

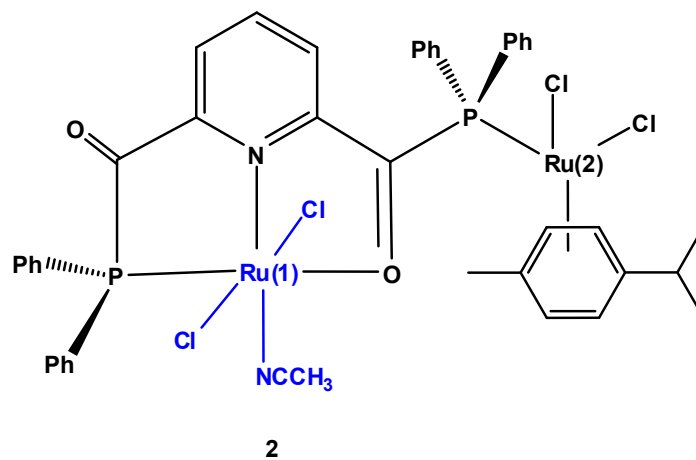
*Supporting Information for*

**A phosphonide based PNP pincer ligand, 2,6- $\{\text{Ph}_2\text{PC}(\text{O})\}_2(\text{C}_5\text{H}_3\text{N})$   
showing PP, PNP and PNO coordination modes**

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Louisiana 70118.*

## AOMix Analysis

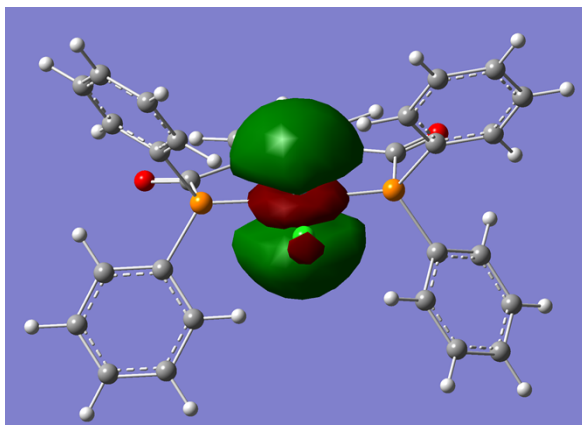


**Fig. S1.** Ruthenium PNO pincer complex **2**

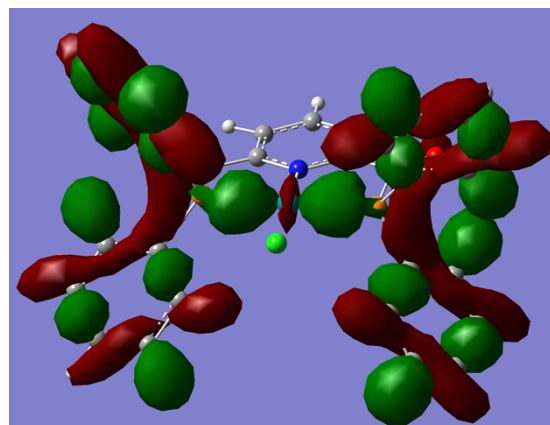
**Table S1.** Composition<sup>a</sup> and energies of important Kohn–Sham orbitals of Ruthenium pincer complex **2** obtained using the wave function generated at the B3LYP/6-31G\*\*, SDD level of theory

Orbital	Energy (eV)	Orbital character
LUMO	-1.849	33.67% $d_{xz}$ Ru, 66.33% PNP
HOMO	-3.191	11.51% $d_{xz}$ Ru, 88.49% PNP
HOMO-19	-9.022	12.78% $d_{xy}$ Ru, 87.22% PNP
HOMO-24	-9.592	1.45% $d_{x^2-y^2}$ Ru, 98.55% PNP
HOMO-37	-10.905	12.06% $d_{x^2-y^2}$ Ru, 87.94% PNP

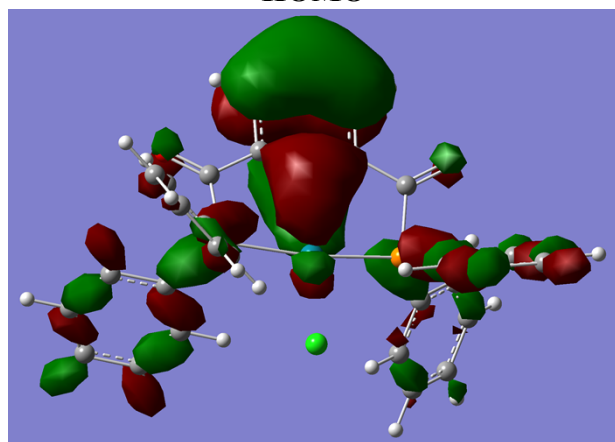
<sup>a</sup>combination of PNP pincer and  $[\text{RuCl}_2(\text{CH}_3\text{CN})]$  are considered as two interacting fragments in AOMix analysis.



