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Supporting Information

Synthesis, Structure and Reactivity of Trigonal Bipyramidal Ruthenium(IV) Trialkyl Complexes

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Table S1. Crystallographic Data for Complexes 1, 2, 4·¼(C_6H_{14})·¼Et_2O, and 5

	1	**2**	**4**·¼(C_6H_{14})·¼($C_4H_{10}O$)	**5**
formula	$C_{30}H_{48}ClPRuSi_3$	$C_{35}H_{58}F_3O_4PRuSSi_3$	$C_{64.5}H_{96}N_2O_{0.25}P_2Ru_2S_2Si_6$	$C_{30}H_{33}F_4OPRuSi$
fw	660.44	848.18	1400.17	645.69
a, Å	11.642(3)	11.72890(10)	20.1717(8)	8.1040(8)
b, Å	16.426(4)	18.1582(3)	19.8722(7)	10.5219(10)
c, Å	20.173(4)	20.2285(3)	20.4513(7)	17.9803(17)
α, deg	111.577(3)			77.7230(10)
β, deg	91.174(3)	93.0830(10)	96.252(4)	79.3130(10)
γ, deg	100.128(3)			85.6750(10)
V, $Å^3$	3516.0(13)	4301.94(10)	8149.3(5)	1471.1(2)
Z	4	4	4	2
cryst system	triclinic	monoclinic	monoclinic	triclinic
space group	*P*-1	$P2_1/c$	$P2_1/c$	*P*-1
ρ_{calcd}, $g\cdot cm^{-3}$	1.248	1.310	1.141	1.458
T, K	298	173	173	298
μ, mm^{-1}	0.686	4.942	4.98	0.675
F(000)	1384	1776	2932	660
no. of reflns	19424	14019	26609	10661
no. of indep reflns	13509	744	14314	6072
R_{int}	0.0363	0.0756	0.0811	0.0227
*R*1,*wR*2 ($I > 2\sigma(I)$)	0.0519, 0.0887	0.0696, 0.1879	0.0607, 0.1409	0.0306, 0.0790
*R*1, *wR*2 (all data)	0.1153, 0.0968	0.0771, 0.1969	0.0917, 0.1583	0.0350, 0.0813

GoF	1.050	1.028	1.008	1.007

Table S2. Selected bond length (Å) from optimized geometries (using different functionals) and crystallographic data of **1**.

	Experimental	M06L/SDD/ 6-31+G* (without C_3 symmetry imposed)	M06L/ SDD/ 6-31+G* (with C_3 symmetry imposed)	B3LYP/SDD /6-31+G*
Ru-Cl	2.411	2.452	2.452	2.424
Ru-C	2.026-2.037	2.043- 2.046	2.042-2.044	2.053
Ru-P	2.269	2.270	2.269	2.352

Table S3. The compositions of the molecular orbitals (MOs) which are involved in the lowest-energy transitions in **1**.

Experimental λ_{max}/cm^{-1} (ε_{max}/dm^3 mol^{-1} cm^{-1})	Excitation energy / cm^{-1} (oscillator strength)	Composition of the excited-state wave functions
19801 (980)	20517(0.0217)	$0.64\psi_{H-1\rightarrow L} - 0.29\ \psi_{H\rightarrow L+1}$
21978 (1034)	21474(0.0096)	$0.28\psi_{H-1\rightarrow L} + 0.64\ \psi_{H\rightarrow L+1}$
	21583(0.0055)	$0.56\psi_{H-1\rightarrow L+1} - 0.41\ \psi_{H\rightarrow L}$

Table S4. Cartesian Coordinates of **1** (without C_3 imposed) from M06L Singlet State Optimized Geometries.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.865406	0.086381	0.030841
2	17	0	3.283842	0.448875	0.212265
3	15	0	-1.383482	-0.191417	-0.096859
4	14	0	2.194966	-2.726161	1.391723
5	14	0	1.217267	2.799374	2.041013
6	14	0	2.018909	0.556868	-3.130368
7	6	0	0.890630	-1.334765	1.501971
8	1	0	1.215965	-0.698601	2.344050
9	1	0	-0.078695	-1.782592	1.764914
10	6	0	0.487759	2.049967	0.445197
11	1	0	1.073447	2.493012	-0.380180
12	1	0	-0.557664	2.377307	0.342330
13	6	0	0.998139	-0.510376	-1.917982
14	1	0	1.609123	-1.417481	-1.758926
15	1	0	0.055316	-0.813494	-2.398130
16	6	0	2.805528	-3.167926	-0.331628
17	1	0	1.998240	-3.476435	-1.009854
18	1	0	3.502119	-4.014127	-0.261985
19	1	0	3.348086	-2.333050	-0.792477
20	6	0	1.323176	-4.244103	2.100797
21	1	0	0.997015	-4.074231	3.134799
22	1	0	1.983952	-5.120830	2.106350
23	1	0	0.429309	-4.507232	1.519900
24	6	0	3.662002	-2.295773	2.480686
25	1	0	4.191554	-1.415488	2.099259
26	1	0	4.376287	-3.128300	2.526285
27	1	0	3.347031	-2.078403	3.509488
28	6	0	1.679382	1.584651	3.399534
29	1	0	0.829001	0.975067	3.732657
30	1	0	2.037944	2.141376	4.275715
31	1	0	2.488855	0.914918	3.082600
32	6	0	-0.140133	3.928308	2.704758

33	1	0	-0.425440	4.692487	1.970539
34	1	0	0.175595	4.450705	3.617167
35	1	0	-1.046695	3.357845	2.947831
36	6	0	2.733202	3.806144	1.579936
37	1	0	3.514963	3.155892	1.169615
38	1	0	3.150234	4.327757	2.451088
39	1	0	2.498987	4.565261	0.822637
40	6	0	2.194395	2.382686	-2.709319
41	1	0	1.235014	2.910793	-2.625951
42	1	0	2.759572	2.878875	-3.509912
43	1	0	2.752984	2.528053	-1.776026
44	6	0	3.730342	-0.192452	-3.312583
45	1	0	4.285757	-0.133219	-2.369606
46	1	0	4.312409	0.332889	-4.080982
47	1	0	3.678099	-1.248788	-3.606312
48	6	0	1.104362	0.425596	-4.776790
49	1	0	1.034483	-0.616060	-5.114868
50	1	0	1.615502	0.992294	-5.566004
51	1	0	0.078573	0.810239	-4.705003
52	6	0	-2.003654	-1.916139	0.031211
53	6	0	-1.230505	-2.938875	-0.532757
54	1	0	-0.271970	-2.692418	-0.991971
55	6	0	-1.662143	-4.260947	-0.491597
56	1	0	-1.044200	-5.044569	-0.928683
57	6	0	-2.870758	-4.581059	0.125718
58	1	0	-3.205199	-5.616269	0.168030
59	6	0	-3.643524	-3.572965	0.698607
60	1	0	-4.584375	-3.817749	1.189169
61	6	0	-3.214144	-2.247281	0.651569
62	1	0	-3.822724	-1.465782	1.107285
63	6	0	-2.185724	0.417607	-1.636039
64	6	0	-1.600046	1.494689	-2.311570
65	1	0	-0.656456	1.902750	-1.948815
66	6	0	-2.201669	2.038620	-3.442777
67	1	0	-1.727040	2.873477	-3.957536
68	6	0	-3.396294	1.503751	-3.921587
69	1	0	-3.865774	1.922211	-4.810283
70	6	0	-3.982365	0.423164	-3.264303

71	1	0	-4.910647	-0.005607	-3.638735
72	6	0	-3.382588	-0.116753	-2.127985
73	1	0	-3.849413	-0.962292	-1.622679
74	6	0	-2.339881	0.678512	1.213785
75	6	0	-2.024502	0.404634	2.552726
76	1	0	-1.250647	-0.326784	2.786730
77	6	0	-2.688394	1.055156	3.587566
78	1	0	-2.431160	0.827063	4.621072
79	6	0	-3.668653	2.005760	3.301009
80	1	0	-4.182281	2.522683	4.109868
81	6	0	-3.977793	2.297897	1.975525
82	1	0	-4.734493	3.045549	1.742804
83	6	0	-3.320004	1.637884	0.936731
84	1	0	-3.574366	1.876119	-0.095504

Table S5. Cartesian Coordinates of **1** (without C_3 imposed) from M06L Triplet State Optimized Geometries.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.840339	-0.332451	0.040159
2	17	0	3.013543	-1.284378	0.370397
3	15	0	-1.402478	0.421823	-0.097952
4	14	0	2.813093	0.573146	-2.744173
5	14	0	0.200474	-3.522110	0.557575
6	14	0	2.411351	1.382439	2.546617
7	6	0	1.128465	0.118611	-2.019246
8	1	0	0.854397	-0.882995	-2.406796
9	1	0	0.372471	0.809699	-2.416874
10	6	0	-0.041923	-1.812395	1.334576
11	1	0	0.541166	-1.749545	2.265021
12	1	0	-1.101957	-1.680700	1.596279
13	6	0	1.415700	1.458908	0.922974
14	1	0	2.071586	1.939464	0.180092
15	1	0	0.552152	2.125147	1.073649
16	6	0	3.863843	1.689663	-1.654726
17	1	0	3.381099	2.656450	-1.455054
18	1	0	4.819665	1.907834	-2.149523
19	1	0	4.091251	1.217287	-0.691626
20	6	0	2.464437	1.527319	-4.340604
21	1	0	1.878766	0.931951	-5.052591
22	1	0	3.391209	1.826873	-4.847848
23	1	0	1.892477	2.443439	-4.139046
24	6	0	3.771044	-0.988116	-3.164739
25	1	0	4.003328	-1.570473	-2.265755
26	1	0	4.720208	-0.748920	-3.661908
27	1	0	3.200755	-1.635911	-3.843271
28	6	0	0.655230	-3.463264	-1.275121
29	1	0	-0.083332	-2.904298	-1.866068
30	1	0	0.678019	-4.483234	-1.683245
31	1	0	1.642215	-3.017636	-1.449635

32	6	0	-1.431797	-4.459104	0.673818
33	1	0	-1.811018	-4.503054	1.702672
34	1	0	-1.326720	-5.491760	0.315393
35	1	0	-2.205774	-3.979036	0.060538
36	6	0	1.543486	-4.440694	1.496022
37	1	0	2.491575	-3.891534	1.455443
38	1	0	1.717635	-5.438929	1.073636
39	1	0	1.277267	-4.570271	2.552602
40	6	0	2.145941	-0.124728	3.643256
41	1	0	1.107996	-0.260252	3.974006
42	1	0	2.753481	-0.007971	4.551333
43	1	0	2.469292	-1.047654	3.147203
44	6	0	4.246828	1.558342	2.192662
45	1	0	4.638747	0.681730	1.664702
46	1	0	4.812322	1.666956	3.127657
47	1	0	4.458583	2.442282	1.577519
48	6	0	1.834873	2.898530	3.518545
49	1	0	2.017969	3.828697	2.965673
50	1	0	2.358352	2.981500	4.480147
51	1	0	0.758336	2.858135	3.732331
52	6	0	-1.762866	1.779761	-1.285684
53	6	0	-0.822762	2.803860	-1.465585
54	1	0	0.138455	2.751397	-0.955035
55	6	0	-1.093268	3.873043	-2.313695
56	1	0	-0.347957	4.655568	-2.446550
57	6	0	-2.304397	3.933328	-3.001328
58	1	0	-2.512181	4.766142	-3.670888
59	6	0	-3.242574	2.917641	-2.836326
60	1	0	-4.188058	2.952113	-3.375206
61	6	0	-2.975272	1.847117	-1.984408
62	1	0	-3.715859	1.055838	-1.870221
63	6	0	-2.102756	1.087717	1.462336
64	6	0	-1.414247	0.920701	2.667530
65	1	0	-0.458865	0.398310	2.665125
66	6	0	-1.940155	1.414649	3.859176
67	1	0	-1.386135	1.280765	4.787606
68	6	0	-3.162826	2.081268	3.858254
69	1	0	-3.574712	2.469382	4.788296

70	6	0	-3.856054	2.257401	2.660399
71	1	0	-4.809496	2.783009	2.652386
72	6	0	-3.327785	1.769075	1.469071
73	1	0	-3.872059	1.920378	0.536381
74	6	0	-2.577523	-0.878691	-0.615044
75	6	0	-2.403519	-1.436489	-1.889758
76	1	0	-1.596121	-1.075846	-2.530592
77	6	0	-3.258275	-2.434229	-2.345981
78	1	0	-3.112599	-2.858531	-3.338006
79	6	0	-4.295992	-2.890250	-1.531960
80	1	0	-4.964205	-3.672622	-1.887515
81	6	0	-4.466752	-2.351084	-0.259352
82	1	0	-5.265970	-2.713159	0.385195
83	6	0	-3.609935	-1.351597	0.201300
84	1	0	-3.749573	-0.937471	1.199465

Table S6. Cartesian Coordinates of **1** (without C_3 imposed) from B3LYP Singlet State Optimized Geometries.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.917507	0.000472	-0.000216
2	17	0	3.341719	0.002575	-0.000625
3	15	0	-1.434268	-0.001096	0.000095
4	14	0	1.895293	-0.770994	3.247194
5	14	0	1.890751	3.200021	-0.955212
6	14	0	1.896274	-2.425585	-2.292205
7	6	0	0.862748	0.308047	2.028726
8	1	0	1.349548	1.297972	2.046449
9	1	0	-0.143105	0.411301	2.450514
10	6	0	0.861328	1.603474	-1.281459
11	1	0	1.350014	1.124456	-2.146894
12	1	0	-0.144728	1.915253	-1.583056
13	6	0	0.864198	-1.910598	-0.747942
14	1	0	1.352237	-2.419988	0.100333
15	1	0	-0.141293	-2.328642	-0.868466
16	6	0	2.296286	-2.533250	2.677741
17	1	0	1.397994	-3.114015	2.433680
18	1	0	2.815027	-3.063147	3.488216
19	1	0	2.958669	-2.529950	1.805381
20	6	0	0.826820	-0.897630	4.817606
21	1	0	0.593470	0.095228	5.224245
22	1	0	1.352191	-1.459587	5.601576
23	1	0	-0.125112	-1.406942	4.621438
24	6	0	3.507588	0.115016	3.692556
25	1	0	4.153414	0.222642	2.814992
26	1	0	4.057218	-0.450313	4.457418
27	1	0	3.313991	1.116791	4.098100
28	6	0	2.290233	3.587883	0.856030
29	1	0	1.391502	3.665640	1.480527
30	1	0	2.807862	4.555280	0.910348
31	1	0	2.953215	2.831301	1.289392

32	6	0	0.820223	4.621739	-1.630868
33	1	0	0.588086	4.477598	-2.694311
34	1	0	1.343757	5.582564	-1.535227
35	1	0	-0.132332	4.704484	-1.092504
36	6	0	3.503682	3.145910	-1.944348
37	1	0	4.150830	2.333199	-1.598673
38	1	0	4.051531	4.091933	-1.836606
39	1	0	3.310952	2.996201	-3.014833
40	6	0	2.295242	-1.050970	-3.533964
41	1	0	1.396318	-0.550387	-3.914926
42	1	0	2.814510	-1.487326	-4.398084
43	1	0	2.956654	-0.296250	-3.094995
44	6	0	3.509740	-3.252615	-1.748538
45	1	0	4.155297	-2.545682	-1.217227
46	1	0	4.059082	-3.632032	-2.620875
47	1	0	3.317456	-4.104729	-1.083389
48	6	0	0.828554	-3.723500	-3.186213
49	1	0	0.596698	-4.572305	-2.529440
50	1	0	1.353690	-4.120928	-4.065247
51	1	0	-0.124134	-3.300068	-3.528466
52	6	0	-2.253132	-0.895896	1.410225
53	6	0	-1.763085	-2.158151	1.787677
54	1	0	-0.904934	-2.581414	1.275822
55	6	0	-2.366945	-2.881042	2.818298
56	1	0	-1.973682	-3.856766	3.092381
57	6	0	-3.465778	-2.348778	3.500258
58	1	0	-3.931685	-2.907998	4.307486
59	6	0	-3.955749	-1.091484	3.140827
60	1	0	-4.806490	-0.665407	3.666697
61	6	0	-3.356492	-0.371260	2.101658
62	1	0	-3.755421	0.601798	1.834556
63	6	0	-2.253571	-0.775497	-1.479309
64	6	0	-1.762359	-0.473783	-2.761297
65	1	0	-0.902812	0.179234	-2.872182
66	6	0	-2.366689	-1.005158	-3.902285
67	1	0	-1.972477	-0.756662	-4.884456
68	6	0	-3.467164	-1.859674	-3.781735
69	1	0	-3.933449	-2.279392	-4.669332

70	6	0	-3.958274	-2.174619	-2.512975
71	1	0	-4.810255	-2.841425	-2.406488
72	6	0	-3.358530	-1.634488	-1.370072
73	1	0	-3.758260	-1.887805	-0.393658
74	6	0	-2.254470	1.666863	0.069705
75	6	0	-1.765929	2.625033	0.974771
76	1	0	-0.908215	2.393828	1.598009
77	6	0	-2.370716	3.878612	1.085147
78	1	0	-1.978631	4.603952	1.793641
79	6	0	-3.468942	4.202526	0.282149
80	1	0	-3.935563	5.180899	0.362546
81	6	0	-3.957339	3.262479	-0.627706
82	1	0	-4.807540	3.504458	-1.260514
83	6	0	-3.357178	2.002815	-0.731472
84	1	0	-3.754871	1.284872	-1.441206

Table S7. Cartesian Coordinates of **1** (with C_3 symmetry imposed) from M06L Singlet State Optimized Geometries.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.000000	0.000000	0.000000
2	17	0	0.000000	0.000000	2.451944
3	15	0	0.062101	0.000000	-2.268247
4	6	0	1.863989	-0.832571	-0.058081
5	1	0	1.640012	-1.746196	0.521185
6	1	0	2.232552	-1.133502	-1.050175
7	6	0	-1.637373	-1.217474	-0.098829
8	1	0	-2.361911	-0.538049	0.385800
9	1	0	-2.009239	-1.450416	-1.108132
10	6	0	-0.269497	2.025712	-0.075789
11	1	0	0.670083	2.339489	0.412205
12	1	0	-0.303215	2.476195	-1.078385
13	6	0	1.674140	0.510451	-2.996091
14	6	0	2.203398	1.755210	-2.624483
15	6	0	2.417740	-0.306737	-3.854531
16	6	0	3.432601	2.181314	-3.116886
17	1	0	1.645672	2.397974	-1.942859
18	6	0	3.655719	0.117007	-4.339245
19	1	0	2.033203	-1.282424	-4.149469
20	6	0	4.163802	1.361360	-3.976907
21	1	0	3.825774	3.152294	-2.818560
22	1	0	4.223921	-0.533249	-5.002580
23	1	0	5.130416	1.689706	-4.355230
24	6	0	-0.238821	-1.620007	-3.085678
25	6	0	-0.779821	-1.726482	-4.372423
26	6	0	0.137560	-2.788666	-2.413056
27	6	0	-0.930198	-2.974493	-4.974225
28	1	0	-1.088901	-0.829470	-4.908917
29	6	0	-0.006165	-4.035004	-3.016111
30	1	0	0.538630	-2.716885	-1.401681
31	6	0	-0.540270	-4.130484	-4.300006

32	1	0	-1.356978	-3.042938	-5.973673
33	1	0	0.287763	-4.933409	-2.474192
34	1	0	-0.660423	-5.104562	-4.771231
35	6	0	-1.130644	1.108736	-3.119513
36	6	0	-0.829673	1.781885	-4.309496
37	6	0	-2.403183	1.266820	-2.556216
38	6	0	-1.785293	2.589669	-4.924528
39	1	0	0.159209	1.679185	-4.756921
40	6	0	-3.359050	2.067593	-3.173530
41	1	0	-2.636748	0.766854	-1.615068
42	6	0	-3.051204	2.732192	-4.360145
43	1	0	-1.536545	3.111983	-5.847065
44	1	0	-4.341404	2.184768	-2.717201
45	1	0	-3.794624	3.367000	-4.839319
46	14	0	-1.662069	2.794796	0.981399
47	14	0	3.275063	0.033173	0.891070
48	14	0	-1.662437	-2.799711	0.972294
49	6	0	-2.646938	-2.461376	2.534328
50	1	0	-2.768406	-3.374602	3.131397
51	1	0	-2.144122	-1.714412	3.159219
52	1	0	-3.651726	-2.084931	2.302924
53	6	0	3.555701	-0.888451	2.502209
54	1	0	3.757416	-1.953254	2.328625
55	1	0	4.409285	-0.477692	3.056829
56	1	0	2.669877	-0.816933	3.144512
57	6	0	-0.938139	3.463368	2.578752
58	1	0	-1.693897	4.016156	3.152026
59	1	0	-0.560159	2.651952	3.210596
60	1	0	-0.106078	4.152369	2.384400
61	6	0	0.007087	-3.525348	1.448587
62	1	0	0.574531	-2.838161	2.088805
63	1	0	-0.156453	-4.447991	2.021724
64	1	0	0.633038	-3.795080	0.587337
65	6	0	-3.128244	1.685921	1.380277
66	1	0	-2.835358	0.840408	2.015005
67	1	0	-3.877895	2.267001	1.933986
68	1	0	-3.629422	1.292687	0.485376
69	6	0	3.032506	1.859678	1.265062

70	1	0	2.183749	2.022754	1.941164
71	1	0	3.929706	2.249064	1.764616
72	1	0	2.881741	2.462907	0.359987
73	6	0	-2.575594	-4.078721	-0.073994
74	1	0	-2.667332	-5.037066	0.453674
75	1	0	-3.590538	-3.743386	-0.322266
76	1	0	-2.059253	-4.271955	-1.023398
77	6	0	4.782894	-0.136080	-0.229420
78	1	0	5.680386	0.298751	0.229407
79	1	0	5.004851	-1.187180	-0.453786
80	1	0	4.622904	0.373418	-1.189096
81	6	0	-2.298151	4.236458	-0.059720
82	1	0	-3.105813	4.776285	0.451745
83	1	0	-1.502249	4.962157	-0.270136
84	1	0	-2.688698	3.896625	-1.028066

Experimental for ESI Mass Spectrometry

All the mass spectrometric experiments were performed using a hybrid quadrupole-time-of-flight (Q-TOF) tandem mass spectrometer (QTOF Premier, Waters Micromass, Manchester, UK) equipped with an electrospray ionization (ESI) source (Z-spray). Instrumental control and data acquisition were conducted via the MassLynx 4.1 system software. TOF mass spectra were acquired in the *m/z* range of 100–2000. The mass scale of the instrument was externally calibrated using sodium formate cluster ions covering the m/z range of 20–1500. The mass accuracy of the m/z data was checked before the sample analysis, and was within 10 ppm.

Sample Preparation

All manipulations were carried out under nitrogen by standard Schlenk techniques. Dry THF was distilled over Na-benzophenone ketyl under argon. To a 2 mL LC vial containing 11.57 mg of complex **2** and 64.05 mg of $NaOC_6F_4H$, 1200 μL dry THF was added. The reaction was stirred at room temperature. 50 μL reaction mixture was diluted to 10^{-4} M for MS analysis. The reaction mixture was monitored over 26 hr.

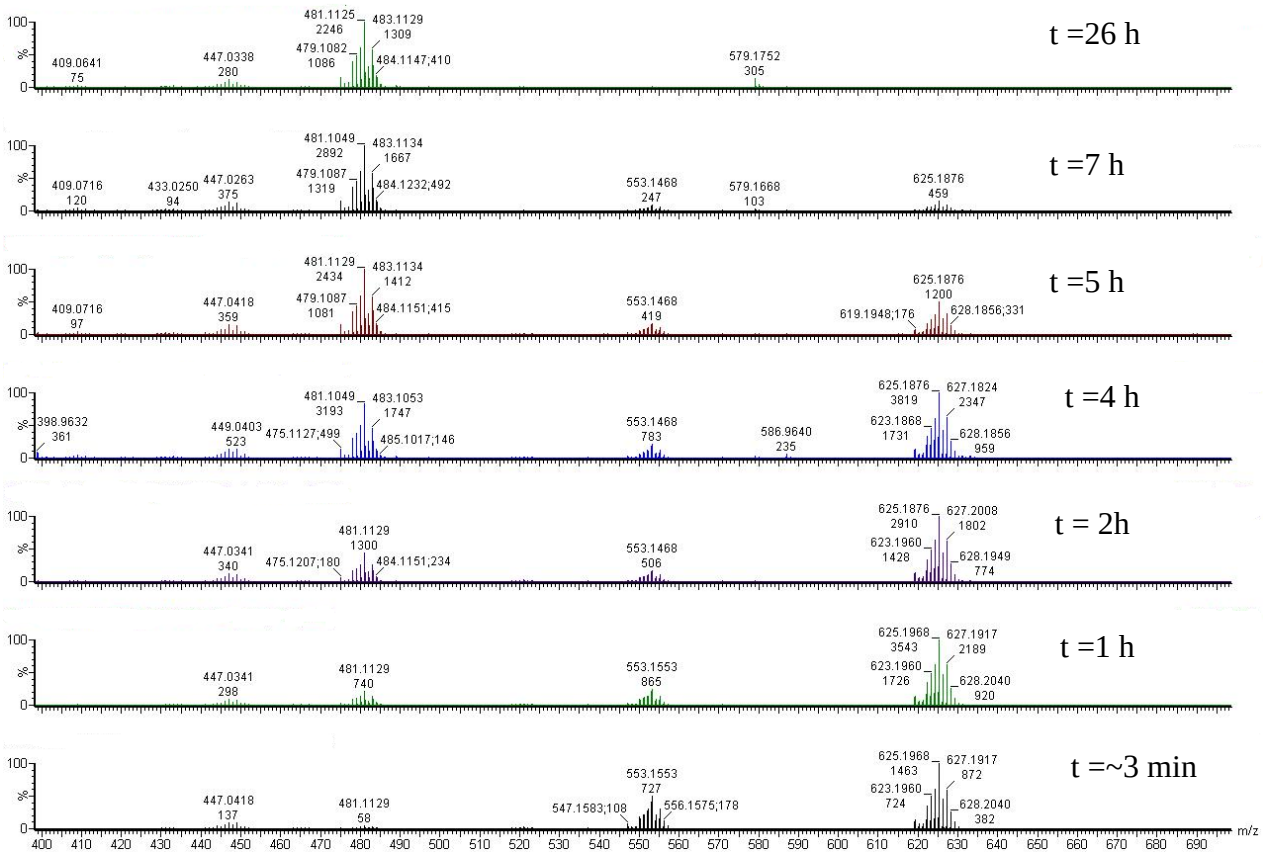

Figure S1. High-resolution ESI mass spectra of the reaction mixture of complex **2** and excess (20 folds) $NaOC_6F_4H$ in THF at room temperature at different time.

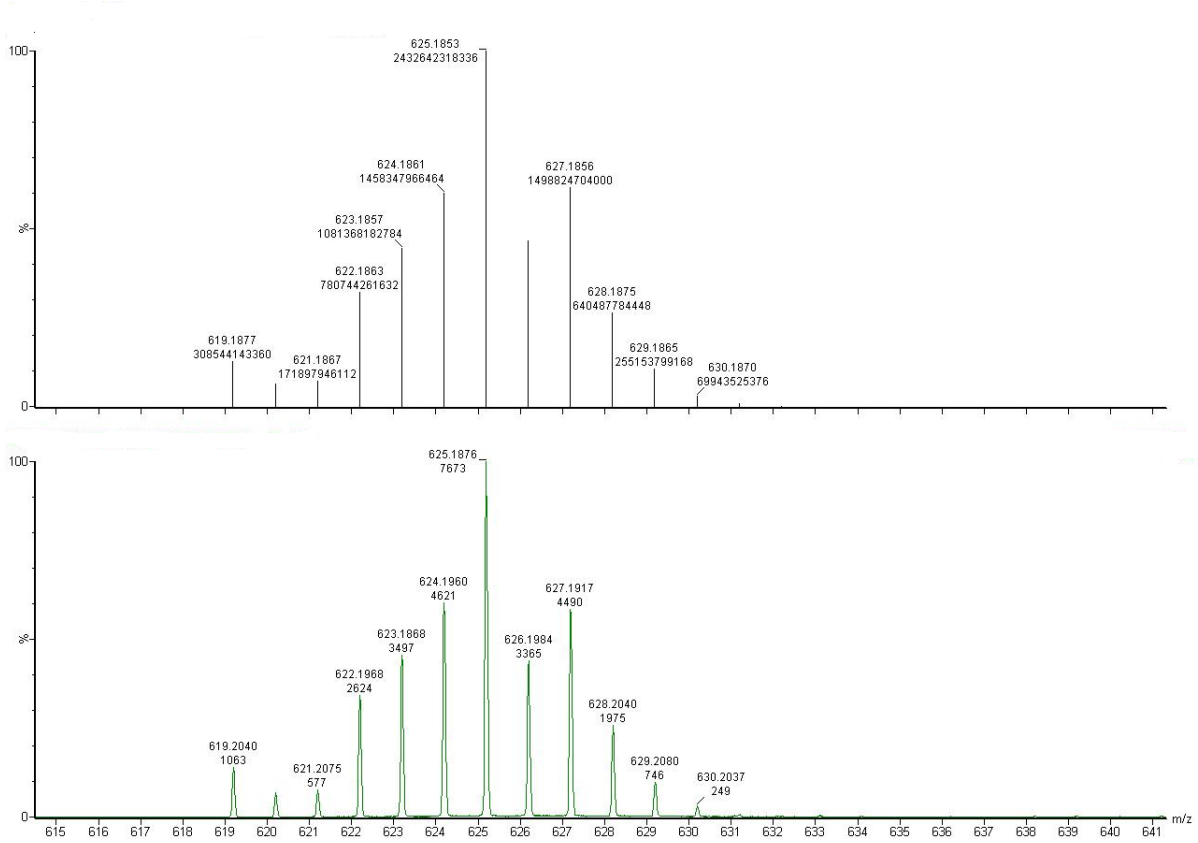

Figure S2. Upper: Simulated mass spectrum of $[Ru(CH_2SiMe_3)_3(PPh_3)]^+$. Lower: Isotopic pattern of the molecular ion at ca. m/z 625.1876 (mass accuracy: 3.7 ppm).

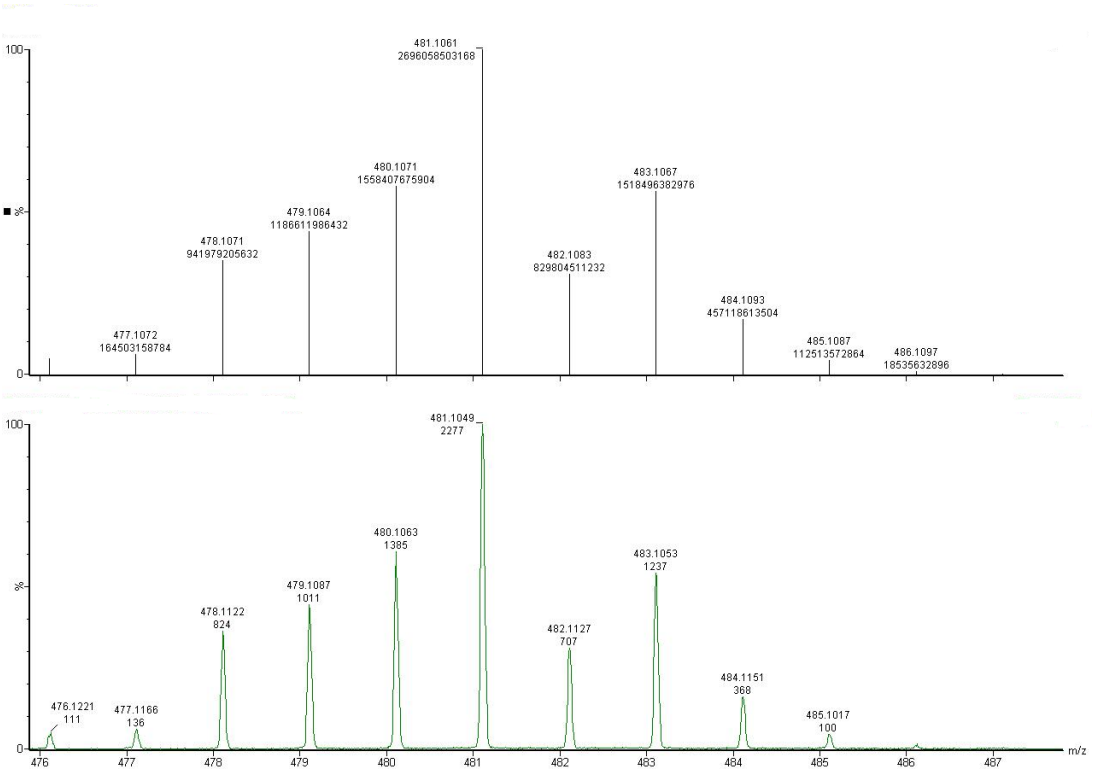

Figure S3. Upper: Simulated mass spectrum of $[Ru(CH_2SiMe_3)Me_2(PPh_3)]^+$. Lower: Isoptic patterns of the molecular ion at ca. m/z 481.1049 (mass accuracy: 2.5ppm).

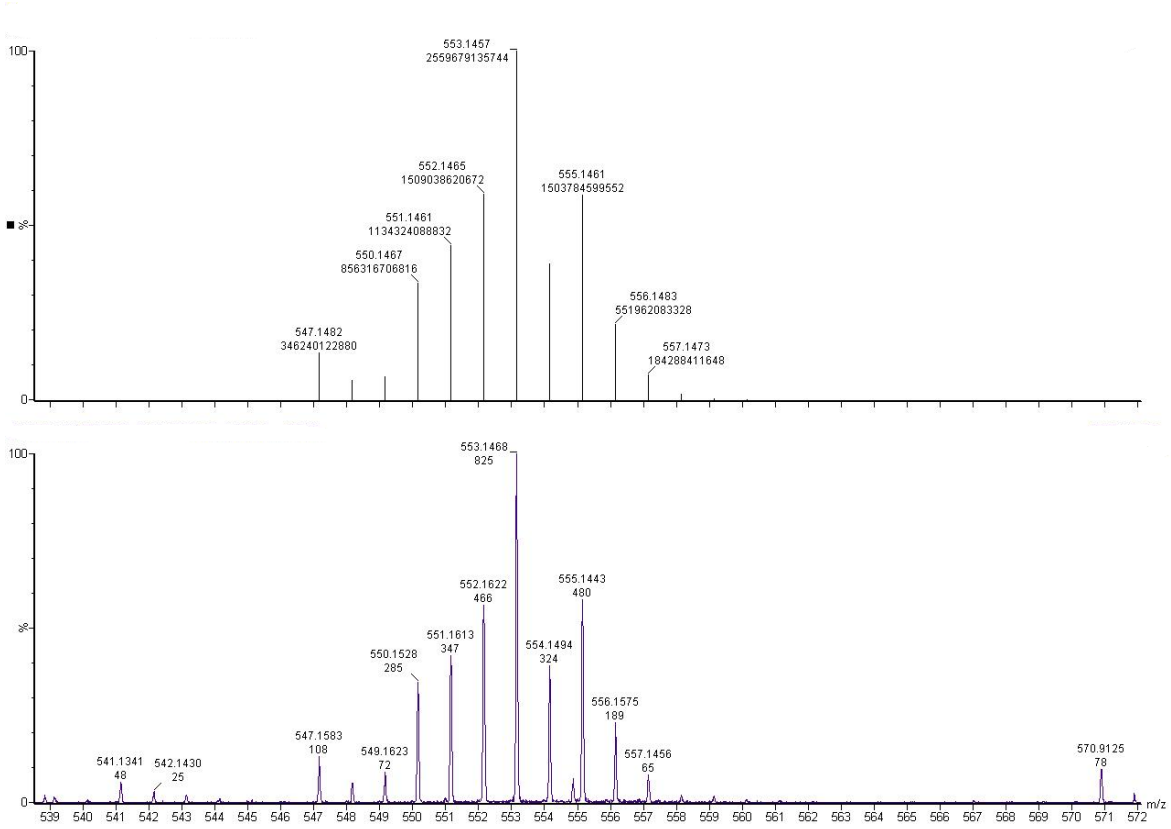

Figure S4. Upper: Simulated mass spectrum of $[Ru(CH_2SiMe_3)_2Me(PPh_3)]^+$. Lower: Isotopic pattern of the molecular ion at ca. m/z 553.1468 (mass accuracy:2.0 ppm).

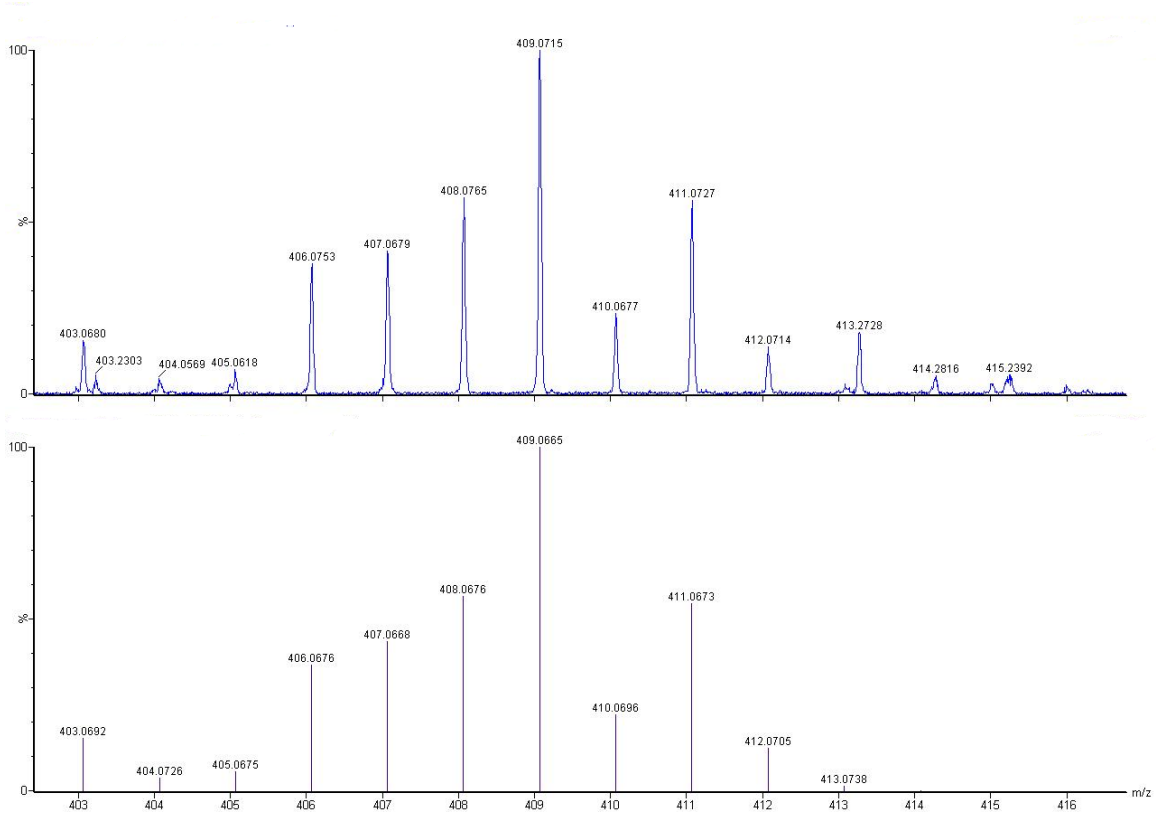

Figure S5. Lower: Simulated mass spectrum of $[RuMe_3(PPh_3)]^+$. Upper: Isotopic pattern of the molecular ion at m/z 409.0665 (mass accuracy: 12 ppm).

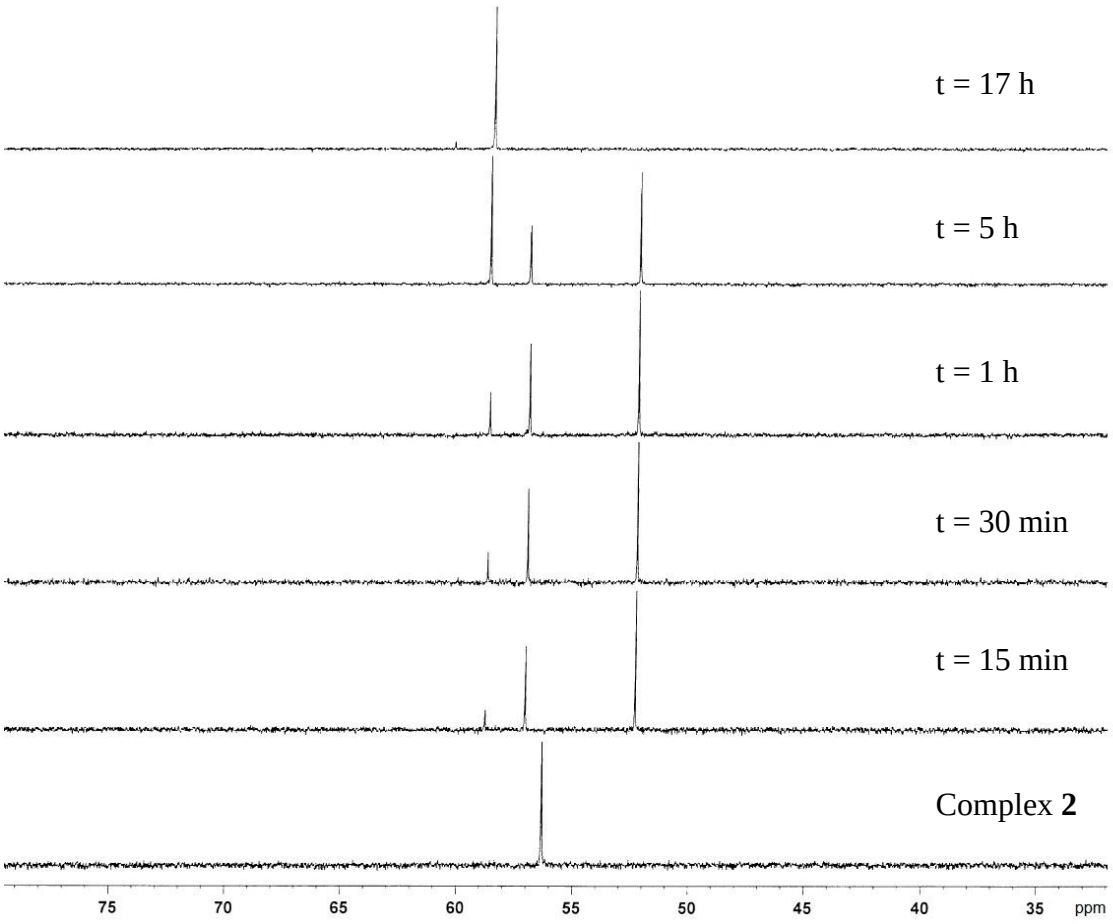

Figure S6. $^{31}P\{^{1}H\}$ NMR spectral change for the reaction of complex **2** with excess (10 folds) $NaOC_6F_4H$ in THF at room temperature at different time.