3(3)
C33-C32-C31	121.1(4)
C32-C33-C34	120.3(4)
C35-C34-C33	119.1(4)
C36-C35-C34	120.9(4)
C35-C36-C31	120.1(4)
C42-C37-C38	119.3(3)
C42-C37-P2	122.0(3)
C38-C37-P2	118.4(2)
C39-C38-C37	120.5(3)
C40-C39-C38	120.3(4)
C41-C40-C39	119.0(3)
C40-C41-C42	121.2(4)
C37-C42-C41	119.6(4)
O3-C43-Rh1	177.3(3)
O4-C44-Rh2	176.1(3)
Cl1S-C1S-Cl3S	110.9(3)
Cl1S-C1S-Cl2S	111.0(2)
Cl3S-C1S-Cl2S	110.1(2)

Table 3. Torsion angles [°] for JM-044_0m.

C43-Rh1-Cl1-Rh2	-53.7(14)
P1-Rh1-Cl1-Rh2	154.67(3)
Cl2-Rh1-Cl1-Rh2	-30.36(3)
C43-Rh1-P1-C3	179.92(17)
Cl1-Rh1-P1-C3	-2.45(12)
Cl2-Rh1-P1-C3	-79.9(3)
C43-Rh1-P1-C19	59.97(17)
Cl1-Rh1-P1-C19	-122.40(12)
Cl2-Rh1-P1-C19	160.2(3)
C43-Rh1-P1-C25	-61.72(16)
Cl1-Rh1-P1-C25	115.91(10)
Cl2-Rh1-P1-C25	38.5(3)
O2-C1-O1-C2	-100.2(2)
C15-C1-O1-C2	143.8(2)
C8-C1-O1-C2	13.5(3)
Rh1-Cl1-Rh2-C44	86.4(7)
Rh1-Cl1-Rh2-P2	-150.27(3)
Rh1-Cl1-Rh2-Cl2	30.32(3)
C43-Rh1-Cl2-Rh2	-151.96(13)
P1-Rh1-Cl2-Rh2	108.1(3)
Cl1-Rh1-Cl2-Rh2	30.02(3)
C44-Rh2-Cl2-Rh1	156.82(11)
P2-Rh2-Cl2-Rh1	-179(100)
Cl1-Rh2-Cl2-Rh1	-30.09(3)
C44-Rh2-P2-C31	-58.59(15)
Cl1-Rh2-P2-C31	128.37(11)
Cl2-Rh2-P2-C31	-83.2(15)
C44-Rh2-P2-C13	179.32(15)
Cl1-Rh2-P2-C13	6.28(11)
Cl2-Rh2-P2-C13	154.7(15)
C44-Rh2-P2-C37	61.05(15)
Cl1-Rh2-P2-C37	-111.99(11)
Cl2-Rh2-P2-C37	36.5(15)
C1-O1-C2-C7	-12.9(3)
C1-O1-C2-C3	165.9(2)
O1-C1-O2-C14	116.8(3)

C15-C1-O2-C14	-126.4(3)
C8-C1-O2-C14	2.7(3)
O1-C2-C3-C4	179.7(3)
C7-C2-C3-C4	-1.6(4)
O1-C2-C3-P1	-3.9(4)
C7-C2-C3-P1	174.8(2)
C19-P1-C3-C2	63.5(2)
C25-P1-C3-C2	172.0(2)
Rh1-P1-C3-C2	-67.1(2)
C19-P1-C3-C4	-120.6(3)
C25-P1-C3-C4	-12.1(3)
Rh1-P1-C3-C4	108.8(2)
C2-C3-C4-C5	-1.1(4)
P1-C3-C4-C5	-177.0(2)
C3-C4-C5-C6	2.8(4)
C3-C4-C5-C17	-178.3(3)
C4-C5-C6-C7	-1.9(4)
C17-C5-C6-C7	179.2(3)
O1-C2-C7-C6	-178.7(3)
C3-C2-C7-C6	2.5(4)
O1-C2-C7-C8	6.3(3)
C3-C2-C7-C8	-172.5(2)
C5-C6-C7-C2	-0.7(4)
C5-C6-C7-C8	173.0(3)
C2-C7-C8-C9	108.3(3)
C6-C7-C8-C9	-65.9(4)
C2-C7-C8-C16	-122.5(3)
C6-C7-C8-C16	63.3(4)
C2-C7-C8-C1	2.3(3)
C6-C7-C8-C1	-171.9(3)
O1-C1-C8-C7	-9.5(3)
O2-C1-C8-C7	104.5(2)
C15-C1-C8-C7	-133.5(3)
O1-C1-C8-C9	-121.5(2)
O2-C1-C8-C9	-7.6(3)
C15-C1-C8-C9	114.4(3)
O1-C1-C8-C16	113.9(3)
O2-C1-C8-C16	-132.1(3)

