Supporting Information for

Trapping a pseudo-Hofmann rearrangement on a ruthenium cluster

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1. Experimental

1.1 General Considerations

Ru$_3$CO$_{12}$ and Ph$_3$PNSiMe$_3$ were purchased pure (Aldrich) and used without prior purification. The solvents were dried and distilled by standard techniques before use. The products were isolated by means of preparative TLC (20x20 cm silica plates, 1mm). The NMR spectra (chemical shifts in ppm) were recorded on Bruker instruments [Avance 300 for ^{1}H (TMS as internal reference), AMX400 for ^{31}P (H$_3$PO$_4$ 85% as external reference) at 300 and 161.98 Mhz, respectively]. The FTIR spectra of the pure solids were recorded on a Nicolet NEXUS spectrometer equipped with a Continuum FTIR microspectrometer. Elemental (C, H, N) analyses were performed on a Carlo Erba EA 1108 instrument.

1.2. Synthesis

Synthesis of compounds 2 and 3

A suspension of solid Ph$_3$PNSiMe$_3$ (200 mg, 0.57 mmol) and Ru$_3$(CO)$_{12}$ (300 mg, 0.47 mmol) in CH$_2$Cl$_2$ (0.5 mL) was placed under vacuum in a teflon sealed tube and then heated to 130°C. The mixture turned to a brownish-red colour after 1 hour. The reaction was stopped after 2 h and the reaction mixture brought to 20°C. Solid Ph$_3$PNSiMe$_3$ was added (1.1 mmol, 285 mg) and the reaction continued at 130°C for 1.5 h. A 0.4/0.6 mixture of compounds **2** and **3** (cumulative yield: 22%, based on Ru$_3$(CO)$_{12}$) was isolated by preparative TLC (2:1 hexane/CH$_2$Cl$_2$ mixture as eluent) as a red microcrystalline solid. Compound **3** can be obtained pure following the same procedure and increasing the reaction time to 3h (yield: 19%, based on Ru$_3$CO$_{12}$).

Compound **3**:

Elemental Analysis, calcd. (%) for $C_{47}H_{39}N_2Cl_1O_9P_2Ru_3Si_1$: N 2.33, C 46.87, H 3.26; found: N 2.34, C 46.92, H 3.23. ^{1}H NMR (300 MHz, CDCl$_3$, 25°C, TMS): δ = 0.26 (s, 9H; μ_3-OSiMe$_3$), 7.9-7.1 (m, 30H; Ph); ^{31}P{^{1}H} NMR (CDCl$_3$) δ = 59.8 (s, μ-Ph$_3$PN), 7.3 (s, μ-Ph$_3$PNCO); FTIR (cm^{-1}): 2047 m(sh), 2034 vs, 2025 vs(sh), 2005 m(sh), 1969 s(sh), 1952 s(sh) [ν(CO)], 1733 m [ν(μ-CO)], 1432 m [ν(μ-Ph$_3$N*CO*)], 1257 m [ν(Ph$_3$*P=N*CO)], 1110 [μ_3-N=P], 852 w [ν(O-Si)].

Compound **2**:

Elemental Analysis, calcd. (%) for $0.4 \cdot (C_{48}H_{39}N_3O_{10}P_2Ru_3Si_1)+0.6 \cdot (C_{47}H_{39}N_2Cl_1O_9P_2Ru_3Si_1)$: N 2.78, C 47.16, H 3.25; found: N 2.81, C 47.21, H 3.23. Spectroscopic data deduced by comparison with those of pure **3**: ^{1}H NMR (CDCl$_3$, 25°C): δ = 0.26 (s, 9H; μ_3-OSiMe$_3$), 7.9-7.1 (m, 30H; Ph); ^{31}P{^{1}H} NMR (CDCl$_3$, 25°C): δ = 58.5 (s, μ-Ph$_3$PN), 6.8 (s, μ-Ph$_3$PNCO); FTIR (cm^{-1}): 2047 m(sh), 2029 vs, 2007 vs, 2005 m(sh), 1969 s(sh), 1954 s(sh) [ν(CO)]; 2177 s [ν(μ-NCO)].
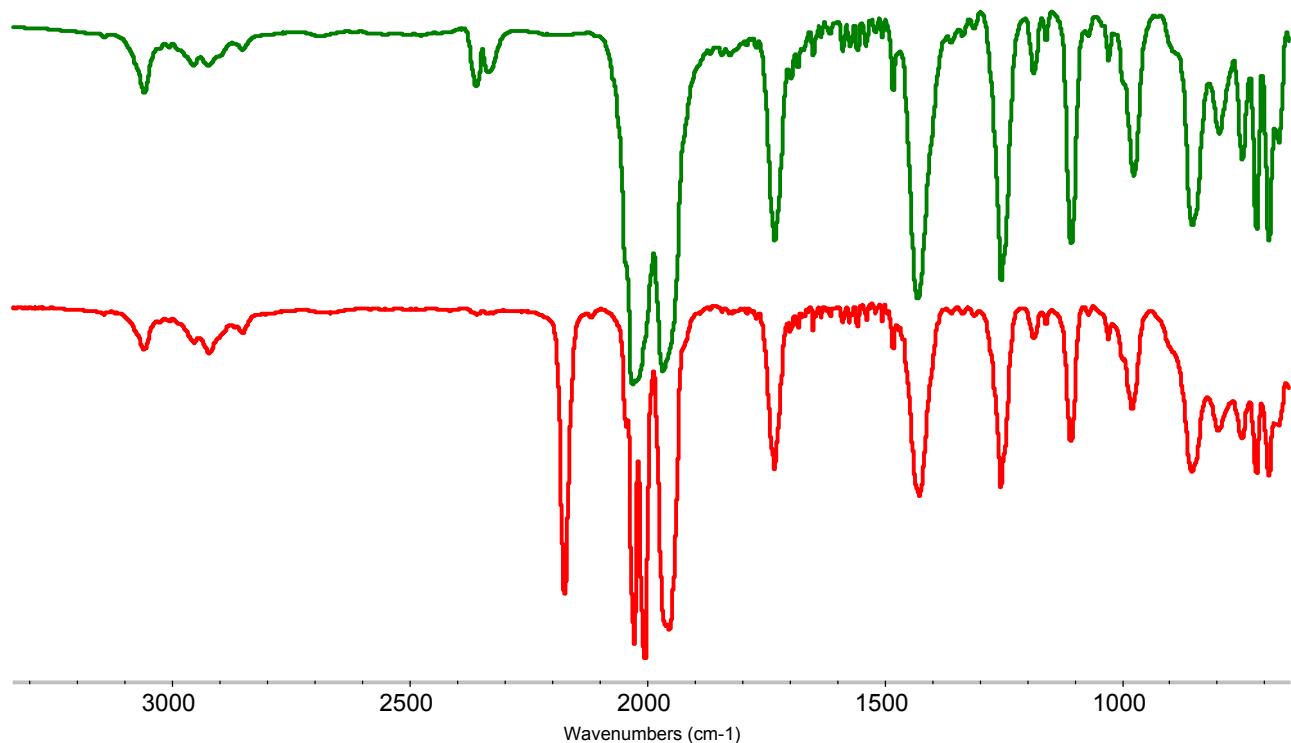

Figure S-1: Comparison between the infrared spectra of (a) pure compound **3,** (b) monocrystal of a mixture of compounds **2** and **3**.

