

Supporting Information for manuscript:

Crystal Structures and DFT Calculations of New chlorido-dimethylsulfoxide- M^{III} ($M = Ir, Ru, Rh$) complexes with N-Pyrazolyl Pyrimidine donor ligand: Kinetic vs thermodynamic isomers.

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1. Plots of the experimental and calculated powder XRD profiles

The calculated powder XRD profiles have been obtained using Mercury from the cif files.

1.1 compound 1a:

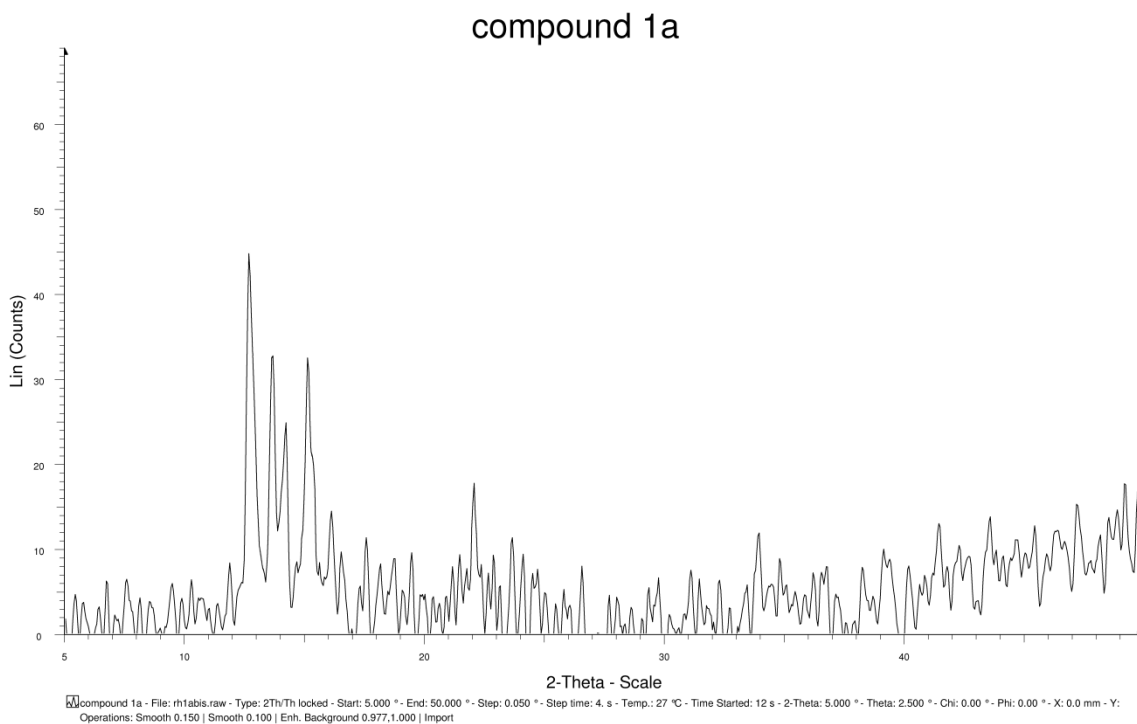


Fig S1. Plot of the experimental powder XRD profile of **1a**.

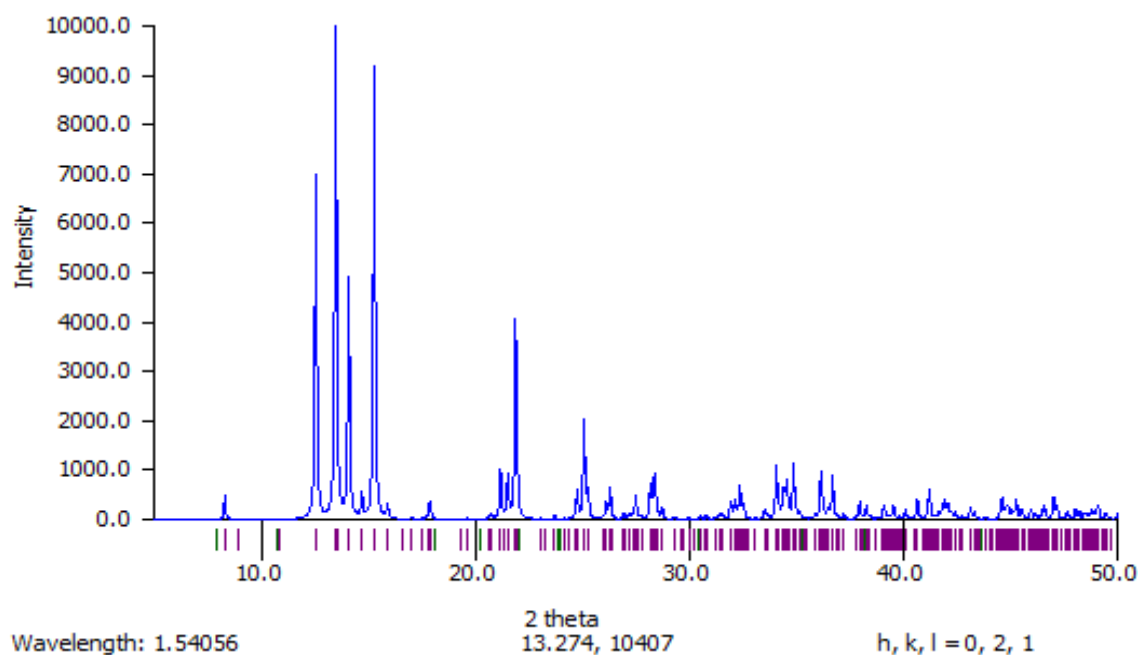


Fig S2. Plot of the calculated powder XRD profile of **1a**.

1.2 compound 1b:

compound 1b

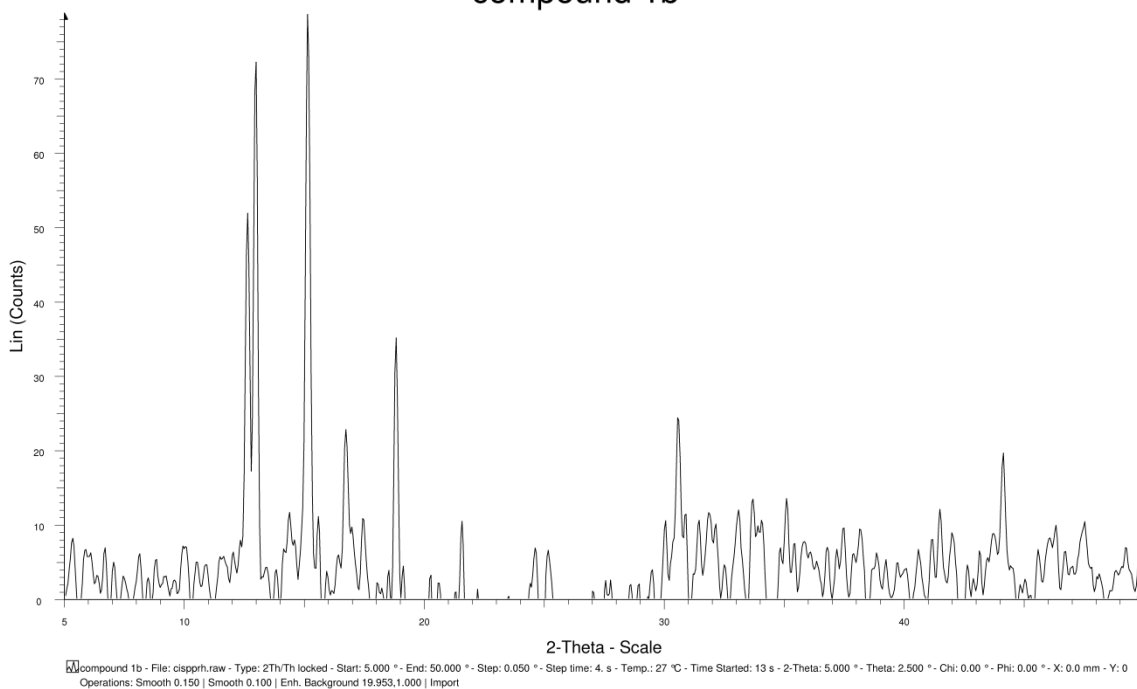


Fig S3. Plot of the experimental powder XRD profile of **1b**.