C15-C1-C8-C16	-10.2(4)
C7-C8-C9-C10	78.2(4)
C16-C8-C9-C10	-50.6(5)
C1-C8-C9-C10	-176.0(3)
C7-C8-C9-C14	-95.8(3)
C16-C8-C9-C14	135.4(3)
C1-C8-C9-C14	10.0(3)
C14-C9-C10-C11	-0.3(5)
C8-C9-C10-C11	-173.8(3)
C9-C10-C11-C12	3.0(5)
C9-C10-C11-C18	-178.8(3)
C10-C11-C12-C13	-2.2(5)
C18-C11-C12-C13	179.7(3)
C11-C12-C13-C14	-1.3(5)
C11-C12-C13-P2	177.0(2)
C31-P2-C13-C14	-76.2(3)
C37-P2-C13-C14	173.3(2)
Rh2-P2-C13-C14	52.9(3)
C31-P2-C13-C12	105.5(3)
C37-P2-C13-C12	-5.0(3)
Rh2-P2-C13-C12	-125.4(2)
C1-O2-C14-C9	4.2(4)
C1-O2-C14-C13	-176.6(3)
C10-C9-C14-O2	175.8(3)
C8-C9-C14-O2	-9.5(4)
C10-C9-C14-C13	-3.4(5)
C8-C9-C14-C13	171.3(3)
C12-C13-C14-O2	-175.0(3)
P2-C13-C14-O2	6.6(4)
C12-C13-C14-C9	4.2(5)
P2-C13-C14-C9	-174.3(2)
C3-P1-C19-C20	-142.6(3)
C25-P1-C19-C20	107.4(3)
Rh1-P1-C19-C20	-17.3(3)
C3-P1-C19-C24	38.9(3)
C25-P1-C19-C24	-71.1(3)
Rh1-P1-C19-C24	164.2(2)
C24-C19-C20-C21	0.5(5)

P1-C19-C20-C21	-178.0(3)
C19-C20-C21-C22	-0.4(6)
C20-C21-C22-C23	0.9(6)
C21-C22-C23-C24	-1.5(6)
C22-C23-C24-C19	1.6(5)
C20-C19-C24-C23	-1.1(5)
P1-C19-C24-C23	177.5(3)
C3-P1-C25-C30	80.2(3)
C19-P1-C25-C30	-173.2(2)
Rh1-P1-C25-C30	-42.0(3)
C3-P1-C25-C26	-104.0(3)
C19-P1-C25-C26	2.6(3)
Rh1-P1-C25-C26	133.7(3)
C30-C25-C26-C27	-0.9(5)
P1-C25-C26-C27	-176.6(3)
C25-C26-C27-C28	1.0(6)
C26-C27-C28-C29	-0.8(6)
C27-C28-C29-C30	0.6(6)
C28-C29-C30-C25	-0.6(5)
C26-C25-C30-C29	0.8(5)
P1-C25-C30-C29	176.7(3)
C13-P2-C31-C32	125.5(3)
C37-P2-C31-C32	-125.3(3)
Rh2-P2-C31-C32	-4.4(3)
C13-P2-C31-C36	-50.9(3)
C37-P2-C31-C36	58.3(3)
Rh2-P2-C31-C36	179.2(2)
C36-C31-C32-C33	-2.0(6)
P2-C31-C32-C33	-178.4(3)
C31-C32-C33-C34	0.4(7)
C32-C33-C34-C35	0.7(7)
C33-C34-C35-C36	0.0(7)
C34-C35-C36-C31	-1.6(6)
C32-C31-C36-C35	2.6(5)
P2-C31-C36-C35	179.0(3)
C31-P2-C37-C42	19.3(3)
C13-P2-C37-C42	127.0(3)
Rh2-P2-C37-C42	-106.5(3)