2. Computational details

All calculations were done using the program system TURBOMOLE.[S1] If not mentioned explicitly otherwise, we used the DFT method with the Becke-Perdew functional (BP86).[S2] The Coulomb terms were treated by the RI-J approximation.[S3] For the structure optimizations we used SV(P) basis sets[S4] (single zeta for core orbitals, double zeta for the valence shells and one set of polarization functions for all centres except hydrogen). Single point energies were calculated with larger triple zeta valence plus polarization basis sets (TZVP).[S5] A comparison between selected crystallographic and computed distances and angles for compound **2** is reported in table S-1. Cartesian coordinates and total energies for optimized models **4a**, **4b, 5a**, **5b** are reported in table S-2. Cartesian coordinates for model **[Ru$_3$(μ$_3$-NPPh$_3$)(μ$_3$-NSiMe$_3$)(μ-NCO)(μ$_{C,O}$-OC=NPPh$_3$)(μ-CO)(CO)$_6$],** are reported in table S-3. The electronic occupation of the frontier orbitals is reported in table S-4. Input and optimized Cartesian coordinates for model **6** are reported in table S-5.

Table S-1: Comparison between computed (model **5a**) and crystallographic bond distances and angles for compound **2**.

[Ru$_3$(μ$_3$-NPPh$_3$)(μ$_3$-OSiMe$_3$)(μ-NCO)(μ$_{C,O}$-OC=NPPh$_3$)(μ-CO)(CO)$_6$]					
E = -4028.0377279230 H = -109608.5458296 eV)					
HOMO-LUMO gap (eV) = 1.66					
Distances (Å)	**Crystallographic**	**Computed**	**Angles (°)**	**Crystallographic**	**Computed**
Ru1···Ru2	3.2189(6)	3.280	Ru2-Ru3-Ru1	65.26(1)	65.70
Ru1···Ru3	3.0815(6)	3.119	O8-C8-N1	178(3)	178.5
Ru2-Ru3	2.8789(7)	2.924	C9-N2-P1	126.3(4)	126.30
P1-N2	1.619(4)	1.634	O9-C9-N2	121.3(5)	123.44
N2-C9	1.345(6)	1.356	O9-C9-Ru1	118.5(4),	117.07
O9-C9	1.255(5)	1.267	N2-C9-Ru1	120.0(4)	119.41
Ru1-N1	2.18(4)	2.243	C9-O9-Ru2	117.0(3)	117.22
Ru3-N1	2.31(4)	2.277			
N1-C8	1.22(5)	1.221			
O8-C8	1.159(16)	1.194			
Ru2-C5	2.031(5)	2.064			
Ru3-C5	2.044(5)	2.061			
Ru1-N3	2.199(3)	2.229			
Ru2-N3	2.180(3)	2.203			
Ru3-N3	2.202(4)	2.233			
Ru1-O10	2.160(3)	2.207			
Ru2-O10	2.184(3)	2.229			
Ru3-O10	2.194(3)	2.236			
Si1-O10	1.688(3)	1.738			

Table S-2: Energies and Cartesian coordinates obtained from BP86/TZVP||BP86/SV(P) calculations for the species **4a**, **4b**, **5a** (**2**) and **5b**

Model 4a
Total energy = -2641.2328156030 H = -71871.6426385 eV
HOMO-LUMO gap (eV) = +1.65903 eV

```
O   -1.8644433    0.1469779   -4.5711264      Ru  -1.9135585    0.1789725   -0.2837721
C   -1.3986974    0.1614498   -3.4762355      P   -0.2114404    3.0339890    0.0025220
O    2.3035364    2.4260725   -2.9624698      N   -0.1259657    1.4249440    0.0423838
O    2.4688529   -1.7631739   -3.1417148      O   -0.0922900   -1.1106698    0.0345085
C    1.8193449    1.5626662   -2.3461309      Si  -0.0593437   -2.8456486    0.0226305
C    1.9059239   -1.0192220   -2.4479251      C    1.7037462   -3.3813181    0.4585206
N   -0.9439623    0.1808931   -2.3406289      H    1.7925793   -4.4897828    0.3936466
H    0.1688164   -3.0603287   -2.4852230      H   -1.1312763    3.6213159    0.9301429
H   -1.5565986   -3.1069443   -1.9914280      H    1.0111892    3.7317386    0.2859846
H   -0.6015895    3.6066353   -1.2532340      O    2.3283169    0.1942684    1.2271441
H   -0.5866348   -4.5843019   -1.6751984      H   -2.3263522   -3.2268724    1.0869058
C   -0.5502047   -3.4707246   -1.6926785      H    1.9736108   -3.0771216    1.4930699
Ru   1.0319000    0.2233744   -1.3525125      H   -1.2397931   -4.6406267    1.2616589
H    6.2447207    0.1172268    0.2797461      C   -1.2775237   -3.5273119    1.2985559
N    3.8884099    0.2067678   -0.4445467      H    4.9241451   -1.0079980    1.6945289
O   -4.0389707    2.2967130   -0.5414983      Ru   0.1052164    0.2133280    1.8394223
O   -4.0958216   -1.8927722   -0.6591177      C   -1.9555621    0.1535244    1.7815009
H    4.9965092    1.2144326    1.7753387      H   -1.0369960   -3.2236215    2.3392703
H    2.4518747   -2.9424471   -0.2375143      O   -2.8123592    0.1195686    2.6135806
C   -3.2513115   -1.1047917   -0.5085621      C    0.2897411   -1.0234686    3.2285582
C   -3.2236075    1.4666313   -0.4404628      C    0.1691371    1.5394553    3.1176164
C    2.5908458    0.2142210   -0.0237366      O    0.4301322   -1.7723843    4.1105963
P    4.9318689    0.1362973    0.8261319      O    0.2118226    2.3994442    3.9075284
```

Model 4b
Total energy = -2641.2358732450 H = -71871.7258412 eV;
HOMO-LUMO gap (eV) = +1.51508 eV

```
O    4.3749983    0.1327799    2.3467499      Ru   1.6440029    0.1595746   -0.9399285
C    3.3026173    0.1609567    1.8327972      P    0.1655666    3.0247671   -0.0956187
O    0.1607038    2.4765810    3.8064240      N    0.0610644    1.4163601   -0.0556495
O    0.1526816   -1.7110528    4.1025282      O    0.0303611   -1.1080442    0.0069294
C    0.1288122    1.6050000    3.0330390      Si  -0.0044088   -2.8416813    0.0561806
C    0.1289834   -0.9785869    3.2006186      C   -1.6493650   -3.3535336    0.8438884
N    2.2142677    0.1949358    1.2733345      H   -1.7135648   -4.4629717    0.9137765
H    1.3749415   -3.2211623    2.1562688      H    0.2890580    3.5951438   -1.4034553
H    2.4210336   -3.0432640    0.7063698      H   -0.9506856    3.7424085    0.4555800
H    1.2717459    3.5926481    0.6175047      O   -2.7595999    0.2099240    2.8023798
H    1.5236150   -4.5732788    0.9884750      H    1.0605240   -3.2559965   -2.2055526
C    1.4612061   -3.4642062    1.0758709      H   -2.5100167   -3.0043661    0.2318685
Ru   0.0798610    0.2480785    1.7842289      H    0.1179264   -4.6628937   -1.6198242
H   -4.7247220   -1.0226857    1.5733006      C    0.1194001   -3.5507358   -1.6930004
N   -2.5626388    0.2346058    0.5739419      H   -4.8260400    0.1141669   -0.3453290
O    3.4517118    2.2574857   -2.1237631      Ru  -1.2909149    0.2091620   -1.2864301
O    3.5590104   -1.9307420   -2.0156658      C    0.3666905    0.1158156   -2.5471232
H   -4.8581680    1.2295518    1.5827891      H   -0.7298978   -3.2618781   -2.3476876
H   -1.7636351   -2.9437666    1.8714784      O    0.4983890    0.0553455   -3.7342252
C    2.8157510   -1.1349522   -1.6024167      C   -2.2946193   -1.0312431   -2.2554552
C    2.7582416    1.4339311   -1.6713638      C   -2.1034751    1.5388368   -2.2670355
C   -1.9634291    0.2410571    1.8271658      O   -2.9507098   -1.7851649   -2.8568976
P   -4.1962593    0.1410329    0.9353903      O   -2.6123146    2.4036147   -2.8669633
```