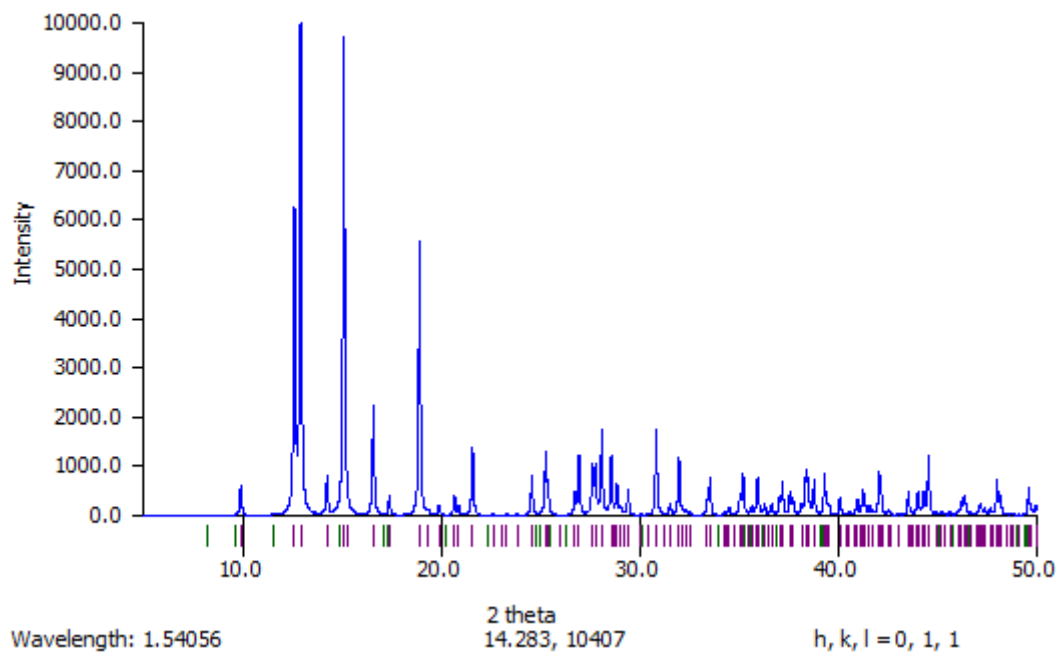


Fig S4. Plot of the calculated powder XRD profile of **1b**.

1.3 compound 2a:

compound 2a

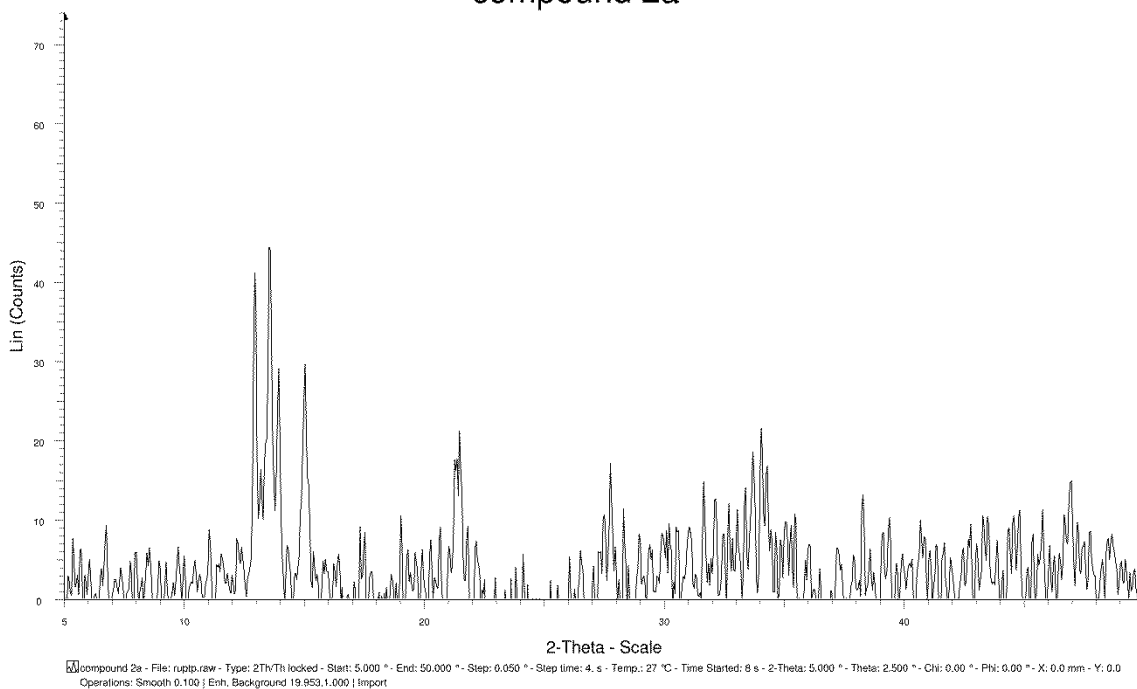


Fig S5. Plot of the experimental powder XRD profile of 2a.

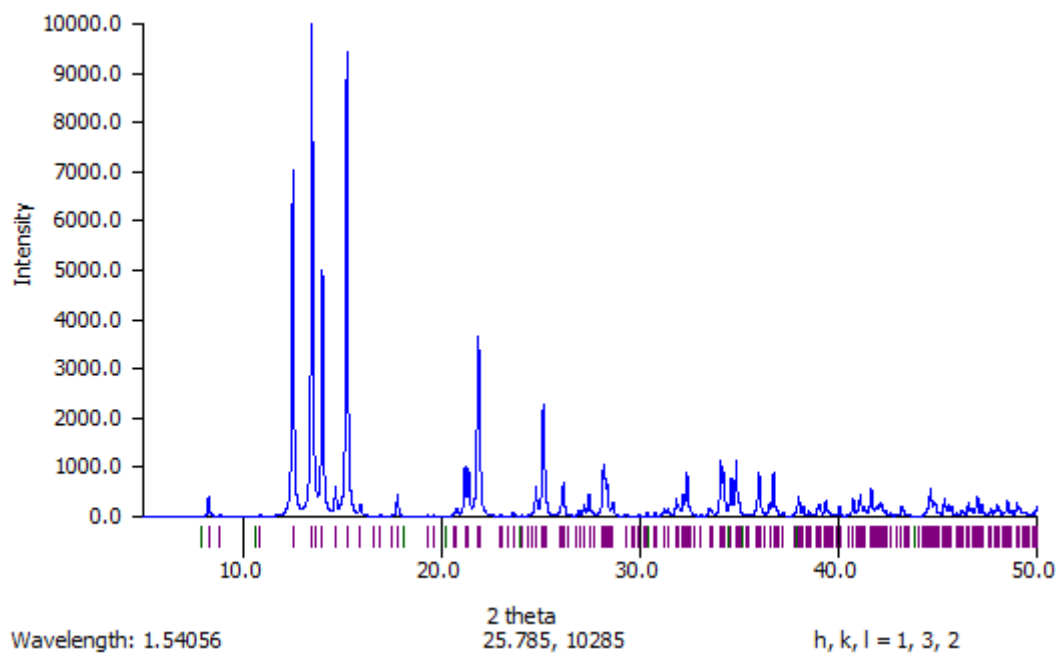


Fig S6. Plot of the calculated powder XRD profile of 2a.