C31-P2-C37-C38	-168.0(2)
C13-P2-C37-C38	-60.4(3)
Rh2-P2-C37-C38	66.1(2)
C42-C37-C38-C39	-2.1(5)
P2-C37-C38-C39	-175.0(2)
C37-C38-C39-C40	1.9(5)
C38-C39-C40-C41	-0.2(5)
C39-C40-C41-C42	-1.4(6)
C38-C37-C42-C41	0.6(5)
P2-C37-C42-C41	173.1(3)
C40-C41-C42-C37	1.2(6)
P1-Rh1-C43-O3	155(8)
Cl1-Rh1-C43-O3	4(9)
Cl2-Rh1-C43-O3	-20(8)
P2-Rh2-C44-O4	-110(4)
Cl1-Rh2-C44-O4	14(5)
Cl2-Rh2-C44-O4	69(4)

Crystallographic details: compound 24.

Table 1. Crystal data and structure refinement for JM236b_0m.

Identification code	JM236b_0m	
Empirical formula	C42.25 H33.50 Cl2.50 O4 P2 Rh2	
Formula weight	961.58	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I-4	
Unit cell dimensions	a = 28.7585(6) Å	α= 90.00 °.
	b = 28.7585(6) Å	β = 90.00 °.
	c = 9.2270(2) Å	γ = 90.00 °.
Volume	7631.2(3) $Å^3$	
Z	8	
Density (calculated)	1.674 Mg/m^3	
Absorption coefficient	1.167 mm^{-1}	
F(000)	3852	
Crystal size	0.02 x 0.03 x 0.3 mm^3	
Theta range for data collection	2.72 to 33.17 °.	
Index ranges	-44 <=h<=28 ,-44 <=k<=43 ,-9 <=l<=13	
Reflections collected	41695	
Independent reflections	12617 [R(int) = 0.0597]	
Completeness to theta =33.17 °	0.940 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9884 and 0.8922	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12617 / 7 / 491	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0411 , wR2 = 0.0921	
R indices (all data)	R1 = 0.0539 , wR2 = 0.0989	
Absolute Structure Flack parameter	x =0.49(2)	
Largest diff. peak and hole	2.473 and -0.644 $e.Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for JM236b_0m.

Bond lengths----	
C1-O2	1.427(4)
C1-O1	1.427(4)
C1-C8	1.565(4)
Cl1-Rh2	2.4017(8)
Cl1-Rh1	2.4037(8)
O1-C14	1.370(4)
P1-C29	1.819(4)
P1-C13	1.820(3)
P1-C35	1.822(3)
P1-Rh1	2.2477(9)
Rh1-C41	1.810(3)
Rh1-Cl2	2.4152(9)
C2-O2	1.372(4)
C2-C7	1.383(4)
C2-C3	1.388(5)
Cl2-Rh2	2.4024(9)
P2-C3	1.814(3)
P2-C17	1.825(3)
P2-C23	1.826(4)
P2-Rh2	2.2411(9)
Rh2-C42	1.813(4)
C3-C4	1.405(5)
O4-C42	1.142(4)
C4-C5	1.396(5)
O3-C41	1.149(4)
C5-C6	1.396(5)
C5-C15	1.502(5)
C6-C7	1.398(5)
C7-C8	1.515(5)
C8-C9	1.511(5)
C9-C10	1.381(4)
C9-C14	1.396(4)
C10-C11	1.390(5)
C11-C12	1.403(5)
C11-C16	1.519(5)

C12-C13	1.403(4)
C13-C14	1.388(5)
C17-C22	1.397(5)
C17-C18	1.398(5)
C18-C19	1.388(5)
C19-C20	1.393(5)
C20-C21	1.376(6)
C21-C22	1.402(5)
C23-C28	1.386(5)
C23-C24	1.414(5)
C24-C25	1.380(6)
C25-C26	1.385(6)
C26-C27	1.390(5)
C27-C28	1.389(6)
C29-C30	1.390(5)
C29-C34	1.391(5)
C30-C31	1.389(6)
C31-C32	1.388(6)
C32-C33	1.400(5)
C33-C34	1.389(6)
C35-C40	1.396(6)
C35-C36	1.415(5)
C36-C37	1.384(5)
C37-C38	1.380(7)
C38-C39	1.385(5)
C39-C40	1.390(5)
C1S-Cl1S	1.744(5)