Model 5a

Total energy = -4028.0499182260 H = -109608.8775448 eV;
HOMO-LUMO gap (eV) = +1.68715 eV

H	-2.6936057	4.0228597	-5.3736021	C	-1.0368555	3.0963350	0.8556068
H	-3.4304373	1.6749980	-4.8507530	H	5.7093974	1.9478633	1.9143545
C	-2.5670279	3.6166170	-4.3563976	H	5.8052359	-2.1032216	0.7554361
C	-2.9801944	2.3043947	-4.0659119	C	1.1654546	4.0256790	1.3485477
H	-1.6582503	5.4357390	-3.5741439	H	-1.9708554	-4.7896549	1.3927336
H	8.3053327	-1.6299204	-3.6415228	H	2.0841246	-3.2161348	1.3214864
C	-2.4251385	-1.7977610	-3.3681222	H	-0.4543255	-5.7346911	1.5229927
C	-1.9869316	4.4073485	-3.3502307	C	-0.8709718	-4.7008610	1.5173652
H	5.8936345	-2.1629638	-4.1036932	C	4.5146504	-0.5303914	1.5533276
C	7.5184536	-1.2725513	-2.9565918	C	-6.3394696	2.4558203	1.7729361
C	6.1703324	-1.5713520	-3.2158645	H	-7.3460124	2.5864625	2.2035750
H	3.8455421	4.9197862	-1.6745987	C	5.3206401	-1.6860262	1.6524599
C	-2.8143143	1.7817981	-2.7739602	C	-1.6177267	4.0464234	1.7245522
C	0.3376457	0.8190708	-2.5732123	H	-2.7068145	4.0612799	1.8819742
C	0.9938254	-1.6356383	-2.5938938	C	-2.6279388	-1.4011296	1.9022482
H	-3.1144130	0.7451470	-2.5571489	C	-4.0584585	1.6237386	1.9589671
H	8.9218311	-0.2701070	-1.6214876	C	0.5822884	4.9620894	2.2202057
C	7.8654688	-0.5115220	-1.8249916	H	-0.6720889	-4.2590030	2.5156905
C	-1.8171008	3.8903611	-2.0547748	H	3.2221895	0.8567693	2.6408512
H	0.0220805	-4.1857712	-2.4091082	H	-3.2940120	1.1074907	2.5542453
H	-1.5765319	-4.6259588	-1.7196910	C	-0.8096180	4.9728633	2.4042786
C	5.1636602	-1.1132772	-2.3480324	C	-5.3379165	1.7980234	2.5069760
H	3.3580177	2.4628429	-1.7145785	H	1.2171379	5.6858377	2.7579231
H	4.1023650	-1.3279838	-2.5477590	C	3.8850393	-0.0189683	2.7119348
C	4.2586528	4.2672453	-0.8881222	H	-1.2752113	5.7026178	3.0869562
C	-2.2265714	2.5718723	-1.7605681	C	-0.0017114	-1.7408367	3.1093940
H	-0.1591051	-5.6922686	-1.4521963	C	-0.8677450	0.6206418	3.0567223
C	-0.4825620	-4.6282258	-1.5250010	C	5.5061628	-2.3124988	2.8969616
H	-1.3604692	4.5183767	-1.2736380	H	-5.5505261	1.4066681	3.5148750
C	3.9839830	2.8906731	-0.9142086	H	6.1344903	-3.2157045	2.9637974
H	5.2680608	5.8923413	0.1555205	C	4.0815279	-0.6447576	3.9517278
C	6.8657731	-0.0519699	-0.9536823	C	4.8915650	-1.7912399	4.0470434
C	5.5108188	-0.3560980	-1.2111329	H	3.5842873	-0.2420610	4.8492015
C	5.0529064	4.8111304	0.1376966	H	5.0364042	-2.2839774	5.0225488
H	-4.5725048	3.1477228	-1.0806255	O	-2.8470085	-2.1987211	-4.4097885
H	7.1462508	0.5513107	-0.0741388	O	0.6784995	1.6957737	-3.2651878
C	4.5077014	2.0467379	0.0907124	O	1.6698110	-2.2404679	-3.3280842
H	2.3325597	-3.1408072	-0.4555214	N	-2.0173569	-1.3688862	-2.2994184
C	-3.5669363	-3.1818751	-0.1873114	Ru	-0.0733444	-0.6059290	-1.4725006
C	-4.4876440	-0.8049280	-0.2640773	N	-0.0521420	-0.8809121	-0.8809121
H	-6.8332644	3.4586391	-0.0969331	O	-5.5979962	-0.4961307	-0.3683543
C	1.5670278	-0.1612478	-0.3020452	O	-4.0999319	-4.2193854	-0.2182310
H	0.8316968	2.3689133	-0.0100428	P	4.1949014	0.2410680	-0.0845716
C	5.5699250	3.9748049	1.1420557	Ru	-2.7652925	-1.5018533	-0.1505917
C	-4.7758523	2.7669666	-0.0682969	P	-2.0797212	1.8840095	-0.0611634
H	6.1881778	4.3972358	1.9512633	N	-1.4983848	0.3398864	-0.0412258
C	5.3019633	2.5947347	1.1204802	O	-0.6232368	-2.1147955	0.0455803
C	1.8193606	-3.7001916	0.3560699	Si	-0.0541533	-3.7531871	0.0973641
H	2.2295729	-4.7356921	0.3699799	O	1.3748650	-0.0580654	0.9474811
C	-6.0539250	2.9424874	0.4874500	Ru	-0.7057750	-0.6706199	1.7499508
C	0.3629309	3.0977905	0.6668998	O	-3.3431219	-1.6809313	2.8211071
C	-3.7660611	2.0982413	0.6597203	O	0.4452235	-2.3682462	3.9862351
H	2.2559910	4.0150021	1.1941204	O	-0.9420189	1.4033748	3.9224807

Model 5b

Total energy = -4028.0348748820 H = -109608.4681944 eV;