1.4 compound 2b:

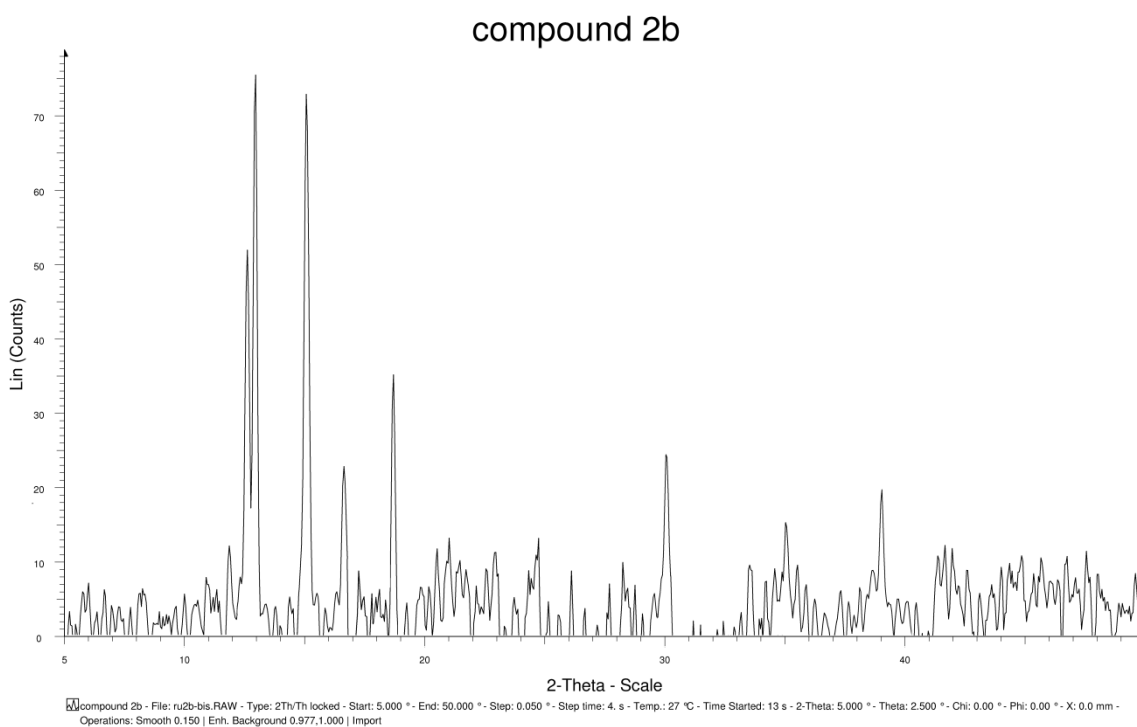


Fig S7. Plot of the experimental powder XRD profile of **2b**.

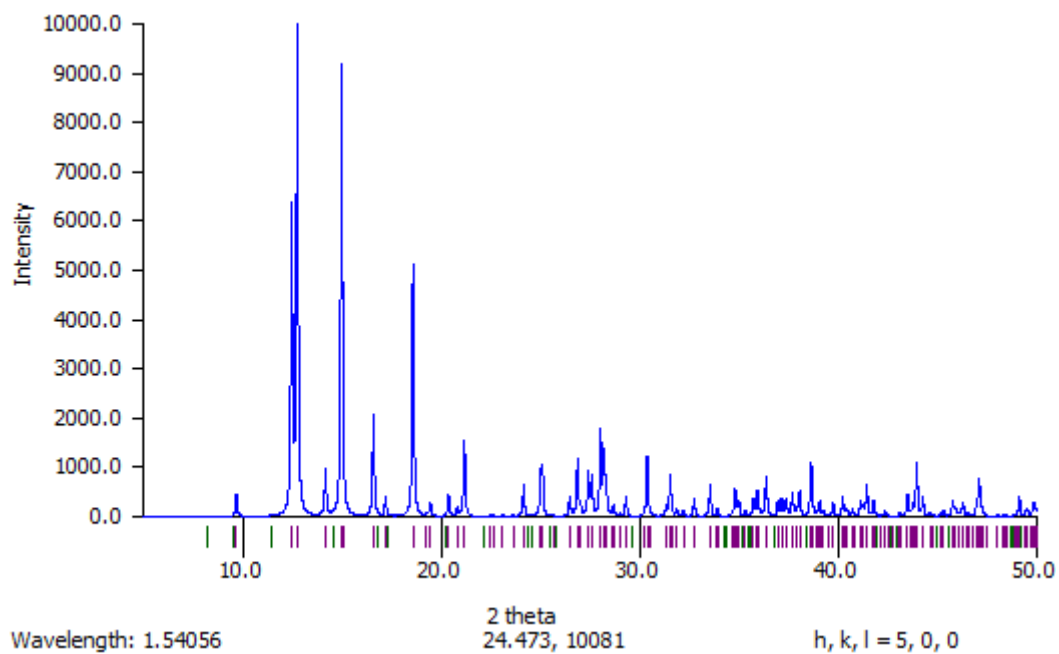


Fig S8. Plot of the calculated powder XRD profile of **2b**.

2. Conversion of 1b to 1a

A solution of 15 mg (0.1 mmols) of *pyrapyr* in 10 ml of EtOH was added to a solution of 48 mg (0.1 mmols) of $[\text{H}(\text{DMSO})_2][\text{trans-RhCl}_4(\text{DMSO})_2]$ in 5 ml of EtOH. The suspension was stirred during 10 h at room temperature and a precipitate was formed that corresponds to 1b (see Figure S1, top), then this suspension is refluxed during 3h with constant stirring. The resulting clear solution was cooled at room temperature, and **1a** precipitates from the reaction mixture (see Figure S1, bottom). The reaction cannot be followed by $^1\text{H-NMR}$ because of the low solubility of both the initial and final products in the reaction solvent (EtOH). The $^1\text{H-NMR}$ spectra have been done in DMSO solvent. In the next Figure we represent the initial (just before heating) and final NMR spectra for this reaction.