Angles----------

O2-C1-O1	107.3(3)
O2-C1-C8	108.0(3)
O1-C1-C8	108.1(2)
Rh2-Cl1-Rh1	84.94(2)
C14-O1-C1	108.2(2)
C29-P1-C13	106.30(17)
C29-P1-C35	103.32(16)
C13-P1-C35	103.96(15)
C29-P1-Rh1	116.93(11)

C13-P1-Rh1	111.33(11)
C35-P1-Rh1	113.84(14)
C41-Rh1-P1	88.74(12)
C41-Rh1-Cl1	173.66(12)
P1-Rh1-Cl1	97.60(3)
C41-Rh1-Cl2	91.45(12)
P1-Rh1-Cl2	178.20(4)
Cl1-Rh1-Cl2	82.21(3)
O2-C2-C7	113.0(3)
O2-C2-C3	123.4(3)
C7-C2-C3	123.6(3)
Rh2-Cl2-Rh1	84.67(3)
C2-O2-C1	108.5(2)
C3-P2-C17	101.89(14)
C3-P2-C23	105.00(17)
C17-P2-C23	103.99(15)
C3-P2-Rh2	112.31(11)
C17-P2-Rh2	112.82(13)
C23-P2-Rh2	119.06(11)
C42-Rh2-P2	90.03(12)
C42-Rh2-Cl1	173.09(11)
P2-Rh2-Cl1	96.49(3)
C42-Rh2-Cl2	91.19(12)
P2-Rh2-Cl2	174.86(3)
Cl1-Rh2-Cl2	82.52(3)
C2-C3-C4	115.9(3)
C2-C3-P2	120.3(2)
C4-C3-P2	122.7(3)
C5-C4-C3	122.6(3)
C4-C5-C6	118.9(3)
C4-C5-C15	119.8(3)
C6-C5-C15	121.3(3)
C5-C6-C7	120.0(3)
C2-C7-C6	118.8(3)
C2-C7-C8	108.8(3)
C6-C7-C8	132.0(3)
C9-C8-C7	110.4(3)
C9-C8-C1	101.5(2)

C7-C8-C1	101.0(2)
C10-C9-C14	120.2(3)
C10-C9-C8	131.4(3)
C14-C9-C8	108.0(3)
C9-C10-C11	119.1(3)
C10-C11-C12	119.9(3)
C10-C11-C16	121.1(3)
C12-C11-C16	119.0(3)
C11-C12-C13	122.0(3)
C14-C13-C12	116.1(3)
C14-C13-P1	121.4(2)
C12-C13-P1	121.2(3)
O1-C14-C13	123.7(3)
O1-C14-C9	113.6(3)
C13-C14-C9	122.7(3)
C22-C17-C18	119.3(3)
C22-C17-P2	121.6(3)
C18-C17-P2	119.0(3)
C19-C18-C17	120.6(3)
C18-C19-C20	120.0(4)
C21-C20-C19	119.6(3)
C20-C21-C22	121.0(4)
C17-C22-C21	119.4(4)
C28-C23-C24	118.6(3)
C28-C23-P2	121.7(2)
C24-C23-P2	119.7(3)
C25-C24-C23	119.8(4)
C24-C25-C26	121.1(3)
C25-C26-C27	119.4(4)
C28-C27-C26	119.9(4)
C23-C28-C27	121.1(3)
C30-C29-C34	118.5(3)
C30-C29-P1	119.3(3)
C34-C29-P1	122.2(2)
C31-C30-C29	120.6(4)
C32-C31-C30	120.6(3)
C31-C32-C33	119.5(4)
C34-C33-C32	119.1(4)

C33-C34-C29	121.7(3)
C40-C35-C36	119.0(3)
C40-C35-P1	119.4(3)
C36-C35-P1	121.6(3)
C37-C36-C35	119.2(4)
C38-C37-C36	121.5(4)
C37-C38-C39	119.6(3)
C38-C39-C40	120.3(4)
C39-C40-C35	120.4(3)
O4-C42-Rh2	176.8(3)
O3-C41-Rh1	177.3(3)

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for JM236b_0m.