HOMO-LUMO gap (eV) = +1.67104 eV

H	-4.5853919	3.0848729	-5.0111910	C	-0.3896190	3.1529651	-0.0147815
H	-5.1989884	1.0799635	-3.6158141	H	5.6243500	2.1209206	0.3307536
C	-4.0358935	2.8680962	-4.0800918	H	5.5263772	-0.5762518	2.0237208
C	-4.3813797	1.7490800	-3.3022508	C	1.6825773	4.0800340	-0.9192639
H	-2.7131950	4.5879717	-4.2744399	H	-1.4049357	-4.2792995	2.4216421
H	6.7191217	-4.5992657	-0.7362723	H	2.2878563	-3.8366760	0.3883973
C	-3.5557722	-1.9831720	-2.3707228	H	-0.2581312	-5.5862072	1.9877430
C	-2.9883864	3.7084706	-3.6691573	C	-0.4019927	-4.4806864	1.9890583
H	5.2236399	-4.3313864	1.2650740	C	3.9029202	0.8086825	1.5425242
C	6.1032829	-3.6915989	-0.6233636	C	-4.8128986	3.4843331	3.0675112
C	5.2687197	-3.5422420	0.4964533	H	-5.5320327	3.8631457	3.8125767
H	4.1369966	2.7851955	-4.4018642	C	4.9496826	0.3041494	2.3450646
C	-3.6793999	1.4694670	-2.1202733	C	-0.4125886	4.1851451	0.9489582
C	-0.5666886	0.2537289	-3.0971681	H	-1.2299959	4.2387443	1.6843586
C	-0.0978869	-2.2373012	-2.9327647	C	-1.6462477	-1.0401287	2.4518937
H	-3.9494638	0.5865419	-1.5231227	C	-2.8911554	2.0962794	2.5054981
H	6.7886940	-2.8013075	-2.4907697	C	1.6490522	5.1083954	0.0392940
C	6.1454706	-2.6840701	-1.6030689	H	0.3576048	-4.0477692	2.6741085
C	-2.2792948	3.4308857	-2.4881757	H	2.4116751	2.3876301	1.3343901
H	-1.3557196	-4.4973323	-1.9713582	H	-2.1247387	1.3848184	2.8347307
H	-2.4760178	-4.7224490	-0.5874702	C	0.6053056	5.1537377	0.9772405
C	4.4796450	-2.3887051	0.6409542	C	-3.8046116	2.5854646	3.4526501
H	3.0719392	1.0069265	-3.0118462	H	2.4426913	5.8738113	0.0547627
H	3.8275942	-2.2871047	1.5232830	C	3.2118804	1.9668600	1.9631705
C	4.4659917	2.6421066	-3.3592172	H	0.5730101	5.9526170	1.7364342
C	-2.6138659	2.3015773	-1.7098380	C	1.2352666	-1.4293305	2.6435112
H	-1.1430676	-5.8900606	-0.8624873	C	0.3296592	0.9618387	2.6316646
C	-1.4169651	-4.8103416	-0.9082767	C	5.2756068	0.9307953	3.5603567
H	-1.4608733	4.1006062	-2.1810830	H	-3.7253756	2.2487912	4.4988191
C	3.8532392	1.6461003	-2.5791675	H	6.0894163	0.5201119	4.1804782
H	5.9747258	4.2149053	-3.4451040	C	3.5443061	2.5912874	3.1744096
C	5.3646998	-1.5269005	-1.4620525	C	4.5735669	2.0723904	3.9786376
C	4.5334452	-1.3674458	-0.3332859	H	2.9850092	3.4845960	3.4946039
C	5.4926519	3.4396835	-2.8262828	H	4.8306683	2.5613270	4.9329584
H	-4.0890456	3.7261268	-0.2729443	O	-4.4031373	-2.3578414	-3.1221675
H	5.3940017	-0.7468010	-2.2382205	O	-0.5089793	0.9652395	-4.0209582
C	4.2514846	1.4445158	-1.2358596	O	0.1651287	-3.0197121	-3.7531317
H	1.7912849	-3.6195456	-1.3188090	N	-2.7072882	-1.5788371	-1.5903228
C	-3.4533643	-2.8966575	1.1960290	Ru	-0.5637135	-0.9347193	-1.6812856
C	-4.1663720	-0.4936755	1.0976014	N	1.8198737	-0.0792867	-0.1471869
H	-5.6960589	4.5911348	1.4108044	O	-5.2048502	-0.0289509	1.3589550
C	1.4463679	-0.5479053	-1.3956126	O	-4.0418135	-3.8418035	1.5435254
H	0.7173519	2.3019007	-1.6975718	P	3.5108479	0.1423956	-0.1234291
C	5.9043202	3.2369575	-1.4988343	Ru	-2.5801382	-1.3379639	0.6612692
C	-3.9960883	3.4010692	0.7742920	P	-1.7623452	1.9229299	-0.1197276
H	6.7122009	3.8499068	-1.0658529	N	-1.2749484	0.3508226	-0.0016013
C	5.2877631	2.2527330	-0.7085116	O	-0.5514931	-2.1535970	0.1431403
C	1.5492843	-4.1557436	-0.3758592	Si	-0.2216821	-3.8590772	0.2097280
H	1.7035080	-5.2441445	-0.5575085	O	2.3205547	-0.7518292	-2.2699009
C	-4.9047923	3.8912330	1.7263637	Ru	0.1157421	-0.4728286	1.5021258
C	0.6750091	3.1029271	-0.9439839	O	-1.9376788	-1.1610305	3.6084260
C	-2.9777753	2.4949527	1.1536621	O	1.9534812	-2.0120003	3.3586423
H	2.5024516	4.0313175	-1.6533502	O	0.4102403	1.8354987	3.4060318

Table S-3 Energies and Cartesian coordinates obtained from BP86/TZVP‖BP86/SV(P) calculations for model **[Ru$_3$(μ$_3$-NPPh$_3$)(μ$_3$-NSiMe$_3$)(μ-NCO)(μ$_{C,O}$-OC=NPPh$_3$)(μ-CO)(CO)$_6$]**
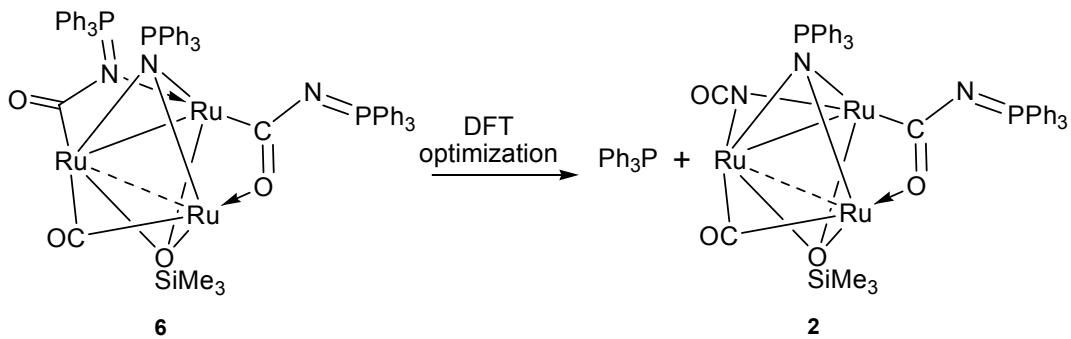
Total energy = -4003.9047887300 H = -108951.8547680 eV
HOMO-LUMO gap +0.38122 eV; **Number of electrons** = 519

Atom	x	y	z	Atom	x	y	z
H	-2.9305441	4.0170153	-5.3796846	C	-0.9825812	3.1160600	0.7703890
H	-3.5272440	1.6215664	-4.8427488	H	5.8144666	2.1393876	1.6099681
C	-2.7620978	3.6191544	-4.3697674	H	5.5450973	-2.0648197	1.1298892
C	-3.0997523	2.2709749	-4.0673157	C	1.2712644	4.0817678	1.0471630
H	-1.9233088	5.4845445	-3.5908219	H	-1.9098701	-4.6961069	1.5729407
H	8.1661988	-2.3535075	-3.2965959	H	2.1262277	-3.1987567	1.2779323
C	-2.5682012	-1.9249374	-3.2456309	H	-0.5115553	-5.8013996	1.4398913
C	-2.1941568	4.4454311	-3.3619462	C	-0.8055180	-4.7378154	1.5642655
H	5.7141668	-2.7282092	-3.7728235	C	4.4112384	-0.2545817	1.6366277
C	7.4026823	-1.8584020	-2.6815197	C	-6.2566249	2.5151804	2.0027646
C	6.0230555	-2.0704804	-2.9491198	H	-7.2342167	2.6513716	2.4849967
H	3.9720359	4.7083251	-2.3113435	C	5.1153426	-1.4568036	1.9349718
C	-2.8730736	1.7533962	-2.7668071	C	-1.4874689	4.0641990	1.7051012
C	0.2598444	0.7627944	-2.6672689	H	-2.5496103	4.0703692	1.9749987
C	0.9208846	-1.7256465	-2.5506042	C	-2.6262286	-1.4151229	1.9967772
H	-3.0994594	0.6992789	-2.5568213	C	-3.9399604	1.6871595	2.0738639
H	8.8575162	-0.8258407	-1.4117235	C	0.7620334	5.0236748	1.9835488
C	7.7924149	-0.9971344	-1.6167951	H	-0.4377036	-4.4013520	2.5497027
C	-1.9700971	3.9291695	-2.0589876	H	3.2501405	1.4038351	2.4913261
H	0.2420427	-4.4354722	-2.2979222	H	-3.1422948	1.1844928	2.6321947
H	-1.4882912	-4.4396109	-1.8405776	C	-0.6203495	5.0108811	2.3108626
C	5.0361129	-1.4264345	-2.1558017	C	-5.1977943	1.8704833	2.6998124
H	3.3745280	2.2882927	-2.0154542	H	1.4339478	5.7547971	2.4526876
H	3.9690842	-1.5745197	-2.3693216	C	3.8396734	0.5033201	2.7025451
C	4.3728811	4.1483509	-1.4560501	H	-1.0215793	5.7292812	3.0379362
C	-2.3080364	2.5800999	-1.7521143	C	0.0650123	-1.7970092	2.9991847
H	-0.4177928	-5.7682608	-1.2964273	C	-0.7179742	0.6596452	3.0175685
C	-0.4676558	-4.6755614	-1.4856547	C	5.2597965	-1.8883882	3.2803993
H	-1.5255697	4.5813403	-1.2984266	H	-5.3533944	1.5032424	3.7229474
C	4.0367364	2.7805503	-1.2897483	H	5.7977909	-2.8202729	3.4989512
H	5.4929874	5.8502355	-0.6495072	C	3.9853938	0.0726295	4.0449023
C	6.8075236	-0.3554071	-0.8240003	C	4.6991149	-1.1239801	4.3390723
C	5.4241711	-0.5724600	-1.0880916	H	3.5298041	0.6546057	4.8568255
C	5.2292634	4.7918257	-0.5194121	H	4.8028768	-1.4616941	5.3790984
H	-4.6498461	3.1362314	-0.9814560	O	-2.9492235	-2.4077433	-4.2664539
H	7.1270071	0.3129935	-0.0148267	O	0.6002910	1.6018451	-3.4044804
C	4.5542696	2.0422264	-0.1856453	O	1.5918475	-2.3595935	-3.2668629
H	2.3484143	-3.2654994	-0.5029510	N	-2.1755890	-1.3909041	-2.2188427
C	-3.4514102	-3.2044070	-0.1008086	Ru	-0.1175962	-0.6441255	-1.4630772
C	-4.4681714	-0.8112413	-0.2320456	N	2.7301828	-0.0342901	-0.8593732
H	-6.8569257	3.4635789	0.1240965	O	-5.5852509	-0.5038290	-0.3484182
C	1.5042070	-0.1847768	-0.3133549	O	-3.9836486	-4.2400685	-0.1264453
H	0.8167922	2.4108252	-0.2698709	P	4.1416213	0.2621257	-0.0965124
C	5.7450645	4.0578854	0.5841723	Ru	-2.6940763	-1.4928093	-0.0873371
C	-4.7837705	2.7851260	0.0478894	P	-2.0816646	1.9095589	-0.0634275
H	6.4062310	4.5502824	1.3098831	N	-1.5049481	0.3740442	-0.0446129
C	5.4114443	2.6876973	0.7499699	N	-0.6488349	-2.0578869	0.0518316
C	1.8397983	-3.7396704	0.3564481	Si	-0.0501734	-3.7423513	0.1236692
H	2.2014252	-4.7861857	0.4399445	O	1.3162251	-0.0747052	0.9505510
C	-6.0434202	2.9725452	0.6747233	Ru	-0.6722974	-0.6894552	1.6786508
C	0.4061798	3.1338757	0.4458871	O	-3.3045505	-1.6900100	2.9291874
C	-3.7186557	2.1378366	0.7384807	O	0.5279035	-2.4164358	3.8710830
H	2.3371808	4.0880359	0.7842662	O	-0.6763442	1.4240660	3.8982153

Table S-4: Electronic occupation of the frontier orbitals for model **[Ru$_3$(μ$_3$-NPPh$_3$)(μ$_3$-NSiMe$_3$)(μ-NCO)(μ$_{C,O}$-OC=NPPh$_3$)(μ-CO)(CO)$_6$]**

Nr.	Orbital	Occupation	Energy	
536.	268		-0.074844 H =	-2.037 eV
535.	268		-0.074882 H =	-2.038 eV
534.	267		-0.076229 H =	-2.074 eV
533.	267		-0.076461 H =	-2.081 eV
532.	266		-0.079519 H =	-2.164 eV
531.	266		-0.079663 H =	-2.168 eV
530.	265		-0.080275 H =	-2.184 eV
529.	265		-0.080864 H =	-2.200 eV
528.	264		-0.081982 H =	-2.231 eV
527.	264		-0.082112 H =	-2.234 eV
526.	263		-0.087613 H =	-2.384 eV
525.	263		-0.087645 H =	-2.385 eV
524.	262		-0.094228 H =	-2.564 eV
523.	262		-0.094364 H =	-2.568 eV
522.	261		-0.096198 H =	-2.618 eV
521.	261		-0.096670 H =	-2.631 eV
520.	260		-0.150827 H =	-4.104 eV
519.	260	1.000	-0.164688 H =	-4.481 eV
518.	259	1.000	-0.189157 H =	-5.147 eV
517.	259	1.000	-0.192537 H =	-5.239 eV
516.	258	1.000	-0.196484 H =	-5.347 eV
515.	258	1.000	-0.198284 H =	-5.396 eV
514.	257	1.000	-0.199212 H =	-5.421 eV
513.	257	1.000	-0.201923 H =	-5.495 eV
512.	256	1.000	-0.211427 H =	-5.753 eV
511.	255	1.000	-0.211601 H =	-5.758 eV
510.	256	1.000	-0.213325 H =	-5.805 eV
509.	255	1.000	-0.215178 H =	-5.855 eV
508.	254	1.000	-0.216272 H =	-5.885 eV
507.	254	1.000	-0.218100 H =	-5.935 eV
506.	253	1.000	-0.218950 H =	-5.958 eV
505.	253	1.000	-0.221106 H =	-6.017 eV
504.	252	1.000	-0.225761 H =	-6.143 eV

Table S-5: Computational details for the DFT model **6 → 2** conversion

Cartesian coordinates of the input model.

Atom	X	Y	Z	Atom	X	Y	Z
H	-2.7433352	5.2553073	2.4278660	H	2.8407035	-4.9034598	0.6832467
H	-2.8961946	2.8575329	3.2128592	H	4.7495712	0.2869036	-2.8601090
C	-1.8627414	4.6004320	2.3762867	H	4.0902737	0.3288908	3.5920929
C	-1.9482358	3.2526211	2.8236244	C	5.1647496	4.1606928	1.1985851
H	-0.5655591	6.1282756	1.4974291	C	4.0917808	1.0248649	5.6420182
H	-1.4246760	-0.9035622	-8.5556965	H	5.8519702	4.7684977	-0.7889891
C	-2.2919703	-0.8272177	2.1688528	C	4.6971023	-0.5851200	-3.5230904
C	-0.6358048	5.0920346	1.8533453	H	5.9669657	4.6871686	1.7323416
H	-2.2225281	-1.2781761	-6.1900828	C	4.1554028	-2.5647480	0.3479690
C	-0.7577949	-0.6935308	-7.7086478	C	4.6577172	-0.2669901	1.2268647
C	-1.2068276	-0.9045825	-6.3770209	C	4.5520209	-2.9234576	-5.1312004
H	1.5114165	5.1686580	-3.8781735	H	4.9332494	0.3778427	5.9231035
C	-0.8135262	2.4057381	2.7527635	H	4.4865047	-3.8337091	-5.7420329
C	-0.5781162	1.4493160	-0.4741251	C	5.8063429	-1.4645861	-3.5982220
C	-1.1814510	-0.9066954	-1.1981039	C	5.7383702	-2.6366740	-4.4034858
H	-0.9004317	1.3619117	3.0794196	H	6.7131064	-1.2501372	-3.0172081
H	0.9057309	-0.0267859	-8.9681888	H	6.5941828	-3.3244049	-4.4472505
C	0.5573288	-0.2006284	-7.9416289	O	-3.4201705	-0.9235121	2.5498175
C	0.4996164	4.2425783	1.7797375	O	-0.9871412	2.4775434	-0.8449318
H	-1.7661918	-3.4764713	-0.3485708	O	-1.9827715	-1.2924911	-1.9525782
H	-1.4143087	-3.8972002	1.3544986	N	-1.1284581	-0.7177599	1.8186189
C	-0.3465902	-0.6251412	-5.2815273	Ru	0.0668141	-0.2171565	-0.0061454
H	0.8696625	2.7872587	-3.4222502	N	1.0839717	0.1626027	-2.7784370
H	-0.6966621	-0.7678421	-4.2506749	O	0.5923611	-0.3929787	5.5915981
C	2.1670037	4.3543942	-4.2141472	O	-0.1257681	-4.0199088	4.0297492
C	0.4196971	2.8930122	2.2270204	P	2.0505596	0.2343137	-4.0939555
H	-1.2839294	-5.1482624	0.0794756	Ru	0.8203622	-1.4307743	2.7715313
C	-1.1087329	-4.0754741	0.3069616	P	1.8812671	1.7908101	2.1933856
H	1.4337186	4.6389240	1.3653994	N	1.5517612	0.3043468	1.5710824
C	1.8028758	3.0076913	-3.9582228	O	1.0572172	-2.0802216	0.6496954
H	3.6607839	5.6905673	-5.1017112	Si	0.7237021	-3.6744940	0.0440220
C	1.4163084	0.0762655	-6.8482105	O	2.6759738	-0.3756189	-1.1935258
C	0.9683614	-0.1388612	-5.5128978	Ru	3.0707564	-1.1592570	0.9286672
C	3.3763519	4.6480286	-4.9042644	O	3.5551416	-2.4156825	3.6358489
H	1.0384165	3.2873675	4.6386565	O	4.8767321	-3.4079875	-0.0126323
H	2.4234302	0.4648450	-7.0461991	O	5.6934730	0.2551000	1.3775115
C	2.6424306	1.9405357	-4.3921586	P	-6.4090262	0.2262126	-0.2968223
H	0.4948835	-3.0311435	-2.3816325	C	-7.3740389	1.3543817	0.8099593
C	0.2423945	-3.0347448	3.5245192	C	-8.4273985	0.9332270	1.6698773
C	0.7124197	-0.7574267	4.4890482	C	-9.0706487	1.8587438	2.5358433
H	1.9048671	3.3431478	6.9703449	C	-8.6783143	3.2239285	2.5443231
C	1.4762726	-0.1144889	-1.5096325	C	-7.6277001	3.6555315	1.6875139
H	2.3091153	2.2365593	-0.7047319	C	-6.9745381	2.7252394	0.8392740
C	4.2174928	3.5853104	-5.3341639	H	-8.7443521	-0.1164382	1.6741365
C	1.8939809	2.6546350	4.8994539	H	-9.8717002	1.5131686	3.2027569
H	5.1538925	3.8058278	-5.8860258	H	-9.1754825	3.9383284	3.2135774
C	3.8519245	2.2364879	-5.0815649	H	-7.3111563	4.7068186	1.6930303
C	1.1545793	-3.6999871	-1.7988293	H	-6.1464429	3.0655211	0.2031574
H	1.0336787	-4.7320814	-2.1913390	C	-7.0991924	-1.4379562	0.1246143
C	2.3865301	2.6907737	6.2300344	C	-6.3846500	-2.2095580	1.0891399
C	3.0957300	2.7756142	-0.1634082	C	-6.8347095	-3.5057121	1.4560305
C	2.4943589	1.8046147	3.9251531	C	-7.9969246	-4.0572882	0.8500445
H	4.0067603	3.5318669	-1.9993543	C	-8.7053543	-3.3010596	-0.1235640
C	3.1554247	2.7244382	1.2600488	C	-8.2600217	-2.0011503	-0.4814739
H	4.5172368	1.4313530	-5.4160575	H	-5.4672843	-1.8115227	1.5489121
H	2.5325558	-2.2791071	-5.6260126	H	-6.2737932	-4.0825830	2.2027538
C	4.0622965	3.5079049	-0.8974798	H	-8.3405946	-5.0624281	1.1277657
H	1.6919398	-4.8668331	2.0569873	H	-9.6011675	-3.7220737	-0.5990533
H	2.2028453	-3.3881859	-1.9669523	H	-8.8146745	-1.4328663	-1.2380011
H	1.4044386	-5.9699585	0.6793685	C	-7.1779620	0.5621471	-1.9493290
C	1.7726835	-4.9598842	0.9583853	C	-6.4426495	0.1310621	-3.0944961
C	3.5065912	-0.8634321	-4.2594665	C	-6.9316913	0.3675936	-4.4050520
C	3.4866233	1.8748941	6.6079287	C	-8.1616654	1.0568668	-4.5931451
H	3.8601144	1.8915749	7.6409672	C	-8.8948566	1.5023129	-3.4593911
C	3.4412521	-2.0410365	-5.0596715	C	-8.4074058	1.2535803	-2.1486416
C	4.1970183	3.4261492	1.9327386	H	-5.4813374	-0.3830493	-2.9586735
H	4.2706654	3.4008986	3.0256701	H	-6.3547002	0.0281230	-5.2751144
C	2.8263925	-1.8943359	2.8412300	H	-8.5413036	1.2461639	-5.6060013
C	3.6038877	0.9955195	4.3122256	H	-9.8438325	2.0378531	-3.5960812
C	5.1009279	4.2038237	-0.2199747	H	-8.9840414	1.6038416	-1.2838249

Cartesian coordinates after optimization.

H	-2.7433352	5.2553073	2.4278660	H	2.8407035	-4.9034598	0.6832467
H	-2.8961946	2.8575329	3.2128592	H	4.7495712	0.2869036	-2.8601090
C	-1.8627414	4.6004320	2.3762867	H	4.0902737	0.3288908	3.5920929
C	-1.9482358	3.2526211	2.8236244	C	5.1647496	4.1606928	1.1985851
H	-0.5655591	6.1282756	1.4974291	C	4.0917808	1.0248649	5.6420182
H	-1.4246760	-0.9035622	-8.5556965	H	5.8519702	4.7684977	-0.7889891
C	-2.2919703	-0.8272177	2.1688528	C	4.6971023	-0.5851200	-3.5230904
C	-0.6358048	5.0920346	1.8533453	H	5.9669657	4.6871686	1.7323416
H	-2.2225281	-1.2781761	-6.1900828	C	4.1554028	-2.5647480	0.3479690
C	-0.7577949	-0.6935308	-7.7086478	C	4.6577172	-0.2669901	1.2268647
C	-1.2068276	-0.9045825	-6.3770209	C	4.5520209	-2.9234576	-5.1312004
H	1.5114165	5.1686580	-3.8781735	H	4.9332494	0.3778427	5.9231035
C	-0.8135262	2.4057381	2.7527635	H	4.4865047	-3.8337091	-5.7420329
C	-0.5781162	1.4493160	-0.4741251	C	5.8063429	-1.4645861	-3.5982220
C	-1.1814510	-0.9066954	-1.1981039	C	5.7383702	-2.6366740	-4.4034858
H	-0.9004317	1.3619117	3.0794196	H	6.7131064	-1.2501372	-3.0172081
H	0.9057309	-0.0267859	-8.9681888	H	6.5941828	-3.3244049	-4.4472505
C	0.5573288	-0.2006284	-7.9416289	O	-3.4201705	-0.9235121	2.5498175
C	0.4996164	4.2425783	1.7797375	O	-0.9871412	2.4775434	-0.8449318
H	-1.7661918	-3.4764713	-0.3485708	O	-1.9827715	-1.2924911	-1.9525782
H	-1.4143087	-3.8972002	1.3544986	N	-1.1284581	-0.7177599	1.8186189
C	-0.3465902	-0.6251412	-5.2815273	Ru	0.0668141	-0.2171565	-0.0061454
H	0.8696625	2.7872587	-3.4222502	N	1.0839717	0.1626027	-2.7784370
H	-0.6966621	-0.7678421	-4.2506749	O	0.5923611	-0.3929787	5.5915981
C	2.1670037	4.3543942	-4.2141472	O	-0.1257681	-4.0199088	4.0297492
C	0.4196971	2.8930122	2.2270204	P	2.0505596	0.2343137	-4.0939555
H	-1.2839294	-5.1482624	0.0794756	Ru	0.8203622	-1.4307743	2.7715313
C	-1.1087329	-4.0754741	0.3069616	P	1.8812671	1.7908101	2.1933856
H	1.4337186	4.6389240	1.3653994	N	1.5517612	0.3043468	1.5710824
C	1.8028758	3.0076913	-3.9582228	O	1.0572172	-2.0802216	0.6496954
H	3.6607839	5.6905673	-5.1017112	Si	0.7237021	-3.6744940	0.0440220
C	1.4163084	0.0762655	-6.8482105	O	2.6759738	-0.3756189	-1.1935258
C	0.9683614	-0.1388612	-5.5128978	Ru	3.0707564	-1.1592570	0.9286672
C	3.3763519	4.6480286	-4.9042644	O	3.5551416	-2.4156825	3.6358489
H	1.0384165	3.2873675	4.6386565	O	4.8767321	-3.4079875	-0.0126323
H	2.4234302	0.4648450	-7.0461991	O	5.6934730	0.2551000	1.3775115
C	2.6424306	1.9405357	-4.3921586	P	-6.4090262	0.2262126	-0.2968223
H	0.4948835	-3.0311435	-2.3816325	C	-7.3740389	1.3543817	0.8099593
C	0.2423945	-3.0347448	3.5245192	C	-8.4273985	0.9332270	1.6698773
C	0.7124197	-0.7574267	4.4890482	C	-9.0706487	1.8587438	2.5358433
H	1.9048671	3.3431478	6.9703449	C	-8.6783143	3.2239285	2.5443231
C	1.4762726	-0.1144889	-1.5096325	C	-7.6277001	3.6555315	1.6875139
H	2.3091153	2.2365593	-0.7047319	C	-6.9745381	2.7252394	0.8392740
C	4.2174928	3.5853104	-5.3341639	H	-8.7443521	-0.1164382	1.6741365
C	1.8939809	2.6546350	4.8994539	H	-9.8717002	1.5131686	3.2027569
H	5.1538925	3.8058278	-5.8640258	H	-9.1754825	3.9383284	3.2135774
C	3.8519245	2.2364879	-5.0815649	H	-7.3111563	4.7068186	1.6930303
C	1.1545793	-3.6999871	-1.7988293	H	-6.1464429	3.0655211	0.2031574
H	1.0336787	-4.7320814	-2.1913390	C	-7.0991924	-1.4379562	0.1246143
C	2.3865301	2.6907737	6.2300344	C	-6.3846500	-2.2095580	1.0891399
C	3.0957300	2.7756142	-0.1634082	C	-6.8347095	-3.5057121	1.4560305
C	2.4943589	1.8046147	3.9251531	C	-7.9969246	-4.0572882	0.8500445
H	4.0067603	3.5318669	-1.9935573	C	-8.7053543	-3.3010596	-0.1235540
C	3.1554247	2.7244382	1.2600488	C	-8.2600217	-2.0011503	-0.4814739
H	4.5172368	1.4313530	-5.4160575	H	-5.4672843	-1.8115227	1.5489121
H	2.5325558	-2.2791071	-5.6260126	H	-6.2737932	-4.0825830	2.2027538
C	4.0622965	3.5079049	-0.8974798	H	-8.3405946	-5.0624281	1.1277657
H	1.6919398	-4.8668331	2.0569873	H	-9.6011675	-3.7220737	-0.5990533
H	2.2028453	-3.3881859	-1.9669523	H	-8.8146745	-1.4328663	-1.2380011
H	1.4044386	-5.9699585	0.6793685	C	-7.1779620	0.5621471	-1.9493290
C	1.7726835	-4.9598842	0.9583853	C	-6.4426495	0.1310621	-3.0944961
C	3.5065912	-0.8634321	-4.2594665	C	-6.9316913	0.3675936	-4.4050520
C	3.4866233	1.8748941	6.6079287	C	-8.1616654	1.0568668	-4.5931451
H	3.8601144	1.8915749	7.6409672	C	-8.8948566	1.5023129	-3.4593911
C	3.4412521	-2.0410365	-5.0596715	C	-8.4074058	1.2535803	-2.1486416
C	4.1970183	3.4261492	1.9327386	H	-5.4813374	-0.3830493	-2.9586735
H	4.2706654	3.4008986	3.0256701	H	-6.3547002	0.0281230	-5.2751144
C	2.8263925	-1.8943359	2.8412300	H	-8.5413036	1.2461639	-5.6060013
C	3.6038877	0.9955195	4.3122256	H	-9.8438325	2.0378531	-3.5960812
C	5.1009279	4.2038237	-0.2199747	H	-8.9840414	1.6038416	-1.2838249

4. Crystallographic details

X-ray data collection, structure solution and refinement for compounds 2/3 and 3·0.5CH$_3$OH.