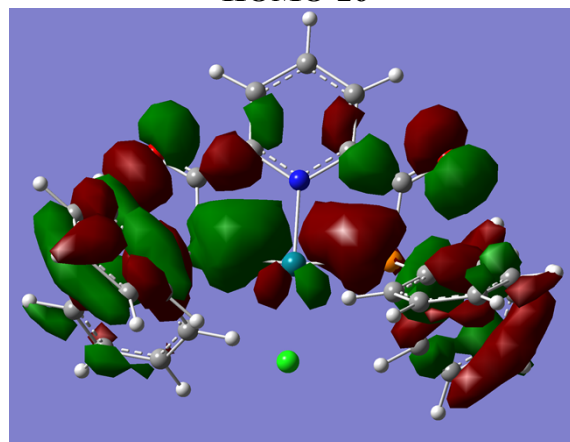
HOMO



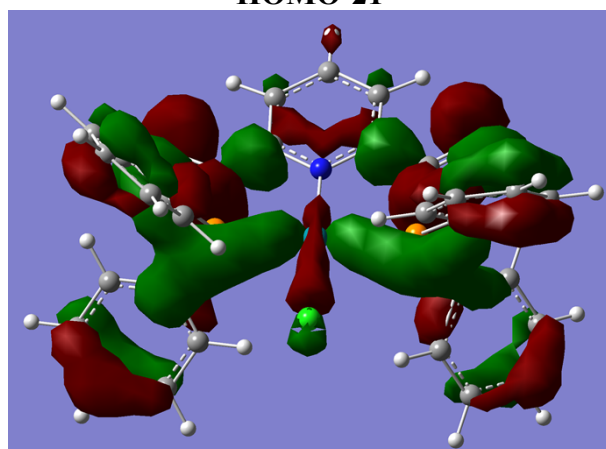
HOMO-26



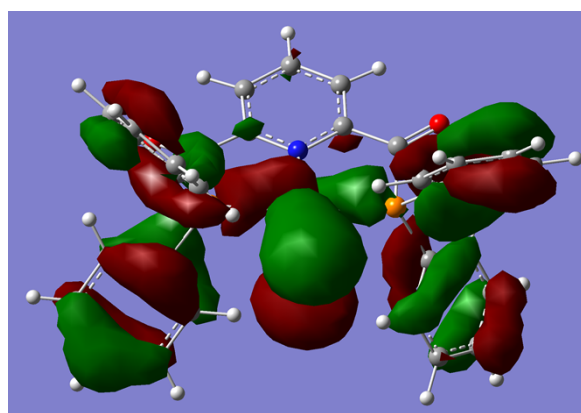
HOMO-21



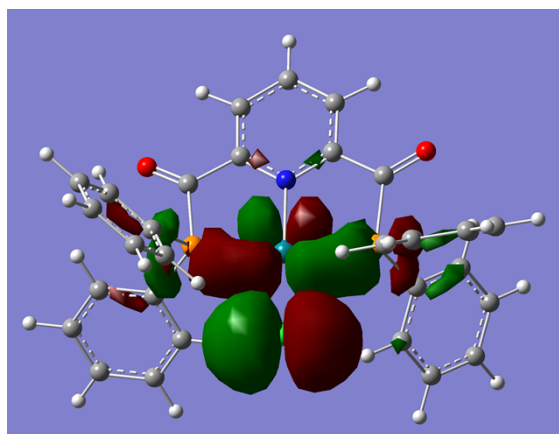
HOMO-18



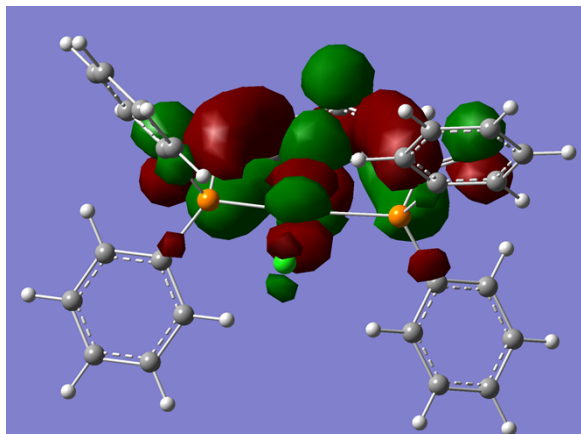
HOMO-14



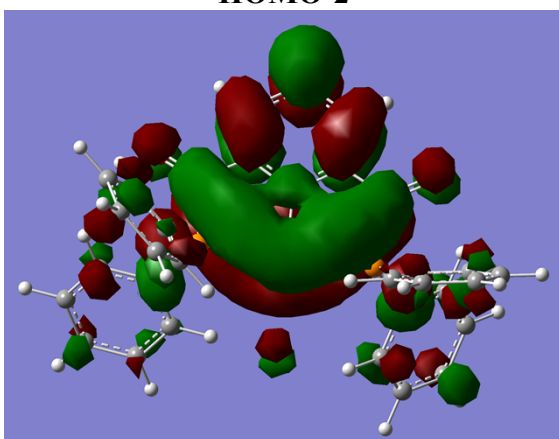
HOMO-13



**HOMO-2**



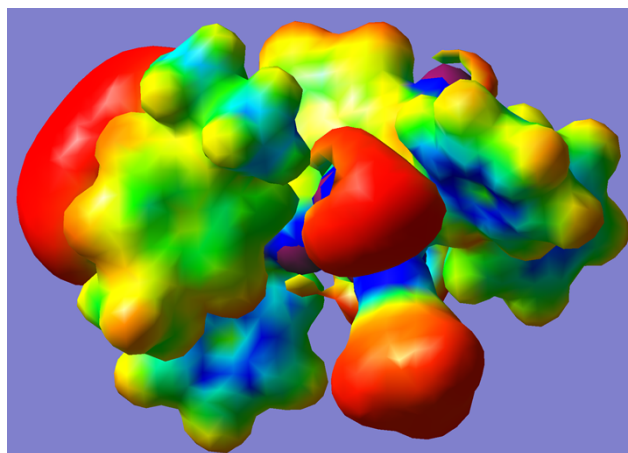
**LUMO**



**LUMO+2**

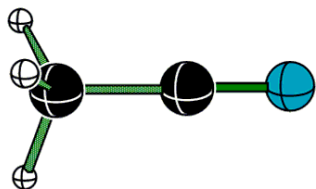
**Fig. S2.** Selected set of Kohn–Sham orbital contours for key orbitals of Rh-PNP pincer complex 5.