O2-C1-O1-C14	-110.6(3)
C8-C1-O1-C14	5.7(4)
C29-P1-Rh1-C41	70.15(17)
C13-P1-Rh1-C41	-167.43(17)
C35-P1-Rh1-C41	-50.32(17)
C29-P1-Rh1-Cl1	-110.11(12)
C13-P1-Rh1-Cl1	12.32(13)
C35-P1-Rh1-Cl1	129.42(12)
C29-P1-Rh1-Cl2	166.1(10)
C13-P1-Rh1-Cl2	-71.5(10)
C35-P1-Rh1-Cl2	45.6(10)
Rh2-Cl1-Rh1-C41	-37.4(11)
Rh2-Cl1-Rh1-P1	144.88(3)
Rh2-Cl1-Rh1-Cl2	-36.92(3)
C41-Rh1-Cl2-Rh2	-143.13(12)
P1-Rh1-Cl2-Rh2	121.0(10)
Cl1-Rh1-Cl2-Rh2	36.93(3)
C7-C2-O2-C1	8.7(4)
C3-C2-O2-C1	-170.7(3)
O1-C1-O2-C2	110.9(3)
C8-C1-O2-C2	-5.5(4)
C3-P2-Rh2-C42	171.14(18)
C17-P2-Rh2-C42	56.66(17)
C23-P2-Rh2-C42	-65.61(18)
C3-P2-Rh2-Cl1	-11.14(13)
C17-P2-Rh2-Cl1	-125.62(11)
C23-P2-Rh2-Cl1	112.10(13)
C3-P2-Rh2-Cl2	67.4(4)
C17-P2-Rh2-Cl2	-47.1(4)
C23-P2-Rh2-Cl2	-169.3(3)
Rh1-Cl1-Rh2-C42	12.7(11)
Rh1-Cl1-Rh2-P2	-147.96(3)
Rh1-Cl1-Rh2-Cl2	37.12(3)
Rh1-Cl2-Rh2-C42	140.22(13)
Rh1-Cl2-Rh2-P2	-116.1(3)
Rh1-Cl2-Rh2-Cl1	-36.93(3)

O2-C2-C3-C4	-177.6(3)
C7-C2-C3-C4	3.1(5)
O2-C2-C3-P2	13.8(5)
C7-C2-C3-P2	-165.5(3)
C17-P2-C3-C2	-166.8(3)
C23-P2-C3-C2	-58.6(3)
Rh2-P2-C3-C2	72.2(3)
C17-P2-C3-C4	25.4(3)
C23-P2-C3-C4	133.6(3)
Rh2-P2-C3-C4	-95.6(3)
C2-C3-C4-C5	-0.5(5)
P2-C3-C4-C5	167.7(3)
C3-C4-C5-C6	-1.8(6)
C3-C4-C5-C15	179.2(4)
C4-C5-C6-C7	1.7(5)
C15-C5-C6-C7	-179.3(3)
O2-C2-C7-C6	177.4(3)
C3-C2-C7-C6	-3.2(5)
O2-C2-C7-C8	-8.3(4)
C3-C2-C7-C8	171.1(3)
C5-C6-C7-C2	0.6(5)
C5-C6-C7-C8	-172.1(4)
C2-C7-C8-C9	-102.5(3)
C6-C7-C8-C9	70.8(5)
C2-C7-C8-C1	4.2(4)
C6-C7-C8-C1	177.5(4)
O2-C1-C8-C9	114.4(3)
O1-C1-C8-C9	-1.5(4)
O2-C1-C8-C7	0.7(3)
O1-C1-C8-C7	-115.1(3)
C7-C8-C9-C10	-69.4(5)
C1-C8-C9-C10	-175.8(4)
C7-C8-C9-C14	103.2(3)
C1-C8-C9-C14	-3.2(4)
C14-C9-C10-C11	-0.3(5)
C8-C9-C10-C11	171.6(4)
C9-C10-C11-C12	-2.3(5)
C9-C10-C11-C16	-179.4(3)