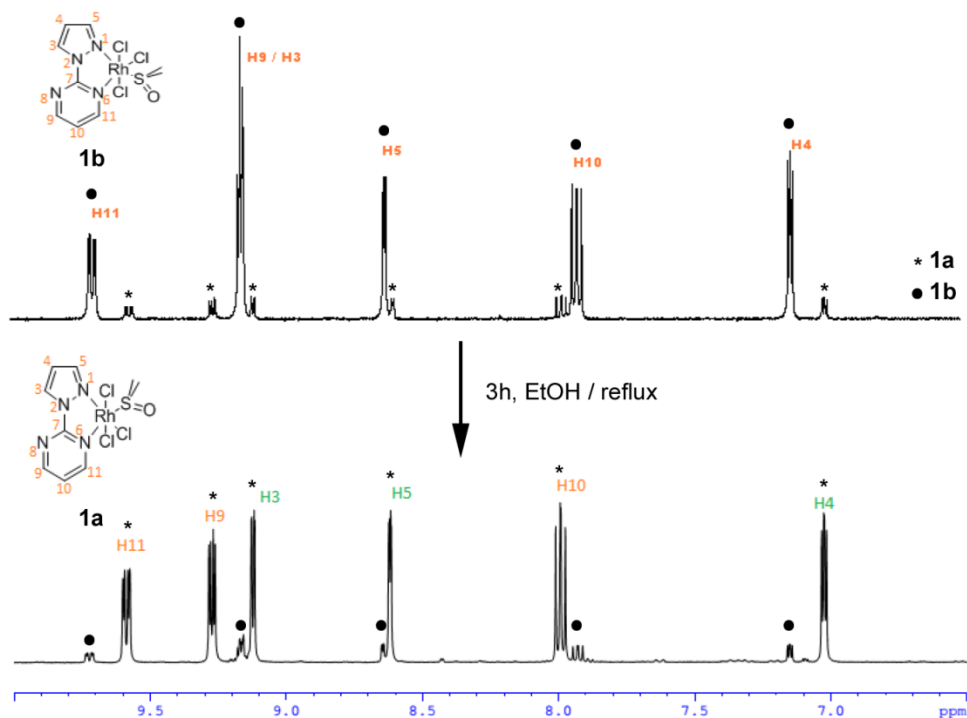


Fig. S1 $^1\text{H-NMR}$ spectra in DMSO- D_6 of reaction mixture at the initial reaction stage and at the final stage, showing the conversion of the *cis* into the *trans* isomer.

3. Figures S1-S3

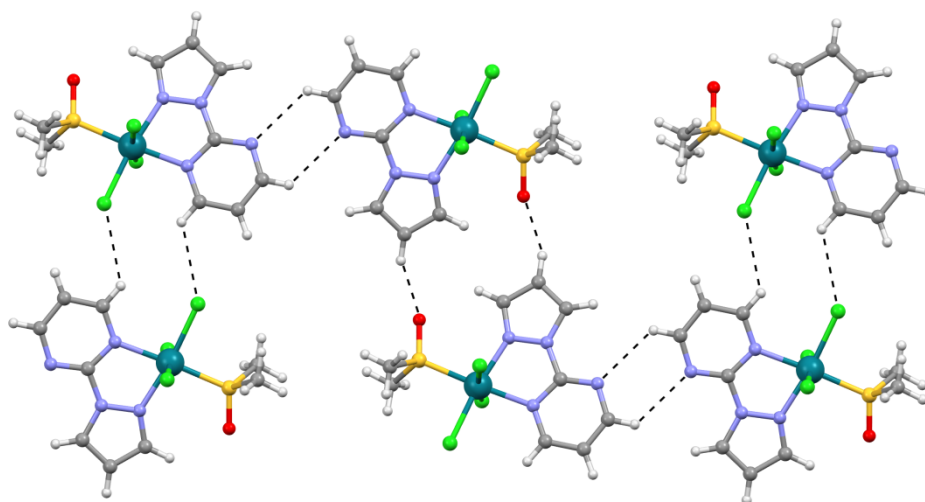


Fig. S2 2D plane observed in the solid state of compound **1a**. The hydrogen bonds are represented by dashed lines.

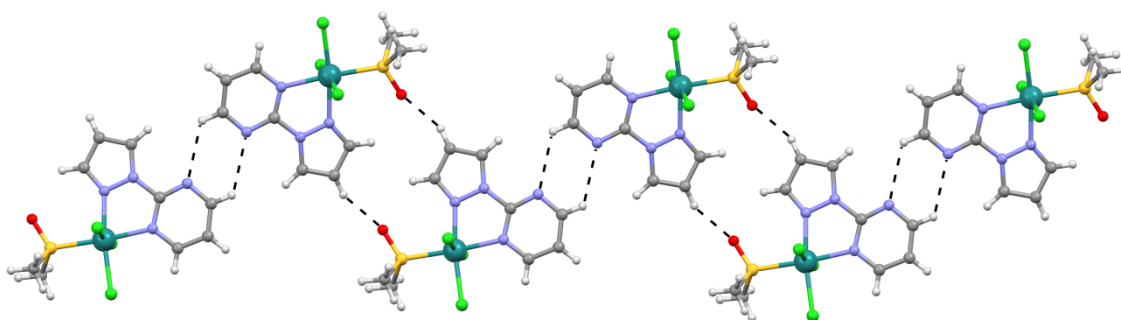


Fig. S3 1D ribbon observed in the solid state of compound **2a**. The hydrogen bonds are represented by dashed lines.

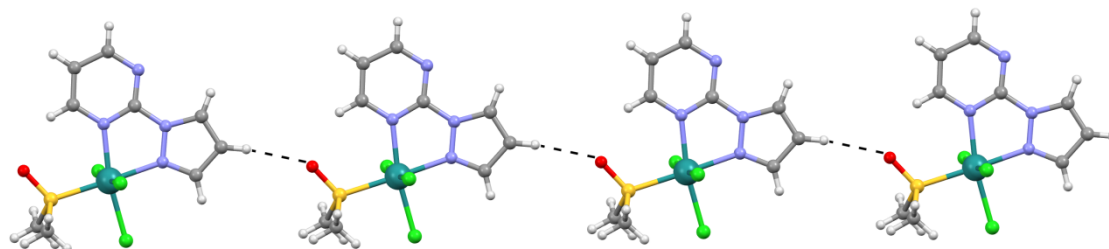


Fig. S4 1D infinite chain observed in the solid state of compound **2b**. The hydrogen bonds are represented by dashed lines.

4. Cartesian Coordinates.

1a.

S	-0.7888311	0.1066504	-2.5278058
O	-2.2424067	0.3947538	-2.4398329
C	-0.5397337	-1.3653598	-3.5287299
H	-1.0153208	-2.1908264	-2.9870074
H	0.5441684	-1.5301074	-3.5944515
H	-1.0091698	-1.1754995	-4.5036483
C	-0.0060814	1.3440422	-3.5706587
H	-0.5161736	1.3145166	-4.5429821
H	1.0597355	1.0856801	-3.6323628
H	-0.1327942	2.3045394	-3.0582623
Cl	-0.1316717	-2.4098001	-0.4275828
Cl	2.3232712	-0.5076296	-1.8011280
Cl	0.8035371	2.2478337	-0.5130603
N	-0.8734699	0.2076549	1.9863048
N	-1.2179361	0.2482699	0.6632834
C	-2.5209542	0.4966572	0.6185407
H	-3.0027763	0.5697690	-0.3521780
C	-3.0345858	0.6204587	1.9354814
H	-4.0614571	0.8215401	2.2182880
C	-1.9652419	0.4320134	2.7826175
H	-1.8562722	0.4314603	3.8605971
N	0.7912010	-0.0775097	3.6052710
C	0.4549419	-0.0438305	2.3228061
N	1.2735188	-0.2293794	1.2661748
C	2.5669050	-0.4718633	1.5236090
H	3.1951411	-0.6139477	0.6422085
C	3.0233757	-0.5271047	2.8385047
H	4.0712229	-0.7228353	3.0578901
C	2.0873543	-0.3222255	3.8538190
H	2.3762106	-0.3524107	4.9069751
Rh	0.3442933	-0.0855101	-0.6026807

2a.

S	-0.7822640	0.1045991	-2.5358298
O	-2.2416917	0.3923425	-2.4590036
C	-0.5430955	-1.3579066	-3.5632658
H	-1.0108024	-2.1929161	-3.0296137
H	0.5394968	-1.5211381	-3.6516395
H	-1.0251029	-1.1632984	-4.5309137
C	-0.0158224	1.3347609	-3.6088419
H	-0.5426094	1.3046803	-4.5719913
H	1.0478018	1.0746268	-3.6966699
H	-0.1299208	2.3012899	-3.1051331
Cl	-0.1845399	-2.3738203	-0.4232479

Cl	2.3462868	-0.5001272	-1.7929662
Cl	0.7217099	2.2441579	-0.5043918
N	-0.8644499	0.2061892	2.0042243
N	-1.2064593	0.2448982	0.6792966
C	-2.5116962	0.4959255	0.6319246
H	-2.9860794	0.5675274	-0.3436163
C	-3.0262483	0.6223741	1.9450438
H	-4.0526049	0.8256404	2.2283108
C	-1.9556101	0.4331435	2.7954304
H	-1.8505846	0.4347362	3.8739872
N	0.7949701	-0.0808761	3.6245074
C	0.4668005	-0.0457181	2.3408886
N	1.2853904	-0.2290002	1.2785300
C	2.5790178	-0.4734463	1.5542541
H	3.2183408	-0.6161394	0.6814793
C	3.0283108	-0.5312570	2.8703874
H	4.0751592	-0.7289289	3.0937062
C	2.0890324	-0.3269071	3.8834642
H	2.3715418	-0.3586937	4.9381026
Ru	0.3657226	-0.0867185	-0.6064130

3a.

S	-0.7979732	0.1084955	-2.5259875
O	-2.2529355	0.3960784	-2.4482853
C	-0.5477723	-1.3622144	-3.5317356
H	-1.0180298	-2.1890818	-2.9874214
H	0.5368416	-1.5232411	-3.5988732
H	-1.0201356	-1.1757958	-4.5052674
C	-0.0161899	1.3445955	-3.5741219
H	-0.5286415	1.3190839	-4.5446901
H	1.0489866	1.0832184	-3.6381848
H	-0.1376021	2.3043767	-3.0590021
Cl	-0.1079667	-2.4270027	-0.4295976
Cl	2.3409194	-0.5108826	-1.8035300
Cl	0.8333052	2.2547005	-0.5170428
N	-0.8720868	0.2079497	1.9941544
N	-1.2104910	0.2467072	0.6642299
C	-2.5171151	0.4958706	0.6140502
H	-2.9894264	0.5668566	-0.3615521
C	-3.0334837	0.6204647	1.9286709
H	-4.0616613	0.8217489	2.2063626
C	-1.9699104	0.4332969	2.7826880
H	-1.8679290	0.4341386	3.8612036
N	0.7923218	-0.0778383	3.6126886
C	0.4533038	-0.0435760	2.3321767
N	1.2726694	-0.2297814	1.2702488
C	2.5691819	-0.4726705	1.5304538
H	3.1953390	-0.6141372	0.6478244

C	3.0236716	-0.5274135	2.8442407
H	4.0716620	-0.7230289	3.0628088
C	2.0883757	-0.3226402	3.8608287
H	2.3778957	-0.3530524	4.9136547
Ir	0.3448764	-0.0852254	-0.6009932

1b.

S	-0.8077742	0.0740377	-2.3967506
O	-2.2461714	0.3730161	-2.1510186
C	-0.6925046	-1.3899344	-3.4320758
H	-1.1131663	-2.2162673	-2.8479307
H	0.3750595	-1.5650274	-3.6226476
H	-1.2671979	-1.1835270	-4.3452347
C	-0.1466844	1.3129128	-3.5183192
H	-0.7669743	1.2881736	-4.4243306
H	0.9034248	1.0504344	-3.7050334
H	-0.2086218	2.2718879	-2.9913701
Cl	0.0378438	-2.4566557	-0.4072215
Cl	2.3507188	-0.5654093	-2.0636477
Cl	1.0008233	2.1944040	-0.5700938
N	1.0971031	-0.1351823	2.2177490
C	3.0190535	-0.5621309	1.3335721
H	3.7182367	-0.7395222	0.5220813
C	3.1975500	-0.5312015	2.7413664
H	4.1202095	-0.6905825	3.2875081
C	1.9567625	-0.2571719	3.2770583
H	1.5906295	-0.1363032	4.2894971
N	-0.9092454	0.3127909	3.3180286
C	-0.2692904	0.1367679	2.1724865
C	-2.1174958	0.4429734	0.8420486
H	-2.5219195	0.4789559	-0.1733403
C	-2.8776202	0.6408556	1.9924938
H	-3.9441790	0.8453824	1.9211667
C	-2.2235725	0.5672624	3.2214888
H	-2.7562380	0.7140901	4.1637400
N	1.7494953	-0.3222331	1.0393128
N	-0.7994994	0.1897007	0.9242875
Rh	0.5512448	-0.1424972	-0.6148710

2b.

S	-0.7951405	0.0680080	-2.4078818
O	-2.2402509	0.3630284	-2.1668741
C	-0.6926872	-1.3826333	-3.4732383
H	-1.1030363	-2.2208486	-2.8987685
H	0.3708889	-1.5530897	-3.6892345
H	-1.2814411	-1.1716875	-4.3761166
C	-0.1582705	1.3057928	-3.5538673
H	-0.7948858	1.2851836	-4.4483826

H	0.8864694	1.0435225	-3.7691102
H	-0.2083308	2.2682374	-3.0321780
Cl	-0.0330828	-2.4140476	-0.3842580
Cl	2.3768404	-0.5644028	-2.0610557
Cl	0.8999891	2.1846105	-0.5357569
N	1.1066140	-0.1363485	2.2341219
C	3.0326933	-0.5678321	1.3648667
H	3.7416949	-0.7486784	0.5627383
C	3.2028928	-0.5343557	2.7736219
H	4.1216387	-0.6940686	3.3264347
C	1.9598878	-0.2574684	3.3005603
H	1.5875093	-0.1338792	4.3102978
N	-0.8987765	0.3168599	3.3350401
C	-0.2580076	0.1352689	2.1882597
C	-2.1082624	0.4396853	0.8552688
H	-2.5066647	0.4724608	-0.1639746
C	-2.8678851	0.6432665	2.0042592
H	-3.9340741	0.8504267	1.9347354
C	-2.2119171	0.5723798	3.2339485
H	-2.7456778	0.7240504	4.1750985
N	1.7650595	-0.3268563	1.0527676
N	-0.7900733	0.1835960	0.9415163
Ru	0.5762863	-0.1501807	-0.6328389

3b.

S	-0.8183001	0.0751840	-2.3894202
O	-2.2595569	0.3717540	-2.1547677
C	-0.7018955	-1.3870793	-3.4302182
H	-1.1143659	-2.2157793	-2.8434915
H	0.3658200	-1.5569880	-3.6255664
H	-1.2823694	-1.1842575	-4.3398597
C	-0.1606510	1.3146455	-3.5152792
H	-0.7851891	1.2951254	-4.4178550
H	0.8881135	1.0498016	-3.7071609
H	-0.2160670	2.2721610	-2.9848512
Cl	0.0743487	-2.4775086	-0.4115482
Cl	2.3631369	-0.5677358	-2.0734214
Cl	1.0426449	2.1987130	-0.5779004
N	1.0978498	-0.1351020	2.2274047
C	3.0241305	-0.5631378	1.3432127
H	3.7208633	-0.7398593	0.5297413
C	3.1991415	-0.5323407	2.7492695
H	4.1209856	-0.6919753	3.2965280
C	1.9573776	-0.2581663	3.2847482
H	1.5913483	-0.1378317	4.2972319
N	-0.9144326	0.3135706	3.3143707
C	-0.2689842	0.1367528	2.1756535
C	-2.1141302	0.4434809	0.8333981

H	-2.5133693	0.4793932	-0.1836813
C	-2.8743855	0.6417272	1.9809008
H	-3.9403901	0.8471386	1.9028517
C	-2.2289499	0.5689044	3.2149290
H	-2.7652952	0.7161727	4.1545828
N	1.7516335	-0.3222562	1.0481088
N	-0.7896268	0.1875813	0.9157797
Ir	0.5505646	-0.1420883	-0.6136901

1a-intermediate.

Rh	-0.9698649	0.1217686	-0.4808475
S	-1.6688382	0.6210784	-2.4407969
O	-2.4657898	1.8278007	-2.6580935
C	-2.5767492	-0.7342029	-3.1564381
H	-3.5151406	-0.7956375	-2.6121995
H	-2.0048954	-1.6521791	-3.0344050
H	-2.7376640	-0.4657597	-4.2021093
C	-0.3069035	0.6813297	-3.5869810
H	-0.7550974	0.7626228	-4.5788580
H	0.3008955	-0.2133810	-3.4657906
H	0.2663481	1.5687087	-3.3327179
Cl	-2.8504820	-1.2143504	-0.0968608
Cl	0.0496081	-1.7774206	-1.4143502
Cl	0.8725186	1.4637362	-0.8053313
N	2.0512908	-0.0873565	1.5124785
C	4.0502799	0.2772909	0.9398235
H	4.9931820	0.8021757	0.9002704
C	3.6552240	-0.8909867	0.2648422
H	4.2252644	-1.4978380	-0.4194343
C	2.3513114	-1.1026214	0.6581705
H	1.6158987	-1.8392784	0.3845749
N	1.0338641	0.4186447	3.5050287
C	0.8586159	0.0787792	2.2312570
C	-1.3966044	-0.1425380	2.4282578
H	-2.3394360	-0.3690715	1.9519872
C	-1.3046090	0.1560604	3.7752923
H	-2.1913603	0.1664783	4.3948632
C	-0.0551602	0.4890252	4.2667970
H	0.0978493	0.7981720	5.2967453
N	3.0737823	0.7653004	1.7172941
N	-0.3172570	-0.1551196	1.6192765
Cl	-2.0400810	1.9387696	0.4382551

2a-intermediate.

S	-1.7523876	0.6496144	-2.5318997
O	-2.5674405	1.8647384	-2.7699352
C	-2.6686676	-0.7452561	-3.2423133
H	-3.5900162	-0.8357983	-2.6572087

H	-2.0539924	-1.6476735	-3.1290205
H	-2.8681115	-0.4864256	-4.2920518
C	-0.3912397	0.6874095	-3.7314380
H	-0.8532425	0.7889414	-4.7234389
H	0.1860050	-0.2394743	-3.6180717
H	0.2224260	1.5556264	-3.4685498
Cl	-2.8678939	-1.2967579	-0.0758047
Cl	0.0647440	-1.8239060	-1.4843592
Cl	0.9265807	1.4757208	-0.8747118
N	2.1252420	-0.0692474	1.6135750
C	4.1853241	0.1698100	1.1592911
H	5.1849890	0.5963059	1.2138577
C	3.7094341	-0.8693512	0.3159824
H	4.2516280	-1.4380303	-0.4321438
C	2.3758333	-0.9923585	0.6330662
H	1.5818700	-1.6097359	0.2226915
N	1.0502881	0.5268982	3.5669062
C	0.9164698	0.1143389	2.3025846
C	-1.3386985	-0.1993439	2.4827854
H	-2.2697805	-0.4851982	1.9937620
C	-1.2844880	0.1382246	3.8303374
H	-2.1844273	0.1179403	4.4433949
C	-0.0545442	0.5696575	4.3141185
H	0.0658122	0.9480169	5.3347221
N	3.2372466	0.6526184	1.9565759
N	-0.2509261	-0.1808514	1.6733275
Cl	-2.1128221	1.9307409	0.4924187
Ru	-0.9752143	0.1328060	-0.5184498

3a-intermediate.

S	-1.6746536	0.6232935	-2.4481723
O	-2.4792663	1.8223888	-2.6931269
C	-2.5739589	-0.7437123	-3.1575595
H	-3.5114371	-0.8101163	-2.6111065
H	-1.9964569	-1.6582668	-3.0307490
H	-2.7434654	-0.4898120	-4.2051697
C	-0.3109983	0.6727758	-3.5951290
H	-0.7471320	0.7625540	-4.5912920
H	0.2883051	-0.2286034	-3.4744049
H	0.2738117	1.5518458	-3.3354851
Cl	-2.8435411	-1.2098436	-0.0600939
Cl	0.0585912	-1.7726616	-1.3620981
Cl	0.8991255	1.4927957	-0.7934982
N	2.0382274	-0.0942355	1.4887077
C	4.0359512	0.3005957	0.9303573
H	4.9674403	0.8451942	0.8889318
C	3.6725986	-0.8885118	0.2747106
H	4.2626682	-1.4968312	-0.3910351

C	2.3698966	-1.1213252	0.6605357
H	1.6550994	-1.8819683	0.3994471
N	1.0350677	0.3447848	3.4973241
C	0.8469201	0.0624206	2.2120069
C	-1.4186269	-0.0859109	2.4210796
H	-2.3726485	-0.2642611	1.9484001
C	-1.3064934	0.1601098	3.7760625
H	-2.1901408	0.1803521	4.3997782
C	-0.0434606	0.4253874	4.2719986
H	0.1287823	0.6863617	5.3120386
N	3.0419942	0.7818147	1.6892133
N	-0.3442721	-0.1104492	1.5995480
Cl	-2.0454197	1.9915776	0.4517019
Ir	-0.9725074	0.1522570	-0.4729215

1b-intermediate.

Rh	0.0515510	0.0292898	-1.0199647
S	-1.3370113	0.5593179	-2.5813927
O	-2.4876331	1.4269767	-2.3133593
C	-1.9660435	-0.8957843	-3.3943651
H	-2.6267469	-1.3820756	-2.6819415
H	-1.1335292	-1.5513873	-3.6436680
H	-2.5086338	-0.5395546	-4.2719539
C	-0.4529610	1.2705665	-3.9539587
H	-1.1753965	1.3638087	-4.7668576
H	0.3886848	0.6260572	-4.2028694
H	-0.0968354	2.2412398	-3.6189182
Cl	-1.2642009	-1.8071262	-0.4914454
Cl	1.2317302	-1.2820967	-2.5597665
Cl	1.3843561	1.8754289	-1.4914643
N	1.5497494	-0.1410989	1.7339717
C	2.8338650	-0.4750042	0.0562663
H	3.0649138	-0.6265845	-0.9841859
C	3.6658758	-0.2752945	1.1606531
H	4.7431348	-0.2770813	1.1789021
C	2.8148615	-0.0548638	2.2249981
H	2.9701894	0.1299864	3.2750399
N	0.2796476	0.8505225	3.4062887
C	0.3794897	-0.1496060	2.5352906
C	-1.5667419	-1.1329181	3.0367449
H	-2.2543885	-1.9570739	2.8766396
C	-1.8672397	-0.0734060	3.8828182
H	-2.8163307	-0.0113140	4.3995064
C	-0.8677322	0.8712021	4.0885251
H	-0.9866850	1.6780934	4.8050838
N	1.5383107	-0.4021342	0.4183103
N	-0.4067718	-1.2018833	2.3822908
Cl	-1.0814783	1.3137977	0.5147817

2b-intermediate.

S	-1.3808720	0.6027745	-2.6876915
O	-2.5301400	1.5180952	-2.4706051
C	-2.0339149	-0.8858432	-3.4962372
H	-2.6941454	-1.3672648	-2.7667990
H	-1.1826506	-1.5402231	-3.7267967
H	-2.5753300	-0.5473194	-4.3913013
C	-0.4513135	1.2438071	-4.1075320
H	-1.1665999	1.3430834	-4.9363131
H	0.3602511	0.5348144	-4.3197559
H	-0.0387548	2.2089656	-3.7946250
Cl	-1.3034812	-1.8443912	-0.5104306
Cl	1.2679921	-1.3432933	-2.6078384
Cl	1.4695264	1.8769410	-1.5849967
N	1.5481809	-0.1302278	1.7928678
C	2.8468544	-0.4625667	0.1122411
H	3.0904381	-0.6266383	-0.9318446
C	3.6802695	-0.2080030	1.2202610
H	4.7640496	-0.1778323	1.2396289
C	2.8172115	0.0126947	2.2742670
H	2.9676576	0.2303739	3.3253755
N	0.3344685	0.7732273	3.5645424
C	0.3851250	-0.1606853	2.6026890
C	-1.5950618	-1.1148341	3.0811529
H	-2.3198014	-1.9079950	2.8764073
C	-1.8470270	-0.1119147	4.0203529
H	-2.7892580	-0.0565033	4.5654195
C	-0.8001910	0.7792186	4.2716419
H	-0.8734562	1.5312878	5.0634576
N	1.5536997	-0.4222813	0.4562718
N	-0.4510376	-1.1766400	2.3957841
Cl	-1.0834667	1.3914464	0.5228015
Ru	0.0307774	0.0377269	-1.0523948

3b-intermediate.

S	-1.3381608	0.5647460	-2.5867599
O	-2.4884274	1.4400794	-2.3332213
C	-1.9789928	-0.8911015	-3.3949013
H	-2.6372905	-1.3742869	-2.6773196
H	-1.1508663	-1.5524544	-3.6465892
H	-2.5274210	-0.5434066	-4.2719134
C	-0.4569110	1.2605585	-3.9716280
H	-1.1767263	1.3598440	-4.7857427
H	0.3791411	0.6083667	-4.2220521
H	-0.0890699	2.2299164	-3.6436255
Cl	-1.2413710	-1.8296903	-0.4796981

Cl	1.2565339	-1.2916106	-2.5464467
Cl	1.4130812	1.8862534	-1.4941826
N	1.5437158	-0.1306930	1.7302743
C	2.8398927	-0.4565851	0.0549047
H	3.0770144	-0.5959645	-0.9858959
C	3.6635172	-0.2790016	1.1676357
H	4.7404534	-0.2909366	1.1933406
C	2.8068738	-0.0636094	2.2281392
H	2.9567685	0.1066554	3.2813737
N	0.2785912	0.8493595	3.4129713
C	0.3730549	-0.1434896	2.5330981
C	-1.5687287	-1.1327510	3.0367418
H	-2.2560026	-1.9566293	2.8738658
C	-1.8657517	-0.0795945	3.8916781
H	-2.8123546	-0.0218231	4.4133911
C	-0.8653275	0.8637224	4.1008444
H	-0.9810592	1.6641967	4.8250325
N	1.5404778	-0.3764855	0.4091829
N	-0.4109862	-1.1962313	2.3772395
Cl	-1.0756651	1.3328959	0.5373133
Ir	0.0519965	0.0397506	-1.0270507

I1b-intermediate.

S	-1.82703300	0.65551220	-2.49282710
O	-2.97523070	1.55192070	-2.74643460
C	-2.14738780	-0.91193460	-3.33066050
H	-3.02321780	-1.34473500	-2.83488510
H	-1.26731530	-1.55078100	-3.17583880
H	-2.33601160	-0.66996510	-4.38623950
C	-0.43459210	1.23463380	-3.48643640
H	-0.78758680	1.27370620	-4.52676270
H	0.39297290	0.52996660	-3.32887900
H	-0.17388990	2.22396310	-3.09418530
Cl	-2.55227200	-1.65573380	-0.19296870
Cl	0.58252830	-1.19187770	-1.36608270
Cl	0.32117700	2.14819850	-0.45706860
N	1.91931670	-0.36130750	1.36430140
C	3.26201361	-1.78760187	0.54303671
H	3.61331338	-2.76085470	0.20802800
C	3.90931942	-0.53327791	0.45676164
H	4.87767933	-0.30123107	0.02552177
C	3.01490485	0.36463726	1.00991669
H	3.02195965	1.44162416	1.12062831
N	1.06336250	0.31353030	3.40995950
C	0.78922880	0.00239300	2.14572210
C	-1.47171580	-0.14866210	2.50239690
H	-2.45093050	-0.35672970	2.07806120
C	-1.26529720	0.08164410	3.85981570

H	-2.10129670	0.05642080	4.55749150
C	0.02734560	0.39975360	4.25691450
H	0.26114440	0.70254390	5.28202680
N	2.05767040	-1.69414156	1.10954966
N	-0.44769800	-0.11890560	1.61510570
Cl	-2.76929550	1.64347120	0.52613120
Rh	-1.09296310	0.21870040	-0.41255080

I2b-intermediate.

S	-1.82677280	0.65610490	-2.49942440
O	-2.96836560	1.56274070	-2.77495980
C	-2.16146330	-0.90568520	-3.35613790
H	-3.03430630	-1.34280040	-2.85863020
H	-1.28407610	-1.55306000	-3.22480120
H	-2.36209650	-0.65658380	-4.40775570
C	-0.43869980	1.21481350	-3.52224230
H	-0.80533160	1.26608070	-4.55725320
H	0.38296560	0.49877270	-3.38888370
H	-0.15330490	2.19939240	-3.13497950
Cl	-2.56877690	-1.64402370	-0.18469980
Cl	0.57230210	-1.19391940	-1.34423840
Cl	0.33590830	2.12097450	-0.46394620
N	1.91820120	-0.35688290	1.37608160
C	3.25454956	-1.77143226	0.52306930
H	3.59887928	-2.73736266	0.16082951
C	3.91593935	-0.52199798	0.48125094
H	4.89203338	-0.28749027	0.06906358
C	3.02567890	0.36661786	1.05650109
H	3.04979407	1.43752365	1.21294517
N	1.06848990	0.31740400	3.42313500
C	0.78798580	0.00335660	2.16194370
C	-1.46644830	-0.15747080	2.52736180
H	-2.44740720	-0.37543350	2.11374700
C	-1.25653270	0.08017500	3.88139330
H	-2.08998370	0.04951680	4.58224710
C	0.03673820	0.40436830	4.27592260
H	0.27354940	0.70946630	5.29942720
N	2.04539507	-1.68169936	1.08029739
N	-0.44986070	-0.12114160	1.62632770
Cl	-2.75705330	1.63952910	0.52803960
Ru	-1.09612300	0.21159430	-0.41278860

I3b-intermediate.