### Electrostatic Potential

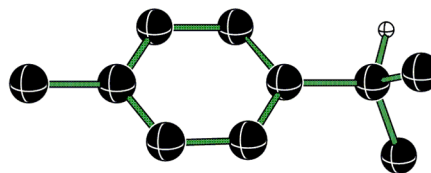


red is  $2.5 \cdot 10^{-5}$ , blue is  $2.5 \cdot 10^{-2}$

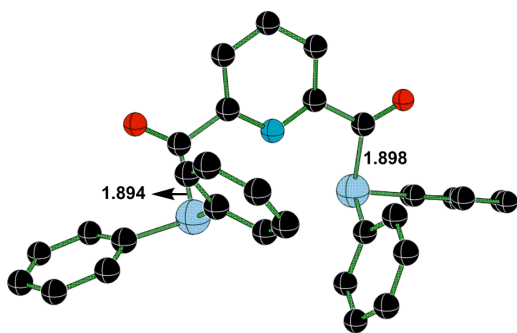
**Fig. S3.** Electrostatic potential map for ruthenium PNO pincer complex 2



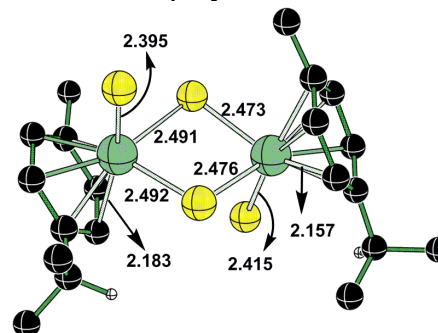
CH<sub>3</sub>CN



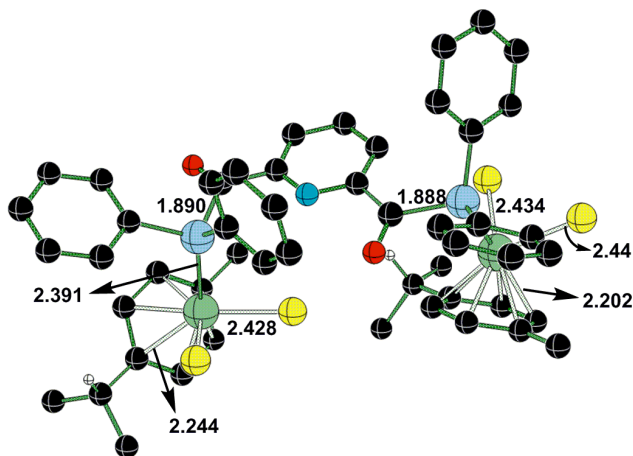
p-cymene



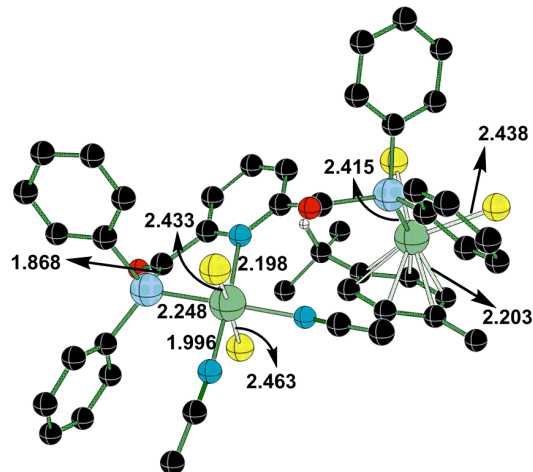
2,6-{Ph<sub>2</sub>PC(O)}<sub>2</sub>(C<sub>5</sub>H<sub>3</sub>N) (PNP) (1)



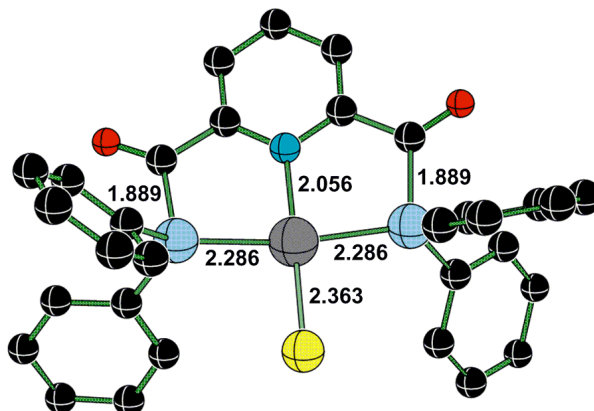
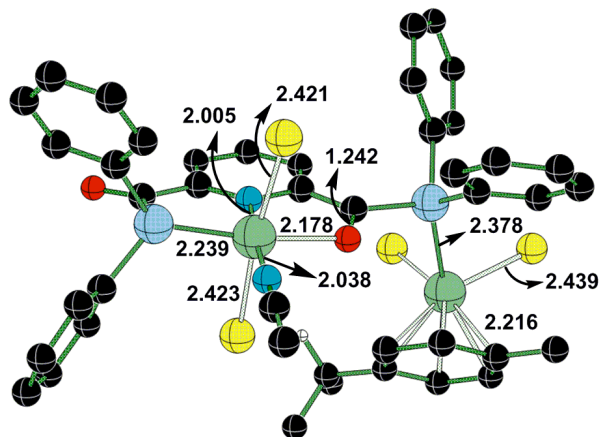
[RuCl<sub>2</sub>(p-cymene)]<sub>2</sub>

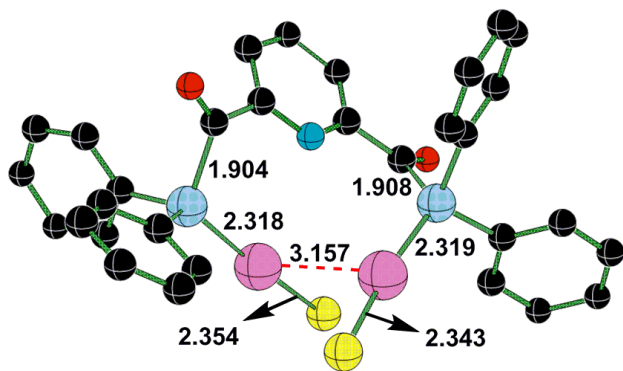
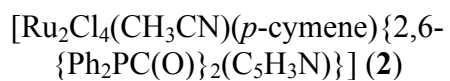


[Ru<sub>2</sub>Cl<sub>4</sub>(p-cymene){2,6-{Ph<sub>2</sub>PC(O)}<sub>2</sub>(C<sub>5</sub>H<sub>3</sub>N)}] (2a)



[Ru<sub>2</sub>Cl<sub>4</sub>(CH<sub>3</sub>CN)<sub>2</sub>(p-cymene){2,6-{Ph<sub>2</sub>PC(O)}<sub>2</sub>(C<sub>5</sub>H<sub>3</sub>N)}] (2b)





**Fig. S4.** The key optimized geometries of complexes PNP (1), p-cymene, CH<sub>3</sub>CN, [RuCl<sub>2</sub>(p-cymene)]<sub>2</sub>, 2a, 2b, 2, 5 and 17 at M06 & B3LYP/6-31G\*\*, SDD level of theory.

Total electronic energies and Gibbs free energies (in a.u.) and Cartesian coordinates of geometries optimized at the M06 & B3LYP/6-31G\*, SDD level of theory

2,6-{Ph<sub>2</sub>PC(O)}<sub>2</sub>(C<sub>5</sub>H<sub>3</sub>N) (PNP) (1)

E<sub>ele</sub> = -2081.9501679  
G = -2081.561652  
N<sub>imag</sub> = 0

6	1.047395	-2.159657	0.788620
6	1.189276	-3.105013	1.806780
6	0.080140	-3.412012	2.582230
6	-1.132440	-2.804106	2.282529
6	-1.179326	-1.906193	1.216032
7	-0.107233	-1.563062	0.500962
1	0.154885	-4.127700	3.397332
1	2.158639	-3.572119	1.958840
1	-2.046953	-3.015103	2.829932
6	2.238281	-1.807683	-0.053027
6	-2.498625	-1.338035	0.786692
8	-3.500900	-1.538925	1.439864
8	3.150382	-2.595152	-0.184715
15	-2.494565	-0.443684	-0.888138
15	2.179846	-0.075385	-0.817713
6	-4.313843	-0.250051	-1.082670
6	-4.895445	-0.956595	-2.139493
6	-5.133204	0.531675	-0.263401
6	-6.266093	-0.891815	-2.371970
1	-4.262438	-1.561498	-2.788558
6	-6.500779	0.601547	-0.496093
1	-4.697614	1.096924	0.558324
1	-6.704504	-1.446644	-3.198454
1	-7.128239	1.214410	0.147535
6	-1.998232	1.229035	-0.293034
6	-2.184999	1.690127	1.015268
6	-1.460168	2.102308	-1.244585
6	-1.870238	3.003013	1.353267
1	-2.593765	1.025629	1.776051
6	-1.151713	3.416782	-0.908777
1	-1.285712	1.743291	-2.257990
1	-2.025996	3.350028	2.372869
1	-0.743728	4.087170	-1.661715
6	3.891052	-0.015620	-1.478039
6	4.268369	-0.964656	-2.435256
6	4.782135	1.014133	-1.163124
6	5.516255	-0.899025	-3.042253
1	3.584294	-1.768895	-2.700255
6	6.027604	1.084048	-1.779388
1	4.503849	1.765996	-0.426530
1	5.799762	-1.651545	-3.774770

p-cymene

E<sub>ele</sub> = -389.19537  
G = -389.020543  
N<sub>imag</sub> = 0

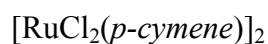
6	-0.031717	-1.037561	0.051344
6	1.349103	-1.180148	0.078897
6	2.191451	-0.067557	0.015807
6	1.600653	1.192392	-0.069208
6	0.217174	1.334667	-0.096783
6	-0.624544	0.225004	-0.037791
1	-0.659927	-1.927203	0.102759
1	1.788040	-2.175241	0.153021
1	2.235637	2.077234	-0.112379
1	-0.221363	2.330624	-0.161585
6	3.682656	-0.226806	0.013818
1	4.069073	-0.370832	-1.003684
1	4.181781	0.657002	0.426202
1	3.995386	-1.096608	0.602322
6	-2.127592	0.385025	-0.048398
6	-2.742027	-0.053844	1.279442
6	-2.770542	-0.363184	-1.213231
1	-2.338793	1.458306	-0.178441
1	-2.296602	0.484804	2.123307
1	-3.824403	0.124141	1.289407
1	-2.581833	-1.126679	1.448823
1	-2.354664	-0.041524	-2.174517
1	-2.605496	-1.445019	-1.124650
1	-3.854523	-0.196934	-1.233963

CH<sub>3</sub>CN

E<sub>ele</sub> = -132.6561071  
G = -132.633726  
N<sub>imag</sub> = 0

6	0.000000	0.000000	0.276667
7	0.000000	0.000000	1.437194
6	0.000000	0.000000	-1.175290
1	0.000000	1.025430	-1.556208
1	0.888048	-0.512715	-1.556208
1	-0.888048	-0.512715	-1.556208

1	6.710624	1.891146	-1.523046
6	2.356446	0.771319	0.814488
6	1.502028	1.832537	1.112526
6	3.297203	0.363688	1.770157
6	1.585506	2.482029	2.341645
1	0.769901	2.156165	0.374487
6	3.378354	1.010512	2.996863
1	3.974455	-0.460169	1.543368
1	0.913353	3.310601	2.556791
1	4.111184	0.686429	3.732639
6	-7.069366	-0.110810	-1.549555
1	-8.140608	-0.052392	-1.729774
6	-1.361592	3.870404	0.390823
1	-1.121777	4.898244	0.654938
6	6.399394	0.126151	-2.716511
1	7.374529	0.180134	-3.195427
6	2.520921	2.070925	3.283931
1	2.585626	2.576222	4.245209

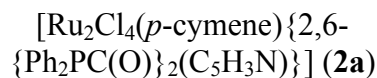


$$E_{\text{ele}} = -2809.0750673$$

$$G = -2808.700503$$

$$N_{\text{imag}} = 0$$

44	1.779199	-0.310382	0.078389
17	-0.028210	-1.898117	0.653870
17	-0.059513	0.984442	-0.958738
17	1.261026	0.817642	2.149786
44	-1.903647	-0.402942	-0.017718
17	-1.914003	-1.563461	-2.112382
6	3.155498	0.518184	-1.360974
6	2.660787	-0.719732	-1.876904
6	2.733217	-1.904647	-1.110577
6	3.324935	-1.821372	0.195914
6	3.824982	-0.597764	0.695692
6	3.749797	0.609593	-0.076291
1	2.951630	1.428298	-1.920284
1	2.090123	-0.723666	-2.803647
1	3.279861	-2.689738	0.850028
1	4.149762	-0.536090	1.732938
6	2.103492	-3.166735	-1.601744
1	1.904291	-3.858347	-0.778266
1	1.148559	-2.955037	-2.096919
1	2.769178	-3.664735	-2.317544
6	4.222680	1.906832	0.524992
1	3.986130	1.846883	1.598376
6	5.737939	2.010699	0.351541
1	6.117913	2.923711	0.823698



$$E_{\text{ele}} = -4891.0838181$$

$$G = -4890.286957$$

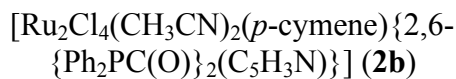
$$N_{\text{imag}} = 0$$

6	-7.319077	3.384644	-0.700537
6	-6.598072	3.180449	-1.870114
6	-5.354893	2.549836	-1.834912
6	-4.826100	2.115931	-0.616974
6	-5.554099	2.333919	0.563295
6	-6.791185	2.963040	0.518110
15	-3.245560	1.207972	-0.381217
6	-2.247145	2.406882	0.567000
6	-1.435106	2.004811	1.626597
6	-0.661157	2.951262	2.289786
6	-0.677017	4.283677	1.890131
6	-1.481477	4.683813	0.825509
6	-2.272650	3.748467	0.169990
44	-3.767483	-1.035571	0.259608
17	-1.399616	-1.464093	0.582838
8	1.197530	0.800537	1.097370
6	1.785768	0.895279	0.041377
6	1.042023	0.876191	-1.262778
6	1.677409	0.693475	-2.494167
6	0.896696	0.618957	-3.643688
6	-0.475483	0.756194	-3.530623
6	-1.011501	0.964287	-2.253034
7	-0.279788	1.016367	-1.148560
6	-2.488973	1.079289	-2.108646



1	6.260016	1.155553	0.797549	8	-3.217055	0.934776	-3.077771
1	6.002515	2.048023	-0.714022	15	3.672169	0.851432	0.114430
6	3.515788	3.130661	-0.037107	6	4.278191	2.054897	-1.122140
1	3.816049	4.021490	0.524993	6	5.370114	1.763570	-1.942149
1	3.785132	3.308482	-1.087361	6	5.817544	2.716020	-2.854248
1	2.426550	3.031759	0.038641	6	5.183642	3.948995	-2.953664
6	-3.212224	1.329798	0.145972	6	4.098017	4.244377	-2.132209
6	-3.962372	0.194393	-0.251532	6	3.649045	3.303321	-1.215735
6	-3.903407	-1.021932	0.496286	44	4.157613	-1.487593	0.073231
6	-3.097367	-1.121405	1.659787	17	4.264401	-1.393219	-2.356892
6	-2.358398	0.034840	2.079732	6	4.739319	-3.310140	1.164186
6	-2.416150	1.228889	1.338360	6	4.329489	-2.319083	2.116173
1	-4.473280	0.192630	-1.210843	6	3.045500	-1.746444	1.940956
1	-4.373301	-1.917150	0.095002	6	2.190217	-2.150729	0.873236
1	-1.619067	-0.058394	2.873799	6	2.607716	-3.124079	-0.062372
1	-1.725023	2.033739	1.586920	6	3.907431	-3.706548	0.103448
6	-2.945243	-2.423561	2.374740	6	5.247152	-1.894871	3.214669
1	-3.686730	-2.500187	3.179805	6	1.652247	-3.545432	-1.155202
1	-3.093424	-3.263801	1.688558	6	0.537434	-4.380108	-0.514892
1	-1.947685	-2.513756	2.815548	6	2.301458	-4.322866	-2.289770
6	-3.170863	2.601869	-0.661765	17	6.527730	-0.908139	0.048500
1	-2.154331	3.008096	-0.544074	6	4.011424	1.714047	1.698087
6	-3.428205	2.393766	-2.146926	6	5.255955	1.483694	2.293033
1	-3.265744	3.333734	-2.685549	6	5.609071	2.156471	3.459231
1	-2.761889	1.633800	-2.571789	6	4.727061	3.060913	4.040219
1	-4.466674	2.090988	-2.337274	6	3.491864	3.300843	3.445373
6	-4.164955	3.595985	-0.060060	6	3.133195	2.637353	2.277877
1	-3.963827	3.783971	1.001401	17	-3.860443	-0.150299	2.517229
1	-4.117905	4.554194	-0.589792	1	1.367005	0.451541	-4.609026
1	-5.190771	3.213066	-0.147350	1	2.754015	0.562531	-2.560114
				1	-1.141939	0.703885	-4.386949
				1	-1.388669	0.957194	1.909187
				1	-2.915141	4.066095	-0.651489
				1	-0.028683	2.634209	3.117126
				1	-1.499987	5.724717	0.510918
				1	5.857819	0.794470	-1.864108
				1	2.804543	3.547762	-0.570305
				1	6.668693	2.485663	-3.490336
				1	3.602451	5.209813	-2.203999
				1	5.947759	0.777550	1.832565
				1	2.158883	2.833956	1.838274
				1	6.580493	1.970576	3.912045
				1	2.796042	4.009629	3.890907
				1	-0.063016	5.015555	2.412684
				1	5.002087	3.582753	4.954118
				1	5.537439	4.686630	-3.670693
				1	2.723546	-0.937735	2.595855
				1	1.223123	-1.661623	0.747158
				1	4.298965	-4.376985	-0.656100
				1	5.765813	-3.669634	1.198554
				1	4.957798	-0.917483	3.615459

1	5.224137	-2.623498	4.034488
1	6.276369	-1.821244	2.844597
1	1.204544	-2.622038	-1.560472
1	-0.024104	-3.814783	0.238020
1	-0.170286	-4.710910	-1.285991
1	0.957090	-5.279087	-0.042172
1	1.553533	-4.538182	-3.061101
1	3.120965	-3.763238	-2.750992
1	2.682689	-5.290752	-1.934660
1	-4.810665	2.386034	-2.759392
1	-5.153436	1.984717	1.515884
1	-6.999913	3.513830	-2.824380
1	-7.344738	3.124150	1.440431
1	-8.289670	3.874317	-0.735757
6	-5.794301	-1.936802	0.603026
6	-4.807895	-2.972560	0.649945
6	-3.886586	-3.126841	-0.406670
6	-3.906507	-2.288550	-1.562488
6	-4.887158	-1.259903	-1.592374
6	-5.827857	-1.092987	-0.533843
1	-4.694031	-3.570492	1.548460
1	-3.062313	-3.829417	-0.291132
1	-4.868023	-0.540767	-2.410269
1	-6.522310	-0.253451	-0.557432
6	-6.798046	-1.716168	1.708733
1	-6.817599	-0.630870	1.896652
6	-8.175327	-2.157366	1.205525
1	-8.171490	-3.229145	0.965194
1	-8.484890	-1.612305	0.306543
6	-6.457835	-2.423359	3.011822
1	-5.465439	-2.136853	3.376446
1	-6.503095	-3.515281	2.895244
6	-2.879284	-2.442841	-2.637329
1	-3.087257	-3.326163	-3.253366
1	-2.868334	-1.565794	-3.293771
1	-1.882730	-2.558472	-2.190598
1	-8.932577	-1.992852	1.980393
1	-7.192330	-2.153030	3.778281

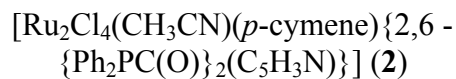


$$E_{\text{ele}} = -4767.2243988$$

$$G = -4766.545506$$

$$N_{\text{imag}} = 0$$

6	-7.629632	-1.894307	1.376089
6	-7.546770	-0.505627	1.292911
6	-6.457906	0.086899	0.662772
6	-5.450339	-0.708967	0.105500



$$E_{\text{ele}} = -4634.5791941$$

$$G = -4633.945333$$

$$N_{\text{imag}} = 0$$

6	6.478168	3.742910	0.606983
6	6.684219	2.547772	1.289102
6	5.934499	1.424255	0.961121
6	4.970943	1.490105	-0.049578

6	-5.529805	-2.100683	0.200207	6	4.760291	2.695035	-0.722468
6	-6.622414	-2.686584	0.831709	6	5.518326	3.813513	-0.397847
15	-3.953488	0.122749	-0.494123	15	3.951381	0.006932	-0.354734
6	-4.546835	1.429524	-1.630756	6	5.211750	-1.316203	-0.400376
6	-3.831301	2.620283	-1.782693	6	5.206557	-2.314620	0.576512
6	-4.233398	3.547552	-2.740419	6	6.215234	-3.274035	0.590700
6	-5.334345	3.290295	-3.549207	6	7.219537	-3.246184	-0.370120
6	-6.039503	2.096810	-3.410765	6	7.225013	-2.253352	-1.347391
6	-5.645973	1.165353	-2.459082	6	6.230597	-1.283855	-1.360882
44	-2.190395	0.275373	0.892184	44	1.919614	-0.217741	0.559355
17	-2.488611	2.659742	1.272739	17	1.889375	-2.637758	0.612051
8	0.499730	2.285367	0.310322	8	-0.229103	-0.441628	0.836977
6	0.981770	1.355275	-0.282471	6	-0.836404	-0.675773	-0.221480
6	0.200180	0.533537	-1.264299	6	-0.109374	-0.526167	-1.489721
6	0.851029	0.205421	-2.452627	6	-0.675987	-0.573033	-2.765763
6	0.184873	-0.500635	-3.442249	6	0.120646	-0.343755	-3.880179
6	-1.117383	-0.888253	-3.183555	6	1.471751	-0.090269	-3.694797
6	-1.706282	-0.536921	-1.974658	6	1.990526	-0.068977	-2.405943
7	-1.086922	0.191843	-1.006684	7	1.218640	-0.275673	-1.318519
6	-3.136526	-0.954485	-1.783424	6	3.438243	0.181631	-2.181129
8	-3.663888	-1.812638	-2.453350	8	4.198532	0.467073	-3.080595
15	2.862934	0.941333	-0.067016	15	-2.658870	-1.029040	-0.064974
6	3.570414	2.052960	-1.355926	6	-3.010000	-2.260817	-1.370561
6	4.927049	1.920767	-1.673325	6	-4.069820	-2.099790	-2.265625
6	5.515010	2.795467	-2.578893	6	-4.289011	-3.062738	-3.247268
6	4.764259	3.799441	-3.182176	6	-3.460960	-4.175248	-3.340412
6	3.416432	3.934917	-2.871529	6	-2.410303	-4.342549	-2.440668
6	2.820557	3.068924	-1.959478	6	-2.188207	-3.393428	-1.451954
44	3.414570	-1.410171	-0.030359	44	-3.645274	1.131332	0.067194
17	3.943381	-1.162679	-2.389854	17	-3.478243	1.210637	-2.358669
6	3.900722	-3.266561	1.052195	6	-4.702833	2.607188	1.312169
6	3.198936	-2.414198	1.961166	6	-4.054838	1.669787	2.177558
6	1.945683	-1.912073	1.537736	6	-2.662571	1.475460	1.985739
6	1.385026	-2.277505	0.279470	6	-1.934011	2.201087	0.998084
6	2.075623	-3.142474	-0.599535	6	-2.591449	3.123277	0.150206
6	3.360303	-3.627775	-0.192040	6	-3.999468	3.321726	0.325413
6	3.801617	-2.093544	3.289910	6	-4.837781	0.909675	3.196376
6	1.439157	-3.525536	-1.914931	6	-1.779290	3.866796	-0.882755
6	0.146177	-4.300398	-1.645103	6	-0.855805	4.845678	-0.151524
6	2.355821	-4.306553	-2.843938	6	-2.614279	4.598260	-1.922050
17	5.711281	-0.747400	0.450627	17	-5.807583	0.030413	-0.178579
6	3.242143	1.892544	1.458096	6	-2.755134	-2.046491	1.457250
6	3.918710	1.256305	2.499464	6	-4.041507	-2.215894	1.984534
6	4.283088	1.958036	3.645392	6	-4.237526	-3.026413	3.097420
6	3.974455	3.308706	3.757892	6	-3.156812	-3.672695	3.689229
6	3.308387	3.956447	2.717906	6	-1.881056	-3.516713	3.157093
6	2.950609	3.258586	1.569432	6	-1.670783	-2.710380	2.042256
7	-3.363895	0.035551	2.488811	7	2.494162	-0.138537	2.512756
6	-4.137517	-0.205181	3.313818	6	2.796015	-0.045684	3.625416
6	-5.151541	-0.535598	4.291877	6	3.169599	0.080240	5.018140
17	-2.006984	-2.179326	0.808418	17	1.681408	2.193560	0.565533

1	0.692365	-0.762229	-4.367020	1	-0.315324	-0.363288	-4.874108
1	1.894302	0.478416	-2.593773	1	-1.738411	-0.762862	-2.876186
1	-1.712174	-1.473723	-3.879334	1	2.156363	0.094093	-4.518771
1	-2.987371	2.825337	-1.125303	1	4.394730	-2.355816	1.300051
1	-6.189934	0.226786	-2.360871	1	6.240088	-0.500603	-2.116748
1	-3.683959	4.480029	-2.846293	1	6.205969	-4.052979	1.349433
1	-6.895680	1.888952	-4.048312	1	8.010602	-2.230749	-2.099060
1	5.515854	1.128715	-1.214948	1	-4.708528	-1.222829	-2.197025
1	1.766834	3.208849	-1.724090	1	-1.369003	-3.536708	-0.746336
1	6.569185	2.681209	-2.819501	1	-5.114563	-2.935774	-3.943272
1	2.820928	4.717983	-3.335085	1	-1.764468	-5.214881	-2.504408
1	4.211653	0.218825	2.377560	1	-4.887398	-1.710631	1.515232
1	2.450239	3.781459	0.759912	1	-0.660030	-2.611855	1.648398
1	4.826147	1.447342	4.438530	1	-5.240175	-3.151601	3.500291
1	3.076420	5.016079	2.794593	1	-1.033254	-4.028837	3.606554
1	-5.646098	4.020466	-4.292940	1	8.002293	-4.001534	-0.360199
1	4.263921	3.864997	4.646849	1	-3.310303	-4.305006	4.560973
1	5.229524	4.476657	-3.894894	1	-3.635209	-4.920585	-4.113434
1	-6.040963	-0.910094	3.770392	1	3.938287	0.849988	5.134390
1	-4.789519	-1.311230	4.972922	1	2.299608	0.361907	5.618734
1	-5.428801	0.348035	4.874134	1	3.561606	-0.869534	5.393662
1	1.395324	-1.220203	2.174655	1	-2.145889	0.712736	2.567877
1	0.408669	-1.883356	0.002757	1	-0.869636	2.006314	0.852298
1	3.968399	-4.199615	-0.885689	1	-4.550203	3.944353	-0.372834
1	4.922316	-3.554261	1.292892	1	-5.788480	2.676317	1.344589
1	3.257130	-1.290456	3.798384	1	-4.297448	0.015449	3.524893
1	3.777060	-2.979005	3.937041	1	-5.035378	1.535974	4.075245
1	4.850499	-1.791004	3.172754	1	-5.799816	0.592724	2.776493
1	1.173975	-2.581892	-2.412370	1	-1.154370	3.114242	-1.390394
1	-0.566851	-3.732805	-1.033247	1	-0.171773	4.330124	0.531414
1	-0.343972	-4.548574	-2.594206	1	-0.250457	5.401726	-0.876389
1	0.362367	-5.243848	-1.125768	1	-1.445121	5.574161	0.422713
1	1.836667	-4.505215	-3.788302	1	-1.953363	5.058187	-2.664825
1	3.271638	-3.748476	-3.070628	1	-3.296765	3.920619	-2.445162
1	2.620954	-5.282591	-2.413724	1	-3.193799	5.410480	-1.460567
1	-6.382917	1.173154	0.604935	1	6.108857	0.482614	1.482771
1	-4.734026	-2.719985	-0.205407	1	4.003274	2.766183	-1.499487
1	-8.332095	0.116982	1.716053	1	7.437176	2.486454	2.071657
1	-6.686154	-3.770073	0.897362	1	5.353869	4.747064	-0.930490
1	-8.483453	-2.360019	1.863850	1	7.068247	4.621398	0.858175
7	-0.557075	0.461089	2.250798				
6	0.067920	0.942701	3.098430				
6	0.832739	1.595119	4.136578				
1	1.548722	0.902972	4.590582				
1	1.388320	2.435949	3.702490				
1	0.156216	1.974328	4.907966				