Suitable crystals for the X-ray analysis of complexes **2/3** and **3**·0.5CH$_3$OH were obtained by evaporation of dichloromethane/methanol solutions. The intensity data was collected at room temperature on a Bruker area detector AXS Smart 1000 (graphite monochromated MoK$_\alpha$ radiation, λ = 0.71073 Å). Crystallographic and experimental details for the structures are summarized in Table S-6. Bruker SADABS software [maximum and minimum transmission coefficient values: 1.000 and 0.860 (**2/3**), 1.000 and 0.671 (**3**·0.5CH$_3$OH)] was used for the absorption correction. The structures were solved by direct methods and refined by full-matrix least-squares procedures (based on $F_o{}^2$, SHELX-97) first with isotropic thermal parameters and then with anisotropic thermal parameters in the last cycles of refinement for all the non-hydrogen. The hydrogen atoms were introduced into the geometrically calculated positions and refined *riding* on the corresponding parent atoms. The occupancy factors for N1, C8, O8 and Cl1 (0.4, 0.4, 0.4 and 0.6, respectively) in **2/3** were refined unconstrained in the isotropic model and then constrained to the obtained value in the anisotropic one. CCDC-xxxxxx (**2/3**), CCDC-xxxxxx (**3**·0.5CH$_3$OH), contain the supplementary crystallographic data for this paper that can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. A list of selected refinement parameters is reported in table S-6. Ortep views of the molecular structures of compound **2** and **3** are reported in figures S-2 and S-3.

Table S-6: X-ray data collection, structure solution and refinement parameters for compounds **2/3**

and **3**·0.5CH$_3$OH.

Complexes	2/3	3·0.5CH$_3$OH
Formula	C$_{47.40}$H$_{39}$Cl$_{0.60}$N$_{2.40}$O$_{9.40}$ P$_2$Ru$_3$Si	C$_{47.50}$H$_{43}$Cl$_1$N$_2$O$_{9.50}$P$_2$Ru$_3$Si
FW	1207.12	1220.51
Crystal System	Triclinic	Triclinic
Space Group	*P-1*	*P-1*
a, Å	11.6159(7)	11.608(3)
b, Å	13.3036(7)	13.277(3)
c, Å	17.140(1)	17.196(3)
α, °	98.473(1)	81.920(3)
β, °	90.88(3)	89.945(3)
γ, °	104.370(1)	76.225(3)
V, Å^3	2535.2(3)	2547(1)
Z	2	1
D_{calcd}, g cm^{-3}	1.581	1.591
F(000)	1203	1281
Crystal size (mm)	0.2 × 0.1 × 0.1	0.2 × 0.2 × 0.1
μ, cm^{-1}	10.55	10.72
Rflns. collected	22509	27031
Rflns. unique	7973	10474
Rflns. observed [*I* > 2σ(*I*)]	4879	7729
Parameters	613	604
R Indices [*I*>2σ(*I*)]	*R1* = 0.0380, *wR2* = 0.0799	*R1* = 0.0350, *wR2* = 0.0539
R Indices (all data)	*R2* = 0.0536, *wR2* = 0.0584	*R2* = 0.0843, *wR2* = 0.0883

Figure S-2: Ortep view of the crystallographic model obtained from the data collected from a crystal formed by a 2:3 mixture by clusters **2** and **3** (Displacement parameters include 30% of the electron density).
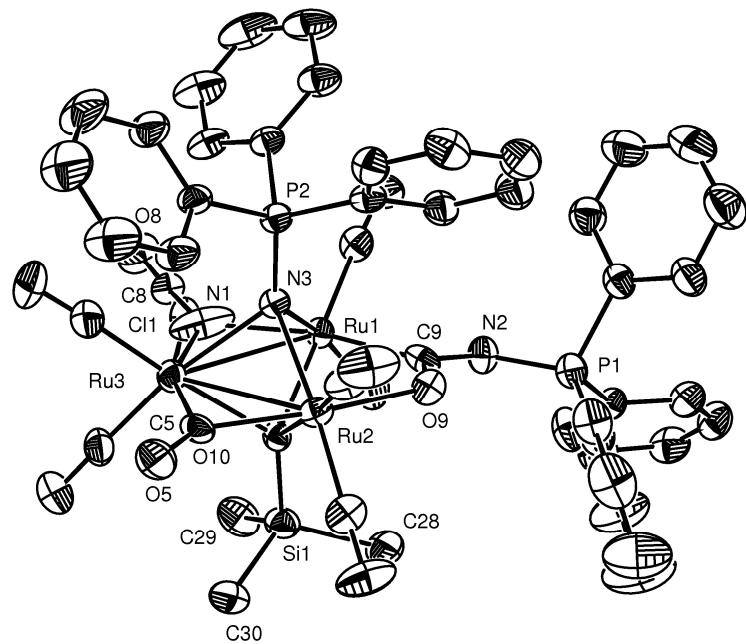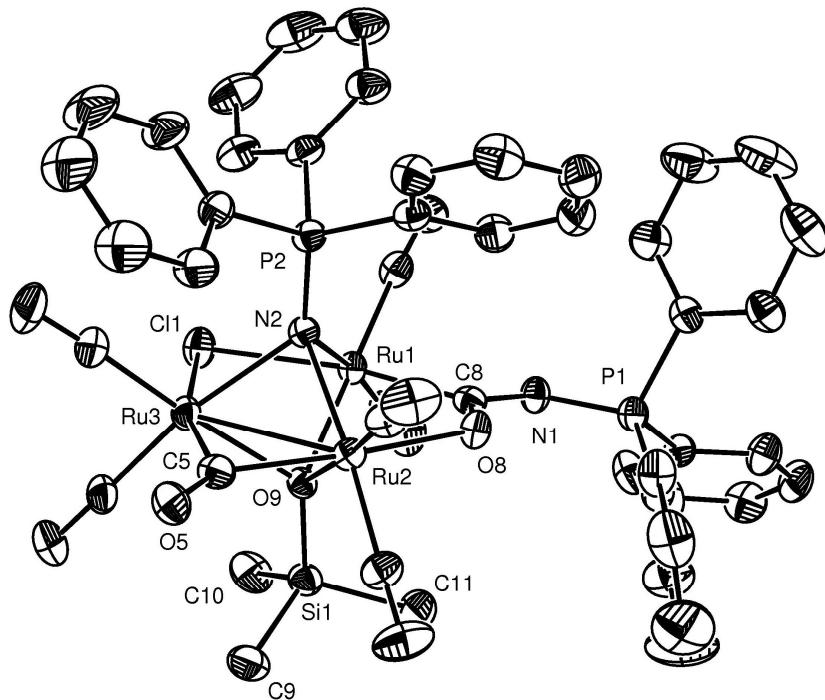

Figure S-3: Ortep view of the crystal structure of cluster **3** in **3**·CH₃OH (Displacement parameters include 30% of the electron density).

5. References

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