S	-1.81969070	0.65798540	-2.48655810
O	-2.96743920	1.55660310	-2.73786190
C	-2.14356100	-0.90489200	-3.33657350
H	-3.01373250	-1.34268600	-2.83502280
H	-1.26100530	-1.54310170	-3.19194900

H	-2.34160810	-0.65845780	-4.38882330
C	-0.43168920	1.23921080	-3.48945070
H	-0.78919580	1.28870420	-4.52721070
H	0.39440050	0.53027790	-3.34168800
H	-0.16428400	2.22391040	-3.08998260
Cl	-2.52639390	-1.68945760	-0.18816890
Cl	0.60422300	-1.19748900	-1.36672350
Cl	0.32771550	2.15119600	-0.44261260
N	1.91135350	-0.35019650	1.35927020
C	3.23824911	-1.79296370	0.54081146
H	3.57867733	-2.77046517	0.20691278
C	3.89960729	-0.54607708	0.45277758
H	4.87053756	-0.32563943	0.02125183
C	3.01530152	0.36248726	1.00432445
H	3.03420487	1.43927182	1.11382149
N	1.05758130	0.34892300	3.39823060
C	0.78573560	0.02402870	2.14012550
C	-1.47456040	-0.16636450	2.51006000
H	-2.45229510	-0.40472620	2.09897080
C	-1.26207430	0.07697460	3.86273370
H	-2.09303260	0.03556160	4.56565390
C	0.02496630	0.42845260	4.25072460
H	0.25806290	0.74788330	5.27060070
N	2.03468711	-1.68519913	1.10595431
N	-0.45663770	-0.11238830	1.60999440
Cl	-2.77256760	1.61982910	0.55415480
Ir	-1.08647910	0.21053510	-0.41117890

N-Pyrazolyl Pyrimidine.

N	-0.9376456	0.1760041	-0.3559729
N	-1.3300057	0.2639733	-1.6416705
C	-2.6440921	0.5045327	-1.5622619
H	-3.2081739	0.6198702	-2.4752467
C	-3.0909377	0.5698695	-0.2284239
H	-4.0900428	0.7485421	0.1339120
C	-1.9636793	0.3535059	0.5323352
H	-1.7898559	0.3085541	1.5934638
N	0.6596218	-0.1314442	1.2862898
C	0.4085613	-0.0752408	-0.0215137
N	1.2643432	-0.2257154	-1.0254830
C	2.5290459	-0.4614549	-0.6646971
H	3.2387713	-0.5865933	-1.4763424
C	2.9240912	-0.5441660	0.6640930
H	3.9517807	-0.7354343	0.9420285
C	1.9310407	-0.3684819	1.6185380
H	2.1471768	-0.4163211	2.6809518

[H(DMSO)₂] [trans-RhCl₄(DMSO)₂]

Rh	0.0001538	0.0000092	-0.0000501
S	-1.0811443	0.1692080	-1.9635907
O	-2.1518583	1.1567372	-2.1568487
C	-1.7259549	-1.4215670	-2.4360315
H	-2.5373114	-1.6402080	-1.7461816
H	-0.9351225	-2.1633547	-2.3337160
H	-2.0874716	-1.3185504	-3.4607368
C	0.0943107	0.3863641	-3.2829814
H	-0.4645661	0.2922481	-4.2157873
H	0.8797542	-0.3606615	-3.1773980
H	0.5073685	1.3849372	-3.1637070
Cl	-1.5635930	-1.5561694	0.7279052
Cl	1.2663359	-1.7071592	-0.9289791
Cl	1.5639544	1.5562343	-0.7280385
Cl	-1.2661431	1.7072163	0.9288983
S	1.0813672	-0.1691358	1.9636049
O	2.1522681	-1.1564371	2.1569904
C	1.7256968	1.4217640	2.4362494
H	2.0885581	1.3182635	3.4604292
H	2.5359830	1.6415175	1.7454962
H	0.9341953	2.1630439	2.3354218
C	-0.0942630	-0.3866528	3.2827932
H	-0.5058823	-1.3859102	3.1642596
H	0.4640538	-0.2909344	4.2157718
H	-0.8806893	0.3591974	3.1762267

[H (DMSO)₂] [trans-RuCl₄ (DMSO)₂]

S	-1.1256003	0.1892201	-2.0250002
O	-2.2077555	1.1830507	-2.2402278
C	-1.7593325	-1.4377327	-2.5056058
H	-2.5538467	-1.6811105	-1.7914360
H	-0.9312970	-2.1534459	-2.4092848
H	-2.1357371	-1.3459507	-3.5344449
C	0.0791877	0.3846385	-3.3625699
H	-0.4737161	0.2940104	-4.3084881
H	0.8440731	-0.3928071	-3.2312016
H	0.5230252	1.3781483	-3.2342579
Cl	-1.6081909	-1.6029222	0.7556454
Cl	1.2964663	-1.7545036	-0.9661506
Cl	1.6085212	1.6030621	-0.7558656
Cl	-1.2966441	1.7541819	0.9662099
S	1.1264278	-0.1885182	2.0246834
O	2.2104101	-1.1804960	2.2391425
C	1.7574333	1.4392522	2.5062199

H	2.1345071	1.3473393	3.5348023
H	2.5511668	1.6845946	1.7918489
H	0.9280632	2.1535403	2.4108657
C	-0.0779334	-0.3866971	3.3622483
H	-0.5197514	-1.3810859	3.2337736
H	0.4747506	-0.2950663	4.3082018
H	-0.8444251	0.3892031	3.2309793
Ru	0.0001979	0.0000947	-0.0000879

[H(DMSO)₂] [trans-IrCl₄(DMSO)₂]

S	-1.1237819	0.1910167	-2.0168158
O	-2.2012796	1.1869825	-2.2146583
C	-1.7544689	-1.4371928	-2.4808554
H	-2.5487177	-1.6716489	-1.7636112
H	-0.9226496	-2.1468049	-2.3681946
H	-2.1255671	-1.3539784	-3.5119123
C	0.0886199	0.3928221	-3.3406798
H	-0.4573664	0.2943612	-4.2893742
H	0.8569776	-0.3787708	-3.1925277
H	0.5235706	1.3893448	-3.2065072
Cl	-1.6190179	-1.6133489	0.7615360
Cl	1.3032770	-1.7680149	-0.9817707
Cl	1.6188060	1.6134243	-0.7617887
Cl	-1.3035794	1.7682041	0.9815024
S	1.1237255	-0.1909416	2.0167710
O	2.2013019	-1.1868355	2.2144367
C	1.7544505	1.4372370	2.4808856
H	2.1259487	1.3538487	3.5117838
H	2.5483945	1.6719316	1.7633804
H	0.9225142	2.1467852	2.3686845
C	-0.0884707	-0.3929728	3.3408115
H	-0.5230460	-1.3896876	3.2068658
H	0.4575682	-0.2941390	4.2894398
H	-0.8571298	0.3783083	3.1926073
Ir	-0.0000793	0.0000696	-0.0000089