[RhCl{2,6-{Ph<sub>2</sub>PC(O)}<sub>2</sub>(C<sub>5</sub>H<sub>3</sub>N)}] (5)

$$E_{\text{ele}} = -2652.8010806$$

$$G = -2652.411237$$

[Au<sub>2</sub>Cl<sub>2</sub>{2,6-{Ph<sub>2</sub>PC(O)}<sub>2</sub>(C<sub>5</sub>H<sub>3</sub>N)}] (17)

$$E_{\text{ele}} = -3273.9928848$$

$N_{\text{imag}} = 0$

$G = -3273.614190$

$N_{\text{imag}} = 0$

6	4.658466	-3.681416	-1.528294	6	0.833712	2.639423	-0.198153
6	5.343576	-2.649227	-0.891062	6	0.675639	4.021343	-0.318764
6	4.652996	-1.536567	-0.428580	6	-0.461777	4.603778	0.222928
6	3.267412	-1.457892	-0.598381	6	-1.410139	3.786962	0.828459
6	2.583051	-2.491561	-1.244092	6	-1.184027	2.410710	0.838190
6	3.281607	-3.602131	-1.707197	7	-0.076428	1.844996	0.359881
15	2.278985	-0.055290	0.014678	1	-0.611601	5.678933	0.170272
6	3.252339	1.448924	-0.342664	1	1.443252	4.599926	-0.824731
6	2.865790	2.174914	-1.475797	1	-2.320065	4.184434	1.271310
6	3.569244	3.317804	-1.838260	6	2.083537	1.999350	-0.712737
6	4.645226	3.750335	-1.068727	6	-2.254455	1.501607	1.352914
6	5.023715	3.037363	0.064876	8	-2.861238	1.721943	2.374438
6	4.333163	1.886170	0.430446	8	2.793156	2.550094	-1.517744
8	-3.494580	0.413620	2.474431	15	-2.780820	0.092014	0.185535
6	-2.448838	0.220083	1.888647	15	2.640572	0.378043	0.124264
6	-1.151327	0.108575	2.615063	6	-3.494321	-1.144695	1.295323
6	-1.178423	0.117082	4.005003	6	-2.728475	-2.287549	1.537469
6	-0.000023	-0.001492	4.726290	6	-4.733966	-0.980794	1.921497
6	1.178405	-0.119499	4.004958	6	-3.195740	-3.260554	2.413670
6	1.151351	-0.109962	2.615025	1	-1.768460	-2.433098	1.041387
7	0.000023	-0.000451	1.893384	6	-5.195672	-1.960556	2.790401
6	2.448874	-0.220902	1.888550	1	-5.342784	-0.101683	1.721352
8	3.494651	-0.414608	2.474213	1	-2.589406	-4.145653	2.591330
15	-2.279014	0.055394	0.014694	1	-6.161625	-1.839017	3.274844
6	-3.252296	-1.448717	-0.343272	6	-4.150810	0.976145	-0.649642
6	-2.865702	-2.174270	-1.476667	6	-4.946780	1.934406	-0.009300
6	-3.569136	-3.317034	-1.839585	6	-4.403749	0.657520	-1.988815
6	-4.645136	-3.749865	-1.070249	6	-5.981379	2.554691	-0.701268
6	-5.023662	-3.037331	0.063620	1	-4.762360	2.197359	1.031143
6	-4.333140	-1.886267	0.429641	6	-5.443619	1.276228	-2.672466
6	-3.267509	1.458209	-0.597756	1	-3.775518	-0.074648	-2.495295
6	-2.583183	2.492099	-1.243147	1	-6.593878	3.299243	-0.198401
6	-3.281758	3.602834	-1.705828	1	-5.631730	1.020301	-3.712036
6	-4.658606	3.682058	-1.526828	6	3.042554	1.110061	1.748643
6	-5.343685	2.649650	-0.889916	6	3.797092	2.287448	1.833874
6	-4.653085	1.536829	-0.427852	6	2.549834	0.518949	2.914078
1	-0.000048	-0.001920	5.812088	6	4.061597	2.855855	3.073550
1	-2.151303	0.221032	4.479222	1	4.184764	2.751389	0.926520
1	2.151280	-0.223759	4.479124	6	2.815805	1.093416	4.153115
1	2.013052	1.834613	-2.065356	1	1.957627	-0.393490	2.842768
1	4.630507	1.330909	1.318406	1	4.651449	3.767238	3.135637
1	3.270439	3.876062	-2.722377	1	2.431926	0.627353	5.057166
1	5.861701	3.377294	0.669287	6	4.208959	0.070125	-0.739571
1	-2.012945	-1.833743	-2.066067	6	4.140291	-0.271259	-2.095407
1	-4.630518	-1.331337	1.317798	6	5.441001	0.085694	-0.083619
1	-3.270300	-3.874949	-2.723908	6	5.305832	-0.570708	-2.788109
1	-5.861661	-3.377504	0.667874	1	3.175107	-0.311977	-2.602859

1	-1.506927	2.404827	-1.392597	6	6.601856	-0.226330	-0.784008
1	-5.191031	0.728202	0.062644	1	5.497888	0.334103	0.974266
1	-2.748881	4.403029	-2.213881	1	5.251006	-0.830436	-3.842253
1	-6.421062	2.711956	-0.755485	1	7.559840	-0.218498	-0.269471
1	5.189819	4.648686	-1.350985	79	-1.120957	-0.462671	-1.333950
1	-5.204415	4.550119	-1.890077	79	1.370382	-1.556895	0.267424
1	-5.189717	-4.648111	-1.352859	17	0.500702	-0.616884	-3.032893
1	5.190962	-0.728098	0.062157	17	0.380559	-3.654184	0.605732
1	1.506790	-2.404220	-1.393470	6	-6.231202	2.226157	-2.030182
1	6.420961	-2.711574	-0.756717	1	-7.039761	2.716051	-2.567496
1	2.748707	-4.402154	-2.215498	6	3.569652	2.259372	4.232472
1	5.204258	-4.549346	-1.891878	1	3.775216	2.707721	5.201733
45	0.000033	0.000123	-0.163148	6	6.535534	-0.548814	-2.134719
17	0.000018	0.000657	-2.526294	1	7.444330	-0.791996	-2.680431
				6	-4.426872	-3.096656	3.038713
				1	-4.797337	-3.859736	3.719598