C10-C11-C12-C13	2.2(6)
C16-C11-C12-C13	179.3(3)
C11-C12-C13-C14	0.6(5)
C11-C12-C13-P1	-166.9(3)
C29-P1-C13-C14	55.2(3)
C35-P1-C13-C14	163.9(3)
Rh1-P1-C13-C14	-73.2(3)
C29-P1-C13-C12	-138.0(3)
C35-P1-C13-C12	-29.3(3)
Rh1-P1-C13-C12	93.6(3)
C1-O1-C14-C13	169.4(3)
C1-O1-C14-C9	-8.3(4)
C12-C13-C14-O1	179.3(3)
P1-C13-C14-O1	-13.2(5)
C12-C13-C14-C9	-3.2(5)
P1-C13-C14-C9	164.2(3)
C10-C9-C14-O1	-179.2(3)
C8-C9-C14-O1	7.3(4)
C10-C9-C14-C13	3.2(5)
C8-C9-C14-C13	-170.4(3)
C3-P2-C17-C22	73.3(3)
C23-P2-C17-C22	-35.7(3)
Rh2-P2-C17-C22	-166.1(2)
C3-P2-C17-C18	-102.0(3)
C23-P2-C17-C18	149.0(3)
Rh2-P2-C17-C18	18.6(3)
C22-C17-C18-C19	1.4(5)
P2-C17-C18-C19	176.8(3)
C17-C18-C19-C20	0.3(5)
C18-C19-C20-C21	-1.5(5)
C19-C20-C21-C22	1.0(5)
C18-C17-C22-C21	-1.8(5)
P2-C17-C22-C21	-177.1(3)
C20-C21-C22-C17	0.6(5)
C3-P2-C23-C28	-19.7(3)
C17-P2-C23-C28	87.0(3)
Rh2-P2-C23-C28	-146.4(2)
C3-P2-C23-C24	160.1(3)

C17-P2-C23-C24	-93.2(3)
Rh2-P2-C23-C24	33.3(3)
C28-C23-C24-C25	0.1(5)
P2-C23-C24-C25	-179.7(3)
C23-C24-C25-C26	1.6(6)
C24-C25-C26-C27	-1.7(6)
C25-C26-C27-C28	0.1(6)
C24-C23-C28-C27	-1.8(5)
P2-C23-C28-C27	178.0(3)
C26-C27-C28-C23	1.7(6)
C13-P1-C29-C30	-159.1(3)
C35-P1-C29-C30	91.8(3)
Rh1-P1-C29-C30	-34.1(3)
C13-P1-C29-C34	23.6(3)
C35-P1-C29-C34	-85.5(3)
Rh1-P1-C29-C34	148.6(2)
C34-C29-C30-C31	-0.3(5)
P1-C29-C30-C31	-177.7(3)
C29-C30-C31-C32	-0.7(6)
C30-C31-C32-C33	0.9(6)
C31-C32-C33-C34	-0.2(6)
C32-C33-C34-C29	-0.8(6)
C30-C29-C34-C33	1.0(5)
P1-C29-C34-C33	178.4(3)
C29-P1-C35-C40	-142.4(3)
C13-P1-C35-C40	106.7(3)
Rh1-P1-C35-C40	-14.6(3)
C29-P1-C35-C36	37.9(3)
C13-P1-C35-C36	-73.0(3)
Rh1-P1-C35-C36	165.7(2)
C40-C35-C36-C37	1.2(5)
P1-C35-C36-C37	-179.1(3)
C35-C36-C37-C38	-0.1(6)
C36-C37-C38-C39	-0.5(6)
C37-C38-C39-C40	0.0(6)
C38-C39-C40-C35	1.1(6)
C36-C35-C40-C39	-1.7(5)
P1-C35-C40-C39	178.5(3)

P2-Rh2-C42-O4	155(7)
Cl1-Rh2-C42-O4	-6(8)
Cl2-Rh2-C42-O4	-30(7)
P1-Rh1-C41-O3	172(100)
Cl1-Rh1-C41-O3	-6(9)
Cl2-Rh1-C41-O3	-6(8)

Symmetry transformations used to generate equivalent atoms: