

Heteroleptic Ruthenium(II) chromophores based on tunable polytopic 4' (amidinato)-2,2':6',2''- terpyridines

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NMR spectroscopy in solution at variable temperature

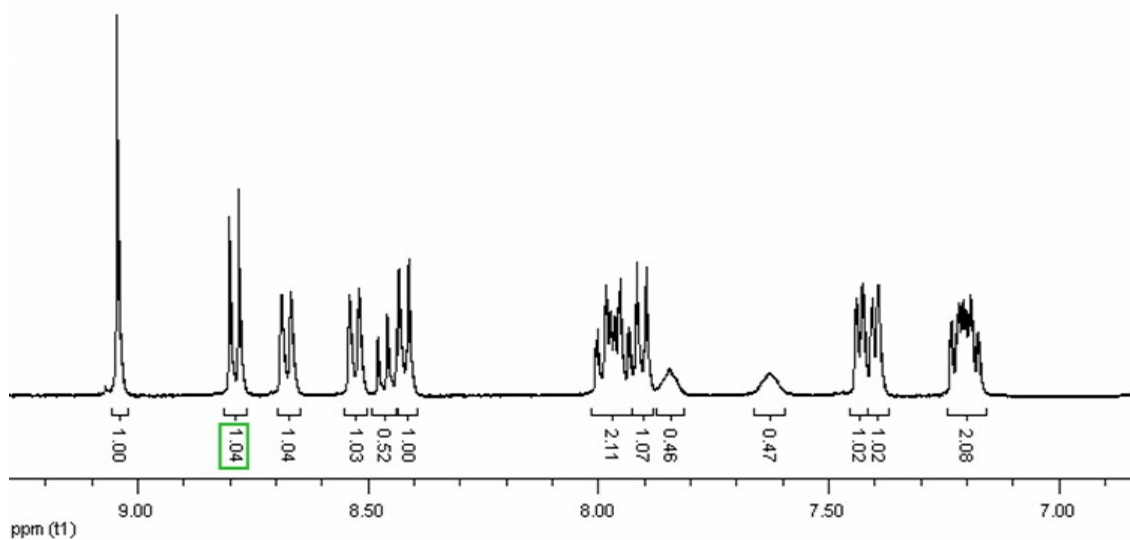


Figure S1. ¹H NMR of complex **1** in CD₃CN at r.t. (aromatic region).

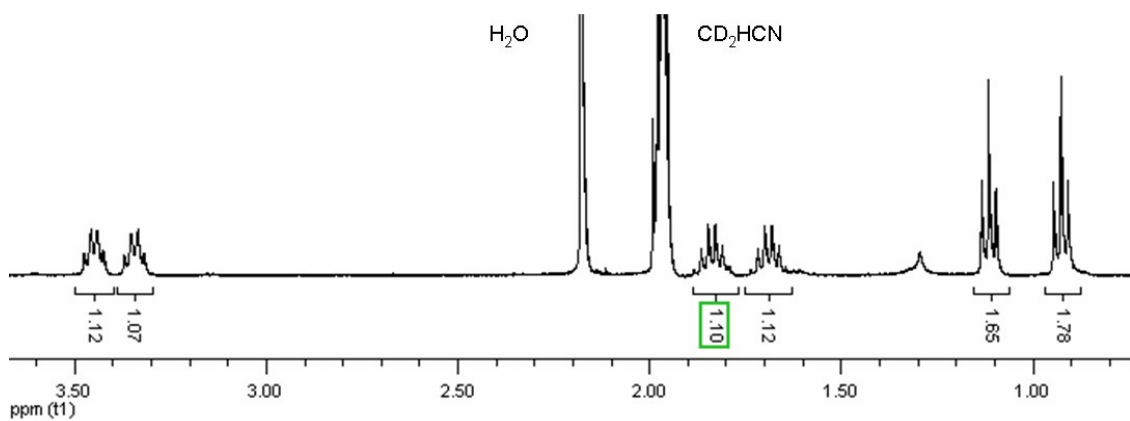


Figure S2. ¹H NMR of complex **1** in CD₃CN at r.t. (aliphatic region).

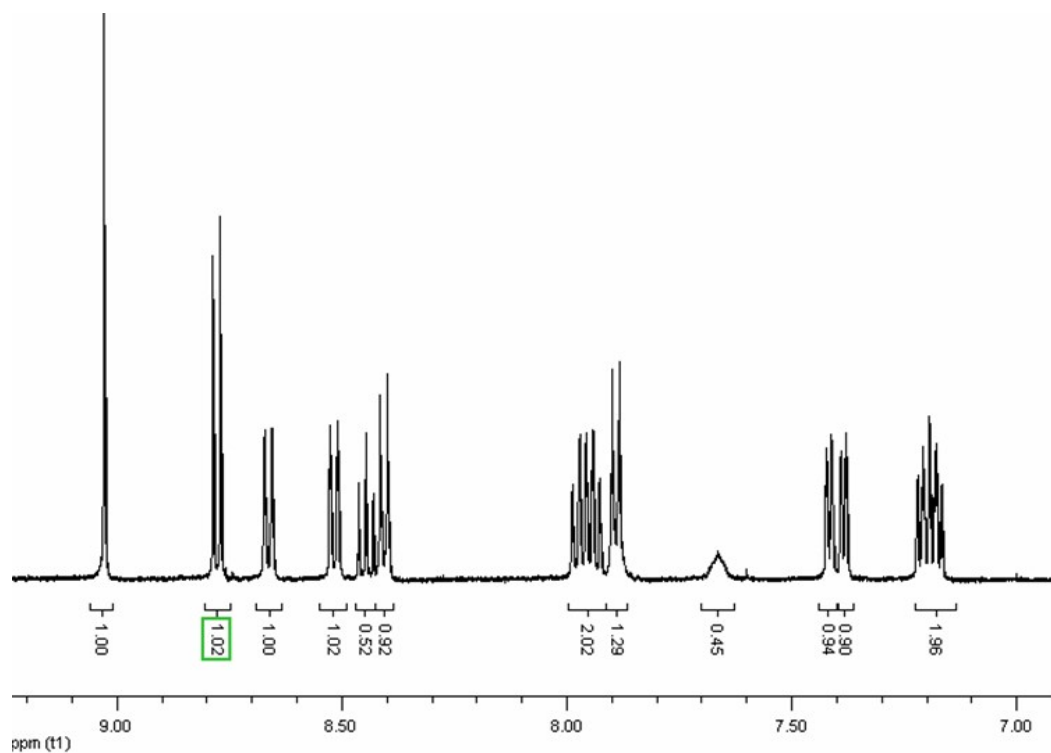


Figure S3. ^1H NMR of complex 1 in CD_3CN at 330 K (aromatic region).

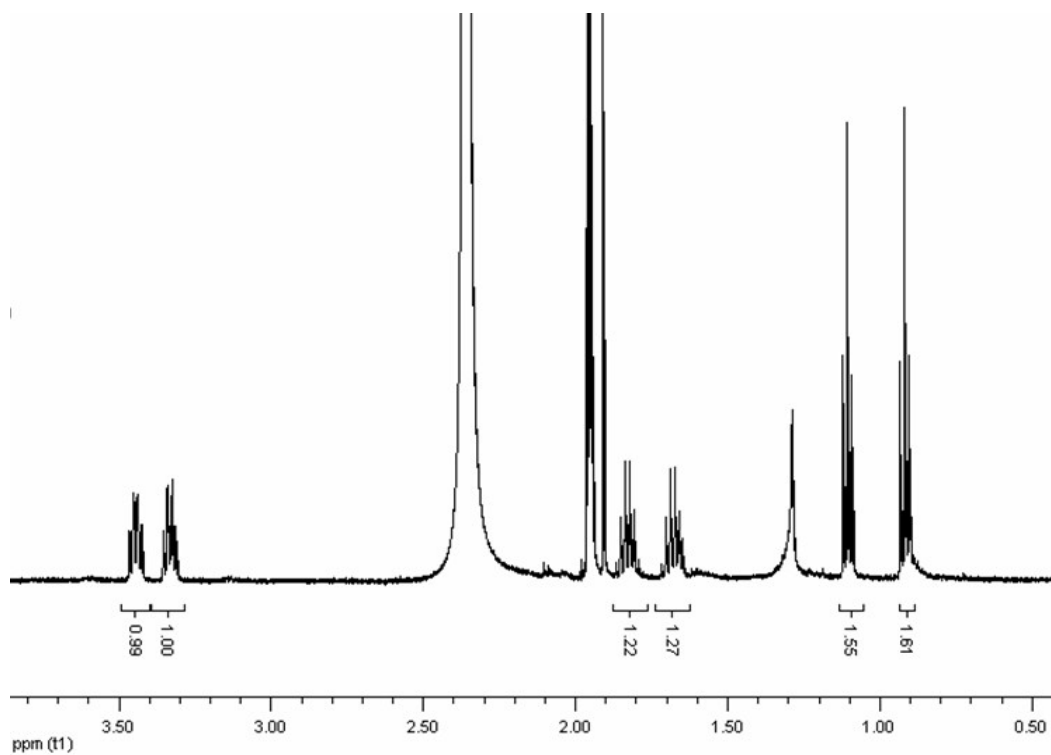


Figure S4. ^1H NMR of complex 1 in CD_3CN at 330 K (aliphatic region).

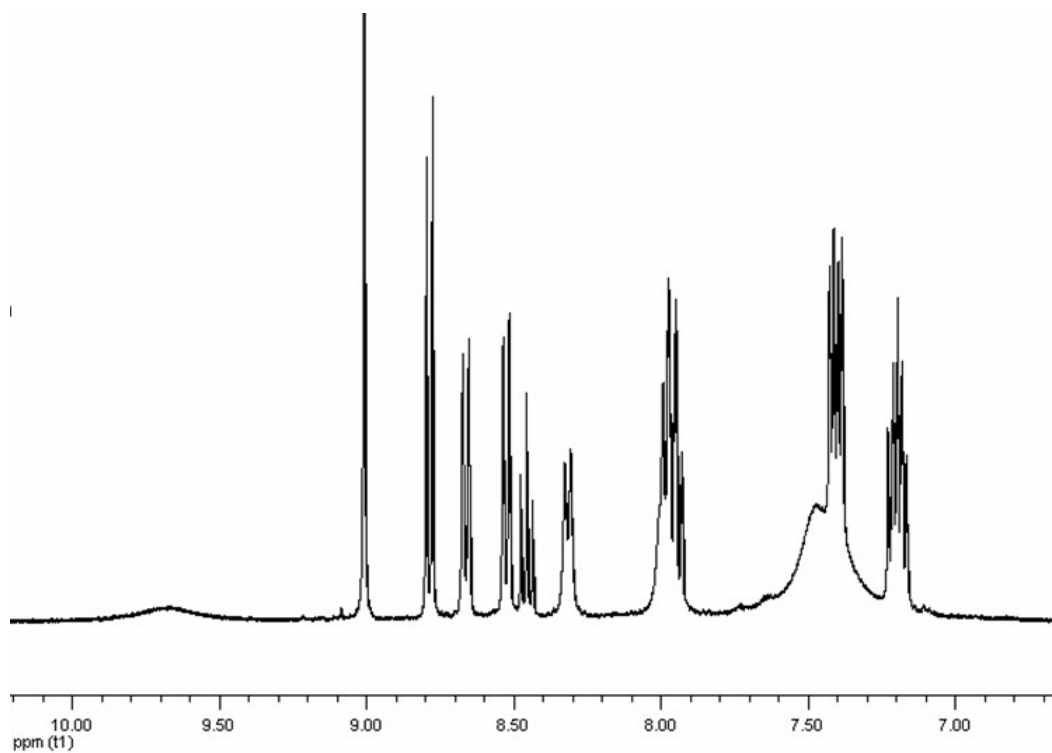


Figure S5. ^1H NMR of complex **2** in CD_3CN at r.t. (aromatic region).

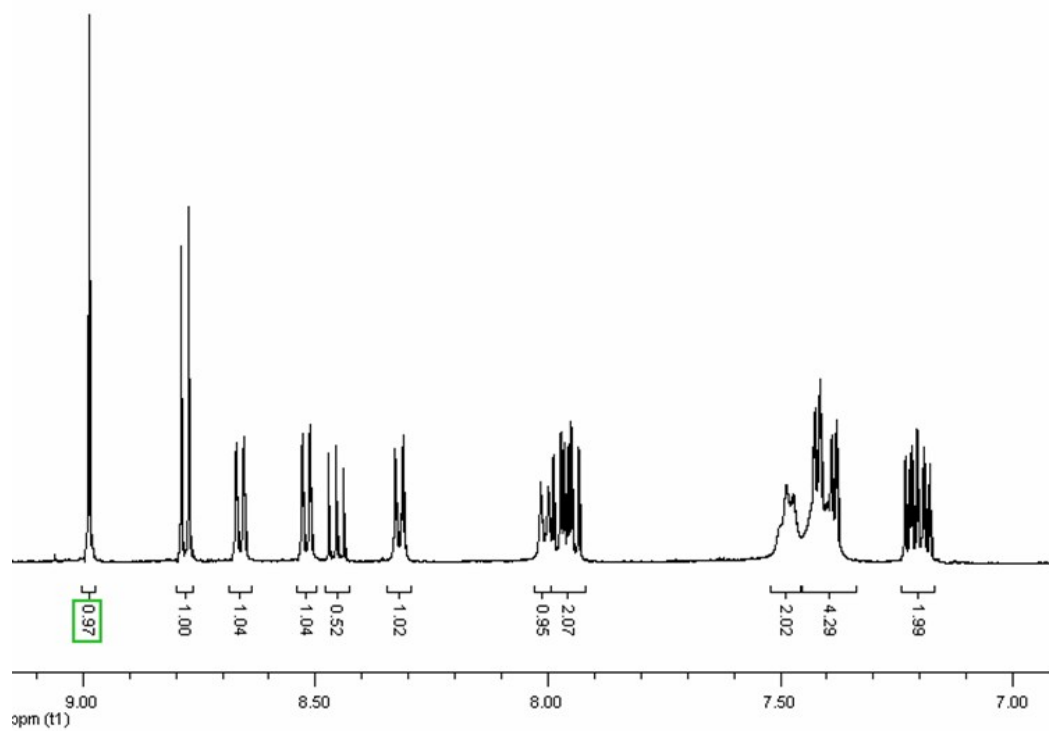
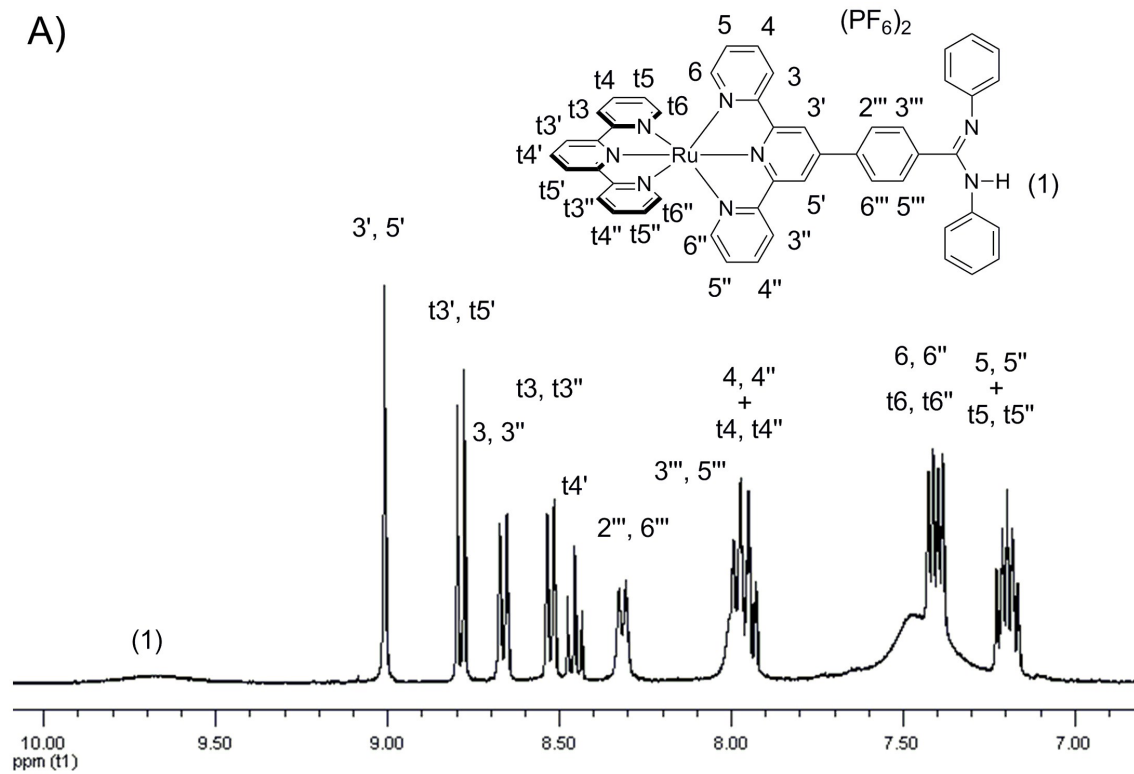


Figure S6. ^1H NMR of complex **2** in CD_3CN at 330 K (aromatic region).

A)



B)

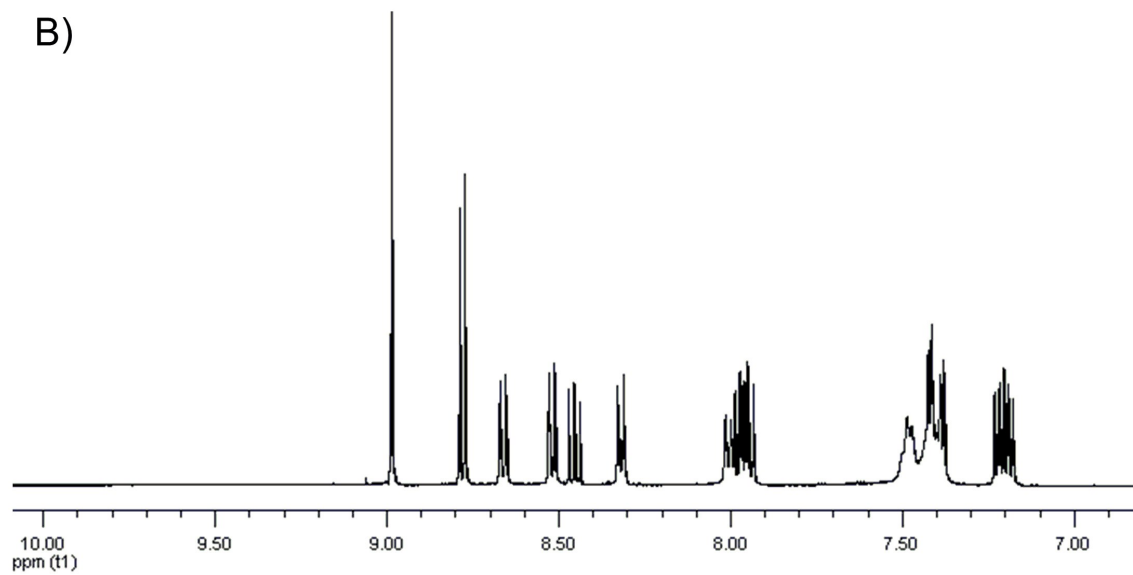


Figure S7. 1H NMR of **2** in CD_3CN at: A) 298 K and B) 330 K.

Electrochemistry

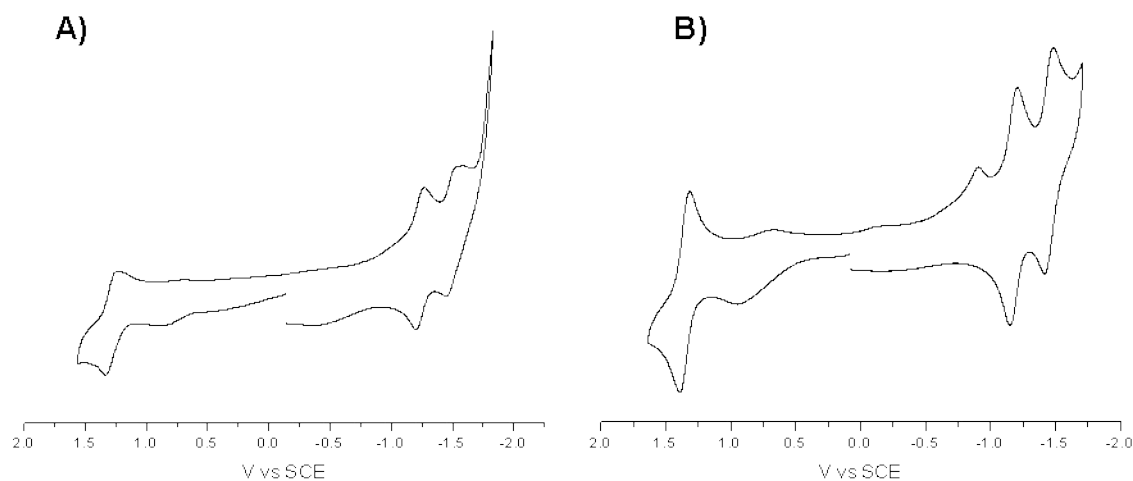


Figure S8. Cyclic voltammograms of **1** (A) and **2** (B) in 0.1 M TBAPF₆ CH₃CN solution at 100 mVs⁻¹.

Spectrophotometric and spectrofluorimetric determination of ground-state pKa values

The ground-state pKa values for complexes **1-4** were determined by UV-Vis and emission measurements over the range of pH = 2-13. Stock solutions (1, 4.6 x 10⁻⁵ M; 2, 5.1 x 10⁻⁵ M; 3, 5.1 x 10⁻⁵ M; 4, 6.1 x 10⁻⁵ M) were prepared in 100 mL of H₂O containing 20% DMSO and 0.1 M KCl, for solubility. The pH of the solution was initially adjusted by addition of 0.2 M NaOH(aq) and subsequently lowered by careful addition of HCl(aq) solution (total volume change kept negligible).

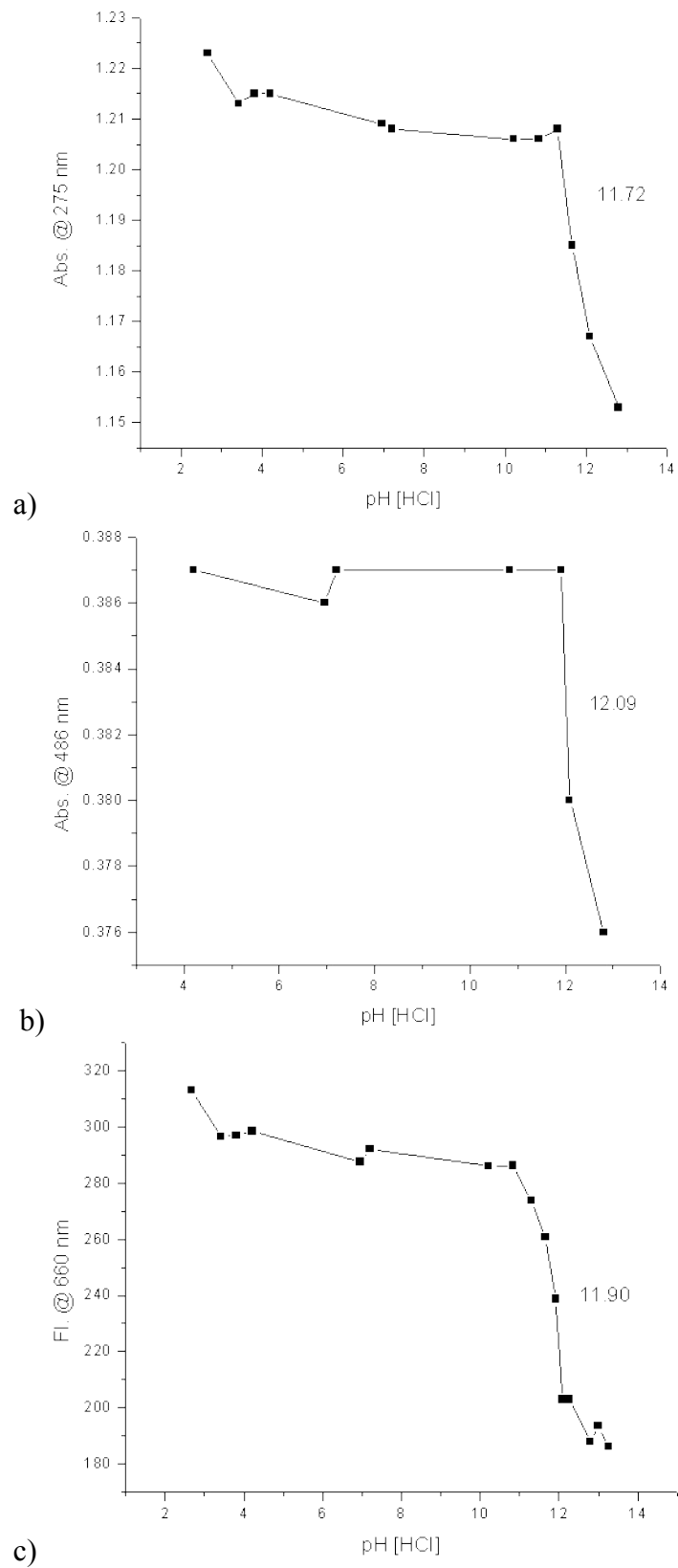


Figure S9. Spectrophotometric titration of **1** at: a) 275 nm; b) 486 nm; c) 660 nm.

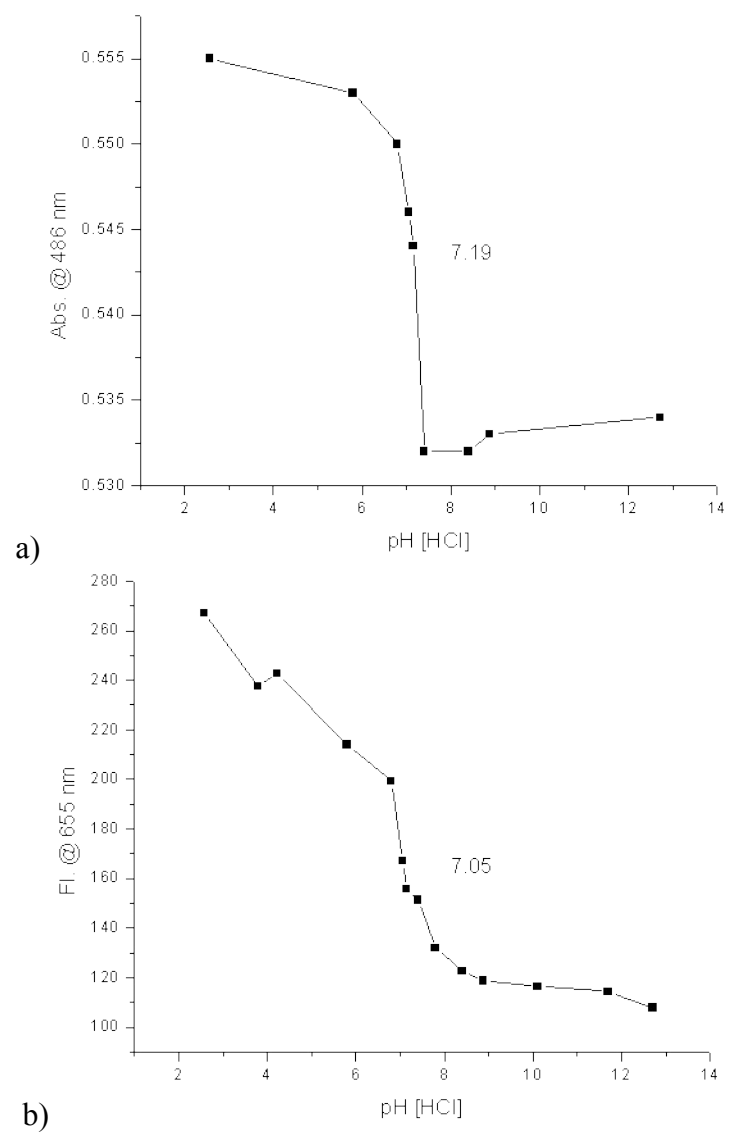
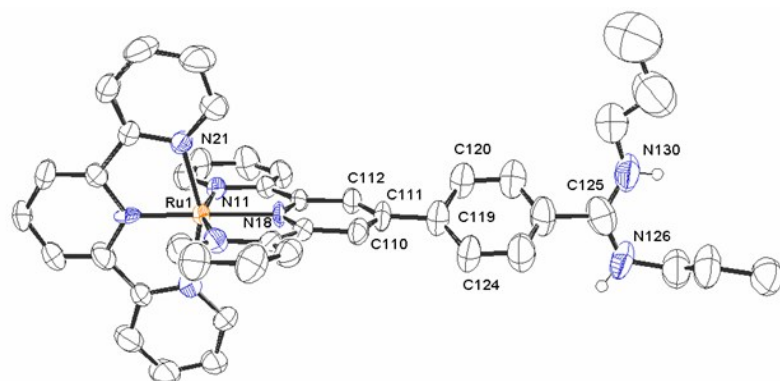


Figure S10. Spectrophotometric titration of **2** at: a) 486 nm; b) 665 nm.

The structure was deposited to the Cambridge Crystallographic Data Centre and was allocated the respective deposition number CCDC 1495788. Full details on data collection strategy and structure resolution can be found in the CIF file.



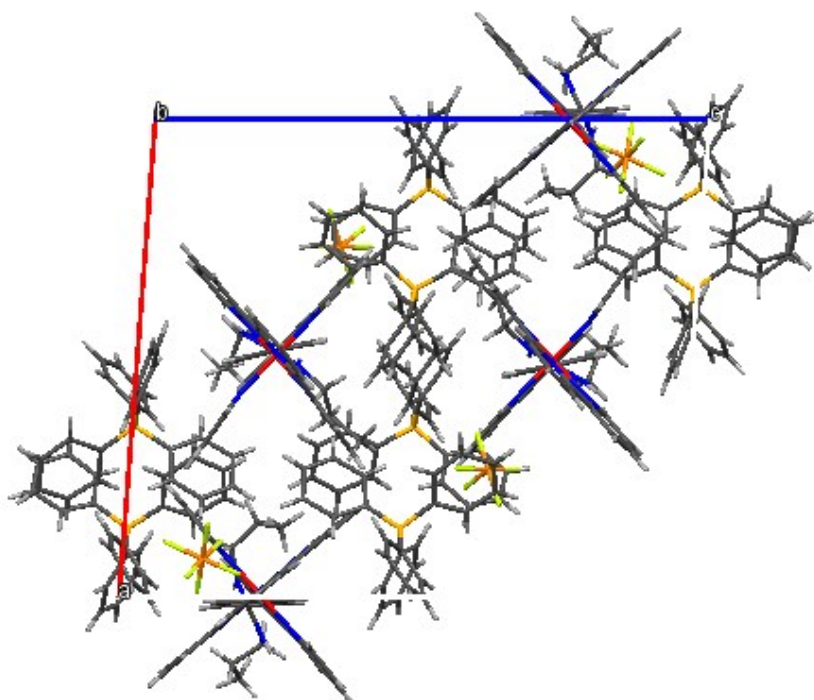
Selected Parameters

$$\begin{aligned} N_{11}\text{-Ru-}N_{21} &= 96.1(2)^\circ \\ N_{11}\text{-Ru-}N_{18} &= 79.9(2)^\circ \\ \text{Tpy-ph}_{(\text{torsion})} &= 44.0^\circ_{(\text{av})} \\ N_{18}\text{-Ru} &= 2.038(5) \text{ \AA} \\ N_{11}\text{-Ru} &= 2.083(6) \text{ \AA} \\ C_{125}\text{-}N_{130} &= 1.318(8) \text{ \AA} \\ C_{125}\text{-}N_{126} &= 1.313(8) \text{ \AA} \end{aligned}$$

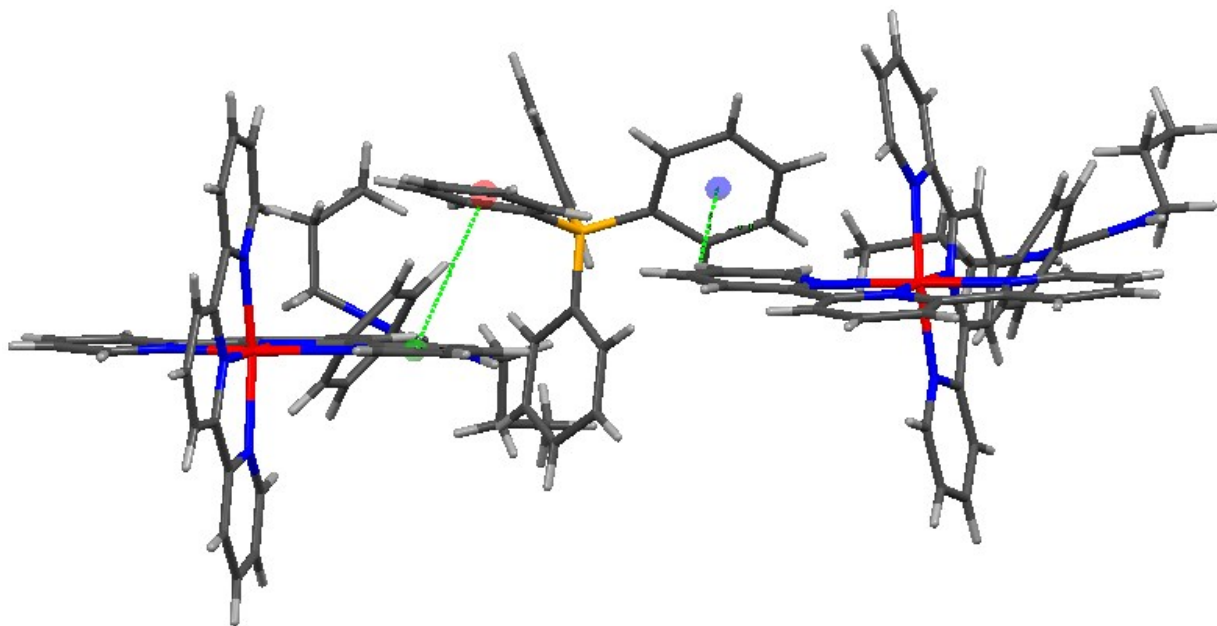
Figure S11. ORTEP of one of the unique complexes constituting the asymmetric unit of **1** (thermal ellipsoids drawn at 50 % probability). Hydrogens, solvent and counter-ions are omitted for clarity.

Table S1. Crystallographic data and parameters for **1** ([1-H](BPh₄)₂(PF₆))

Formula	C ₉₁ H ₈₁ B ₂ F ₆ N ₈ PRu
M_v (g/mol); F(000)	1554.30; 3224
T (K); wavelength (Å)	220(2); 1.54178
Crystal System	Monoclinic
Space Group	P2 ₁
Unit Cell: a (Å)	18.6928(8)
b (Å)	22.4646(7)
c (Å)	21.6484(8)
β (°)	94.336(3)
V (Å³); Z; d_{calcd} (g/cm³)	9064.7(6); 4; 1.139
θ range (°); completeness	2.05 to 72.81; 0.979
collected reflections; R_σ	72843; 0.0901
unique reflections; R_{int}	33931; 0.027
μ (mm⁻¹); Abs. Corr.	2.033; Multi-scan
R₁(F); wR(F²) [I > 2σ(I)]	0.0647; 0.1421
R_{1a}(F); wR(F²) (all data)	0.1058; 0.1564
GoF(F²)	0.857
Residual electron density (e⁻/Å³)	1.785; -0.571



(a)



(b)

Figure S12. Crystal structure of **1**. (a) Packing view of unit cell along b axis, showing alternance of cations and anions. (b) Capped-sticks view showing inter-annular interactions (“face-to-face” and “edge-to-face”) between phenyl rings of one BPh_4^- anion and of the two independent cations within the asymmetric unit.

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotr. displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.
 U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru (1)	4954 (1)	1315 (1)	2495 (1)	36 (1)
N (11)	4167 (3)	1481 (2)	3105 (3)	45 (2)
C (12)	3789 (4)	1093 (3)	3397 (4)	51 (2)
C (13)	3255 (4)	1261 (4)	3761 (4)	66 (2)
C (14)	3093 (5)	1859 (4)	3826 (4)	71 (2)
C (15)	3492 (4)	2273 (3)	3520 (3)	53 (2)
C (16)	4018 (4)	2085 (3)	3163 (3)	43 (2)
C (17)	4481 (4)	2473 (3)	2821 (3)	37 (2)
N (18)	4947 (3)	2222 (2)	2484 (2)	35 (2)
C (19)	5384 (4)	2483 (3)	2139 (3)	37 (2)
C (110)	5357 (4)	3117 (3)	2117 (3)	42 (2)
C (111)	4891 (4)	3428 (3)	2459 (3)	49 (2)
C (112)	4444 (4)	3103 (3)	2816 (3)	44 (2)
C (113)	5872 (4)	2099 (3)	1829 (3)	42 (2)
N (114)	5747 (3)	1493 (3)	1904 (3)	48 (2)
C (115)	6180 (4)	1114 (4)	1670 (4)	60 (2)
C (116)	6773 (4)	1283 (4)	1335 (4)	71 (2)
C (117)	6909 (4)	1891 (4)	1260 (4)	70 (2)
C (118)	6444 (4)	2295 (3)	1522 (3)	50 (2)
C (119)	4850 (4)	4084 (3)	2441 (4)	62 (2)
C (120)	4726 (4)	4411 (3)	2983 (4)	68 (2)
C (121)	4706 (4)	5018 (4)	2998 (5)	81 (2)
C (122)	4848 (5)	5322 (3)	2450 (5)	79 (3)
C (123)	5010 (5)	5016 (4)	1924 (4)	84 (3)
C (124)	4991 (4)	4409 (3)	1923 (4)	66 (2)
C (125)	4855 (5)	6012 (4)	2442 (4)	85 (3)
N (126)	4528 (4)	6264 (3)	1952 (3)	84 (2)
C (127)	4517 (4)	6898 (3)	1832 (4)	92 (3)
C (128)	5198 (4)	7121 (3)	1655 (5)	93 (3)
C (129)	5215 (5)	7791 (3)	1517 (4)	95 (3)
N (130)	5158 (4)	6314 (3)	2914 (3)	85 (2)
C (131)	5654 (5)	6104 (4)	3406 (4)	104 (3)
C (132)	6231 (6)	6524 (5)	3574 (6)	149 (5)
C (133)	6728 (7)	6253 (6)	4130 (6)	189 (6)
N (21)	5763 (3)	1107 (2)	3171 (3)	37 (1)
C (22)	6222 (4)	1489 (4)	3469 (4)	55 (2)
C (23)	6783 (4)	1313 (5)	3872 (4)	72 (3)
C (24)	6910 (4)	687 (4)	3955 (4)	66 (3)
C (25)	6434 (4)	297 (3)	3642 (4)	56 (2)
C (26)	5876 (4)	511 (3)	3255 (3)	42 (2)
C (27)	5356 (4)	115 (3)	2894 (3)	46 (2)
N (28)	4906 (3)	453 (3)	2506 (2)	42 (2)
C (29)	4392 (4)	149 (4)	2135 (4)	53 (2)
C (210)	4321 (5)	-441 (3)	2163 (4)	67 (3)
C (211)	4769 (5)	-782 (4)	2562 (4)	72 (3)
C (212)	5304 (4)	-479 (3)	2929 (4)	63 (2)
C (213)	3956 (4)	578 (3)	1745 (3)	42 (2)
N (214)	4148 (3)	1163 (3)	1808 (3)	43 (2)

C(215)	3778(4)	1573(3)	1462(3)	52(2)
C(216)	3228(4)	1429(4)	1036(4)	59(2)
C(217)	3031(5)	827(4)	959(4)	72(3)
C(218)	3401(5)	409(4)	1317(4)	64(3)
Ru(3)	10077(1)	61(1)	7499(1)	42(1)
N(31)	9263(3)	208(2)	6824(3)	45(2)
C(32)	8890(4)	-194(3)	6481(3)	48(2)
C(33)	8340(4)	-39(4)	6062(4)	63(2)
C(34)	8162(4)	541(3)	5966(4)	56(2)
C(35)	8546(4)	974(3)	6303(4)	52(2)
C(36)	9115(4)	790(3)	6726(3)	44(2)
C(37)	9544(4)	1198(3)	7095(3)	36(2)
N(38)	10044(3)	967(3)	7487(3)	48(2)
C(39)	10506(4)	1234(3)	7879(3)	38(2)
C(310)	10473(4)	1870(3)	7907(3)	51(2)
C(311)	9960(4)	2164(4)	7507(3)	50(2)
C(312)	9509(4)	1833(3)	7087(3)	49(2)
C(313)	10993(4)	866(3)	8266(3)	44(2)
N(314)	10901(3)	267(2)	8172(3)	40(2)
C(315)	11320(4)	-108(3)	8514(3)	51(2)
C(316)	11877(4)	105(4)	8930(3)	51(2)
C(317)	11969(5)	682(4)	9006(4)	64(2)
C(318)	11542(4)	1078(3)	8676(3)	46(2)
C(319)	9917(3)	2823(3)	7516(3)	49(2)
C(320)	9873(4)	3098(3)	8092(4)	66(2)
C(321)	9803(4)	3710(3)	8130(4)	72(2)
C(322)	9817(4)	4047(3)	7598(4)	70(2)
C(323)	9865(5)	3778(4)	7032(4)	88(3)
C(324)	9920(4)	3157(3)	6984(4)	64(2)
C(325)	9744(5)	4710(3)	7645(5)	103(3)
N(326)	9159(4)	4947(3)	7373(5)	138(4)
C(327)	8999(6)	5576(4)	7340(6)	144(5)
C(328)	8582(8)	5732(5)	7868(6)	177(6)
C(329)	8284(9)	6382(6)	7721(8)	272(9)
N(330)	10285(4)	5044(4)	7878(4)	119(3)
C(331)	11009(5)	4844(4)	8046(6)	127(4)
C(332)	11529(8)	4928(8)	7600(8)	252(10)
C(333)	11450(13)	5487(9)	7184(10)	338(14)
N(41)	9344(3)	-105(3)	8168(3)	53(2)
C(42)	9029(5)	301(4)	8489(4)	79(3)
C(43)	8597(7)	162(6)	8922(6)	127(4)
C(44)	8450(7)	-453(6)	9035(6)	124(4)
C(45)	8799(5)	-860(4)	8703(5)	79(3)
C(46)	9254(5)	-688(4)	8272(4)	58(2)
C(47)	9642(5)	-1104(4)	7914(4)	57(2)
N(48)	10075(3)	-797(4)	7511(3)	52(2)
C(49)	10476(4)	-1127(4)	7129(4)	55(2)
C(410)	10449(5)	-1722(4)	7107(5)	75(3)
C(411)	10062(5)	-2004(6)	7504(5)	92(4)
C(412)	9650(5)	-1701(4)	7924(5)	78(3)
C(413)	10876(4)	-722(3)	6741(4)	50(2)
N(414)	10797(3)	-128(3)	6845(3)	48(2)
C(415)	11152(5)	251(4)	6517(4)	63(2)
C(416)	11589(5)	73(5)	6076(4)	85(3)
C(417)	11677(5)	-542(5)	5957(5)	87(3)
C(418)	11307(5)	-926(4)	6317(4)	75(3)
B(5)	3574(4)	8832(3)	9948(4)	40(2)

C (511)	3085 (4)	8799 (3)	9272 (3)	43 (2)
C (512)	2439 (4)	8477 (3)	9217 (4)	51 (2)
C (513)	2053 (4)	8386 (3)	8654 (4)	61 (2)
C (514)	2311 (5)	8635 (4)	8107 (4)	69 (3)
C (515)	2929 (5)	8953 (4)	8142 (4)	73 (3)
C (516)	3324 (4)	9023 (3)	8742 (3)	50 (2)
C (521)	3069 (4)	8806 (3)	10529 (4)	47 (2)
C (522)	3294 (5)	8482 (4)	11102 (4)	58 (2)
C (523)	2888 (5)	8514 (4)	11584 (4)	77 (3)
C (524)	2246 (6)	8838 (5)	11602 (5)	85 (3)
C (525)	2054 (5)	9163 (4)	11064 (5)	75 (3)
C (526)	2434 (4)	9148 (4)	10539 (4)	55 (2)
C (531)	4039 (4)	9462 (3)	10050 (4)	49 (2)
C (532)	4593 (4)	9495 (4)	10501 (4)	58 (2)
C (533)	4963 (5)	10005 (5)	10642 (4)	74 (3)
C (534)	4807 (5)	10536 (5)	10303 (5)	82 (3)
C (535)	4274 (5)	10521 (4)	9854 (4)	74 (3)
C (536)	3886 (4)	9988 (4)	9740 (4)	58 (2)
C (541)	4140 (4)	8268 (3)	9913 (3)	50 (2)
C (542)	4821 (4)	8330 (3)	9699 (4)	57 (2)
C (543)	5271 (5)	7848 (4)	9643 (5)	80 (3)
C (544)	5071 (6)	7269 (4)	9772 (5)	78 (3)
C (545)	4373 (5)	7196 (3)	9967 (4)	73 (3)
C (546)	3925 (4)	7686 (3)	10039 (3)	52 (2)
B (6)	6444 (4)	8790 (3)	5084 (4)	39 (2)
C (611)	6049 (4)	9443 (3)	5067 (4)	52 (2)
C (612)	6314 (5)	9946 (4)	5367 (4)	76 (3)
C (613)	5958 (6)	10502 (5)	5295 (6)	101 (4)
C (614)	5346 (6)	10559 (5)	4922 (6)	94 (4)
C (615)	5073 (5)	10066 (5)	4603 (5)	92 (3)
C (616)	5417 (5)	9527 (4)	4682 (4)	66 (3)
C (621)	6851 (4)	8762 (3)	4453 (4)	51 (2)
C (622)	7494 (5)	9055 (4)	4380 (4)	66 (2)
C (623)	7816 (6)	9092 (5)	3821 (5)	90 (3)
C (624)	7498 (8)	8802 (6)	3313 (5)	114 (4)
C (625)	6849 (6)	8497 (4)	3369 (5)	94 (3)
C (626)	6549 (5)	8491 (3)	3896 (4)	61 (2)
C (631)	7037 (4)	8694 (3)	5705 (4)	50 (2)
C (632)	6903 (5)	8928 (4)	6264 (4)	65 (2)
C (633)	7388 (7)	8804 (5)	6811 (5)	97 (4)
C (634)	7961 (6)	8417 (6)	6735 (7)	113 (5)
C (635)	8096 (5)	8204 (5)	6175 (5)	93 (4)
C (636)	7622 (4)	8342 (4)	5669 (4)	62 (2)
C (641)	5861 (4)	8250 (3)	5166 (3)	50 (2)
C (642)	5962 (4)	7668 (3)	4964 (3)	59 (2)
C (643)	5483 (5)	7207 (3)	5061 (4)	75 (3)
C (644)	4894 (5)	7300 (4)	5375 (4)	80 (3)
C (645)	4791 (5)	7866 (4)	5615 (4)	76 (3)
C (646)	5264 (4)	8331 (4)	5497 (4)	62 (2)
B (7)	8565 (5)	7680 (4)	59 (5)	56 (3)
C (711)	8111 (4)	7656 (3)	660 (4)	52 (2)
C (712)	7479 (5)	7343 (4)	654 (4)	60 (2)
C (713)	7077 (5)	7262 (4)	1163 (5)	77 (3)
C (714)	7360 (6)	7488 (5)	1711 (5)	84 (3)
C (715)	7936 (6)	7799 (4)	1752 (5)	77 (3)
C (716)	8312 (5)	7874 (4)	1216 (5)	71 (3)
C (721)	9168 (4)	8206 (3)	54 (4)	56 (2)

C (722)	9064 (5)	8774 (4)	298 (4)	77 (3)
C (723)	9563 (6)	9243 (4)	253 (5)	95 (3)
C (724)	10175 (6)	9147 (5)	-29 (5)	96 (4)
C (725)	10304 (5)	8616 (4)	-304 (5)	81 (3)
C (726)	9799 (5)	8154 (4)	-244 (4)	72 (3)
C (731)	8056 (5)	7779 (4)	-580 (4)	68 (3)
C (732)	7458 (5)	8152 (5)	-588 (5)	101 (4)
C (733)	7020 (6)	8321 (5)	-1112 (6)	110 (4)
C (734)	7215 (7)	8039 (7)	-1642 (7)	120 (5)
C (735)	7801 (6)	7714 (5)	-1719 (5)	105 (4)
C (736)	8201 (6)	7581 (4)	-1153 (5)	92 (3)
C (741)	8979 (4)	7015 (3)	62 (3)	47 (2)
C (742)	8698 (5)	6507 (4)	-253 (4)	69 (3)
C (743)	9027 (6)	5971 (4)	-195 (5)	85 (3)
C (744)	9670 (6)	5889 (4)	181 (5)	84 (3)
C (745)	9960 (5)	6369 (4)	493 (4)	67 (2)
C (746)	9606 (5)	6924 (4)	433 (4)	56 (2)
B (8)	8568 (5)	2472 (4)	4972 (5)	54 (3)
C (811)	9034 (4)	1852 (3)	5020 (4)	48 (2)
C (812)	8800 (4)	1325 (4)	4728 (4)	57 (2)
C (813)	9186 (5)	801 (4)	4798 (5)	81 (3)
C (814)	9807 (6)	777 (4)	5205 (5)	80 (3)
C (815)	10039 (5)	1276 (4)	5489 (4)	70 (2)
C (816)	9657 (4)	1803 (4)	5413 (4)	54 (2)
C (821)	8108 (4)	2558 (3)	4328 (4)	53 (2)
C (822)	7468 (5)	2895 (4)	4251 (4)	70 (3)
C (823)	7100 (5)	3008 (4)	3672 (5)	82 (3)
C (824)	7324 (6)	2768 (5)	3169 (5)	87 (3)
C (825)	7949 (5)	2417 (5)	3180 (5)	85 (3)
C (826)	8327 (5)	2320 (4)	3759 (5)	78 (3)
C (831)	9120 (4)	3060 (3)	5013 (4)	55 (2)
C (832)	9769 (5)	3065 (4)	4754 (4)	70 (3)
C (833)	10233 (5)	3553 (4)	4752 (5)	90 (3)
C (834)	10039 (6)	4058 (5)	5031 (6)	93 (3)
C (835)	9405 (6)	4095 (4)	5278 (5)	86 (3)
C (836)	8937 (4)	3605 (3)	5292 (4)	64 (2)
C (841)	8050 (4)	2436 (3)	5545 (4)	51 (2)
C (842)	7440 (4)	2102 (4)	5510 (4)	61 (2)
C (843)	7007 (5)	1996 (4)	5984 (4)	76 (3)
C (844)	7212 (5)	2255 (4)	6568 (5)	74 (3)
C (845)	7804 (5)	2607 (4)	6641 (4)	68 (2)
C (846)	8221 (4)	2675 (3)	6136 (4)	56 (2)
P (1)	2663 (1)	9481 (1)	3520 (2)	101 (1)
F (11)	3065 (3)	8997 (3)	3110 (3)	129 (2)
F (12)	2676 (3)	9024 (2)	4078 (3)	111 (2)
F (13)	3427 (3)	9735 (2)	3770 (3)	133 (2)
F (14)	2660 (4)	9944 (3)	2969 (4)	181 (3)
F (15)	1907 (3)	9224 (2)	3262 (3)	140 (2)
F (16)	2280 (4)	9941 (3)	3906 (4)	165 (3)
P (2)	790 (2)	6599 (2)	8548 (2)	133 (1)
F (21)	474 (4)	6395 (3)	7886 (4)	168 (3)
F (22)	1496 (4)	6209 (4)	8502 (4)	196 (3)
F (23)	1166 (5)	7139 (4)	8223 (5)	211 (4)
F (24)	101 (5)	6982 (4)	8607 (5)	221 (4)
F (25)	412 (5)	6038 (3)	8807 (4)	204 (4)
F (26)	1138 (6)	6765 (4)	9237 (4)	226 (4)

Table S3. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.

	x	y	z	U_{eq}
H(12)	3889	685	3354	61
H(13)	2999	970	3966	80
H(14)	2724	1980	4070	85
H(15)	3399	2682	3560	64
H(110)	5661	3325	1866	50
H(112)	4117	3301	3054	53
H(115)	6097	705	1727	72
H(116)	7066	994	1167	85
H(117)	7296	2023	1043	84
H(118)	6527	2706	1487	60
H(120)	4654	4200	3348	81
H(121)	4602	5225	3358	97
H(123)	5132	5225	1571	101
H(124)	5077	4206	1556	79
H(126)	4301	6033	1680	101
H(12A)	4146	6985	1500	110
H(12B)	4389	7108	2205	110
H(12C)	5326	6904	1287	111
H(12D)	5566	7033	1990	111
H(12E)	4856	7884	1183	143
H(12F)	5686	7900	1394	143
H(12G)	5113	8012	1885	143
H(130)	5044	6689	2929	102
H(13A)	5864	5728	3279	125
H(13B)	5391	6024	3772	125
H(13C)	6030	6905	3699	179
H(13D)	6514	6596	3218	179
H(13E)	6926	6572	4391	283
H(13F)	7115	6029	3967	283
H(13G)	6446	5991	4372	283
H(22)	6155	1898	3398	66
H(23)	7077	1595	4088	87
H(24)	7301	546	4212	79
H(25)	6493	-116	3695	68
H(210)	3961	-630	1907	80
H(211)	4717	-1197	2587	86
H(212)	5627	-693	3199	75
H(215)	3903	1976	1517	62
H(216)	2986	1728	798	70
H(217)	2654	715	670	86
H(218)	3280	5	1272	77
H(32)	9009	-599	6530	58
H(33)	8081	-337	5837	76
H(34)	7785	647	5675	67
H(35)	8431	1379	6252	63
H(310)	10786	2085	8185	61
H(312)	9186	2028	6802	59
H(315)	11241	-520	8477	61
H(316)	12183	-164	9153	62

H(317)	12334	823	9291	77
H(318)	11617	1490	8725	55
H(320)	9892	2866	8454	79
H(321)	9747	3893	8514	87
H(323)	9862	4013	6672	106
H(324)	9957	2974	6598	77
H(326)	8842	4705	7198	166
H(32A)	8721	5668	6949	173
H(32B)	9445	5807	7357	173
H(32C)	8889	5728	8256	212
H(32D)	8187	5451	7904	212
H(32E)	8664	6627	7577	407
H(32F)	8114	6554	8093	407
H(32G)	7891	6360	7402	407
H(330)	10195	5419	7935	142
H(33A)	11182	5050	8428	153
H(33B)	10991	4418	8141	153
H(33C)	11517	4578	7331	302
H(33D)	12005	4941	7824	302
H(33E)	10948	5548	7052	507
H(33F)	11721	5432	6823	507
H(33G)	11632	5832	7415	507
H(42)	9114	705	8408	95
H(43)	8389	462	9153	152
H(44)	8127	-570	9325	149
H(45)	8725	-1267	8771	95
H(410)	10698	-1935	6817	89
H(411)	10063	-2422	7506	110
H(412)	9388	-1913	8205	93
H(415)	11102	661	6591	76
H(416)	11831	357	5851	102
H(417)	11968	-680	5652	105
H(418)	11358	-1339	6265	90
H(512)	2262	8317	9577	61
H(513)	1627	8163	8633	74
H(514)	2052	8578	7722	83
H(515)	3098	9125	7785	88
H(516)	3761	9231	8764	60
H(522)	3718	8256	11129	70
H(523)	3045	8300	11942	92
H(524)	1969	8836	11947	102
H(525)	1644	9406	11059	90
H(526)	2268	9367	10187	66
H(532)	4723	9147	10724	70
H(533)	5326	10006	10967	88
H(534)	5069	10887	10390	98
H(535)	4158	10863	9616	88
H(536)	3501	9992	9434	70
H(542)	4979	8711	9590	69
H(543)	5733	7916	9512	97
H(544)	5382	6945	9732	93
H(545)	4206	6811	10049	88
H(546)	3466	7623	10177	62
H(612)	6741	9920	5625	91
H(613)	6150	10837	5509	122
H(614)	5110	10928	4881	113
H(615)	4656	10099	4335	110

H(616)	5219	9196	4465	79
H(622)	7727	9239	4729	80
H(623)	8240	9312	3792	108
H(624)	7712	8806	2934	137
H(625)	6628	8296	3025	113
H(626)	6106	8296	3909	73
H(632)	6498	9169	6300	78
H(633)	7317	8977	7197	116
H(634)	8259	8304	7084	136
H(635)	8502	7967	6127	111
H(636)	7712	8183	5281	75
H(642)	6372	7583	4754	71
H(643)	5571	6826	4904	91
H(644)	4565	6992	5431	96
H(645)	4403	7938	5856	91
H(646)	5171	8712	5649	74
H(712)	7305	7170	277	72
H(713)	6634	7062	1130	92
H(714)	7125	7414	2072	101
H(715)	8105	7972	2130	92
H(716)	8738	8097	1257	85
H(722)	8645	8847	500	92
H(723)	9470	9620	418	114
H(724)	10518	9453	-35	115
H(725)	10712	8559	-525	97
H(726)	9898	7783	-419	86
H(732)	7337	8304	-205	121
H(733)	6639	8593	-1105	133
H(734)	6893	8081	-1994	144
H(735)	7935	7588	-2108	126
H(736)	8604	7333	-1175	110
H(742)	8272	6542	-511	82
H(743)	8821	5643	-412	102
H(744)	9891	5514	215	101
H(745)	10389	6331	745	81
H(746)	9807	7250	657	67
H(812)	8368	1327	4477	68
H(813)	9031	460	4574	97
H(814)	10056	417	5275	96
H(815)	10469	1270	5745	84
H(816)	9825	2141	5635	65
H(822)	7278	3051	4607	84
H(823)	6693	3256	3645	99
H(824)	7059	2833	2788	105
H(825)	8108	2253	2815	102
H(826)	8745	2087	3772	94
H(832)	9912	2713	4563	84
H(833)	10667	3530	4561	108
H(834)	10351	4387	5054	111
H(835)	9268	4459	5446	104
H(836)	8506	3639	5486	77
H(842)	7302	1927	5125	73
H(843)	6592	1761	5923	91
H(844)	6937	2182	6906	89
H(845)	7929	2799	7019	82
H(846)	8647	2897	6197	68

Table S4. Anisotropic parameters ($\text{\AA}^2 \times 10^3$) for **1**.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Ru (1)	47 (1)	22 (1)	39 (1)	1 (1)	-9 (1)	-4 (1)
N (11)	62 (4)	29 (3)	41 (3)	5 (2)	-9 (3)	-12 (3)
C (12)	52 (5)	43 (4)	58 (5)	2 (3)	6 (4)	-9 (3)
C (13)	72 (5)	47 (4)	81 (6)	11 (4)	16 (4)	-18 (4)
C (14)	75 (6)	60 (5)	81 (6)	-11 (4)	34 (5)	-6 (4)
C (15)	62 (5)	41 (4)	57 (5)	-5 (3)	14 (4)	-6 (3)
C (16)	54 (4)	30 (3)	45 (4)	1 (3)	-9 (4)	-6 (3)
C (17)	52 (4)	24 (3)	34 (4)	4 (3)	1 (3)	-13 (3)
N (18)	54 (4)	11 (2)	42 (4)	-1 (2)	8 (3)	1 (2)
C (19)	45 (4)	30 (4)	35 (4)	5 (3)	1 (3)	0 (3)
C (110)	41 (4)	30 (4)	54 (4)	7 (3)	1 (4)	-7 (3)
C (111)	58 (5)	21 (3)	67 (5)	6 (3)	5 (4)	-2 (3)
C (112)	52 (4)	27 (3)	52 (4)	0 (3)	0 (4)	2 (3)
C (113)	47 (4)	38 (4)	40 (4)	9 (3)	-4 (3)	-2 (3)
N (114)	55 (4)	38 (3)	50 (4)	-7 (3)	-12 (3)	5 (3)
C (115)	56 (4)	50 (4)	72 (6)	-2 (4)	-10 (4)	5 (3)
C (116)	68 (5)	62 (5)	83 (6)	1 (5)	9 (4)	9 (4)
C (117)	60 (5)	66 (5)	85 (6)	18 (4)	17 (4)	-5 (4)
C (118)	46 (4)	49 (4)	54 (4)	9 (3)	0 (4)	-5 (3)
C (119)	72 (5)	37 (3)	81 (5)	6 (4)	22 (4)	-2 (3)
C (120)	79 (5)	44 (4)	82 (6)	6 (4)	23 (5)	1 (4)
C (121)	84 (5)	53 (4)	108 (7)	9 (5)	14 (5)	-5 (4)
C (122)	97 (6)	42 (4)	100 (7)	-6 (5)	30 (6)	8 (4)
C (123)	105 (6)	55 (5)	95 (6)	2 (5)	22 (5)	-12 (5)
C (124)	78 (5)	40 (4)	82 (6)	8 (4)	30 (4)	1 (3)
C (125)	92 (7)	59 (5)	105 (7)	-25 (5)	20 (6)	4 (5)
N (126)	107 (6)	40 (3)	106 (6)	23 (4)	6 (5)	8 (4)
C (127)	94 (6)	59 (5)	121 (8)	7 (5)	-4 (6)	-6 (5)
C (128)	79 (6)	52 (5)	146 (8)	17 (5)	-2 (6)	1 (4)
C (129)	93 (6)	67 (5)	121 (8)	11 (5)	-23 (6)	-1 (5)
N (130)	114 (6)	41 (4)	100 (6)	8 (4)	11 (5)	0 (4)
C (131)	122 (8)	77 (6)	113 (8)	5 (6)	5 (7)	-13 (6)
C (132)	148 (10)	127 (9)	168 (11)	-28 (9)	-16 (9)	-13 (8)
C (133)	165 (11)	212 (13)	186 (12)	-35 (11)	-2 (10)	29 (11)
N (21)	36 (3)	33 (3)	41 (3)	6 (2)	-5 (3)	-3 (2)
C (22)	56 (5)	54 (5)	54 (5)	0 (4)	-4 (4)	-7 (3)
C (23)	59 (5)	87 (6)	68 (5)	9 (5)	-21 (4)	-20 (5)
C (24)	54 (5)	80 (6)	61 (5)	28 (5)	-19 (4)	-8 (4)
C (25)	66 (5)	39 (4)	63 (5)	14 (4)	-6 (4)	-3 (3)
C (26)	50 (4)	31 (4)	44 (4)	5 (3)	-2 (4)	1 (3)
C (27)	49 (4)	36 (4)	50 (4)	0 (3)	-12 (3)	-8 (3)
N (28)	38 (4)	53 (4)	31 (3)	4 (3)	-21 (3)	3 (3)
C (29)	49 (4)	43 (4)	66 (5)	-10 (4)	-7 (4)	-14 (4)

C(210)	89(6)	38(4)	69(5)	-14(4)	-17(5)	-12(4)
C(211)	119(7)	22(4)	71(6)	3(3)	-11(5)	-16(4)
C(212)	77(5)	30(4)	77(6)	8(4)	-15(5)	6(4)
C(213)	47(4)	32(4)	46(4)	-4(3)	-9(4)	-3(3)
N(214)	49(4)	38(4)	43(4)	-3(3)	2(3)	1(3)
C(215)	58(5)	44(4)	51(5)	5(3)	-12(4)	12(3)
C(216)	63(5)	54(5)	55(5)	-6(4)	-19(4)	13(4)
C(217)	64(5)	78(6)	69(6)	-17(5)	-29(5)	23(5)
C(218)	66(6)	64(5)	59(5)	-16(4)	-7(5)	3(4)
Ru(3)	50(1)	28(1)	46(1)	-3(1)	-10(1)	5(1)
N(31)	55(4)	30(3)	48(4)	-3(3)	-5(3)	4(3)
C(32)	53(4)	33(4)	54(5)	-3(3)	-17(4)	-9(3)
C(33)	65(5)	60(5)	60(5)	2(4)	-23(4)	-24(4)
C(34)	49(4)	46(4)	70(5)	7(4)	-21(4)	-2(3)
C(35)	50(4)	42(4)	61(5)	11(3)	-15(4)	-1(3)
C(36)	45(4)	38(4)	46(4)	5(3)	-6(4)	-7(3)
C(37)	47(4)	24(3)	36(4)	3(3)	-8(3)	6(3)
N(38)	61(4)	20(3)	62(4)	-8(3)	8(4)	-5(3)
C(39)	48(4)	28(4)	37(4)	-2(3)	-1(3)	4(3)
C(310)	61(5)	41(4)	47(4)	-1(3)	-8(4)	8(3)
C(311)	53(4)	35(4)	59(5)	4(3)	-9(4)	-1(3)
C(312)	61(4)	33(4)	52(4)	0(3)	-11(4)	-1(3)
C(313)	50(4)	39(4)	45(4)	-9(3)	7(4)	3(3)
N(314)	42(3)	38(3)	39(3)	-3(3)	-9(3)	5(2)
C(315)	60(5)	37(4)	55(5)	-2(3)	-7(4)	20(3)
C(316)	55(4)	44(4)	54(4)	1(4)	-5(4)	15(4)
C(317)	71(6)	57(5)	62(5)	-9(4)	-22(5)	2(4)
C(318)	43(4)	48(4)	44(4)	-7(3)	-17(4)	2(3)
C(319)	62(4)	26(3)	57(4)	-1(3)	-8(3)	-7(3)
C(320)	77(5)	42(4)	73(5)	-3(3)	-27(4)	1(3)
C(321)	86(6)	58(5)	68(5)	-12(4)	-25(5)	21(4)
C(322)	81(5)	39(4)	84(6)	-12(4)	-32(5)	11(3)
C(323)	105(7)	60(5)	95(7)	13(5)	-27(6)	-12(5)
C(324)	72(5)	52(4)	65(5)	2(4)	-19(4)	-3(4)
C(325)	101(6)	45(4)	155(9)	-23(5)	-53(6)	8(4)
N(326)	114(6)	58(5)	228(10)	-15(6)	-87(7)	19(4)
C(327)	128(9)	99(8)	198(12)	-45(8)	-33(9)	44(7)
C(328)	196(12)	133(10)	199(13)	-62(10)	1(11)	28(9)
C(329)	288(16)	215(15)	305(17)	-52(14)	-24(14)	51(13)
N(330)	119(6)	55(4)	170(8)	-14(5)	-68(6)	13(5)
C(331)	108(8)	82(7)	185(11)	-32(7)	-38(8)	8(6)
C(332)	254(16)	263(17)	240(16)	-50(14)	34(14)	37(14)
C(333)	350(20)	330(20)	340(20)	-44(17)	26(16)	14(16)
N(41)	63(4)	41(4)	56(4)	7(3)	18(3)	8(3)
C(42)	112(8)	50(5)	81(6)	8(4)	34(6)	4(5)
C(43)	155(10)	90(8)	144(10)	6(7)	71(8)	-8(7)
C(44)	136(9)	109(9)	137(10)	12(8)	72(8)	-21(7)
C(45)	84(6)	62(5)	89(7)	22(5)	-3(6)	-1(5)
C(46)	61(5)	52(5)	60(5)	9(4)	-4(4)	-8(4)
C(47)	53(5)	49(5)	66(6)	6(4)	-21(5)	3(4)
N(48)	38(4)	66(5)	47(4)	-2(3)	-25(4)	3(3)
C(49)	45(4)	48(5)	70(6)	-18(4)	-18(4)	14(4)
C(410)	81(6)	45(5)	97(7)	-12(5)	1(6)	-8(4)
C(411)	106(9)	50(6)	118(10)	-10(6)	-3(8)	13(5)
C(412)	90(7)	53(5)	88(7)	12(5)	-9(6)	2(5)
C(413)	51(4)	47(4)	51(5)	-18(3)	-5(4)	15(3)
N(414)	46(4)	38(3)	58(4)	-6(3)	-16(3)	3(3)

C(415)	66(6)	52(5)	70(6)	-8(4)	2(5)	8(4)
C(416)	77(6)	96(7)	82(6)	-10(6)	12(5)	-3(6)
C(417)	78(6)	95(7)	91(7)	-21(6)	20(5)	4(5)
C(418)	65(5)	72(5)	88(7)	-31(5)	-1(5)	10(4)
B(5)	47(4)	24(3)	49(5)	-4(3)	4(4)	1(3)
C(511)	46(4)	39(4)	45(4)	-6(3)	0(3)	4(3)
C(512)	53(4)	40(4)	59(5)	-16(3)	-6(4)	3(3)
C(513)	45(4)	54(5)	84(6)	-24(4)	0(4)	7(3)
C(514)	73(6)	74(6)	58(5)	-31(4)	-8(5)	24(4)
C(515)	102(7)	67(5)	52(5)	0(4)	17(5)	32(5)
C(516)	57(4)	50(4)	43(4)	1(3)	-2(4)	9(3)
C(521)	46(4)	48(4)	46(4)	-14(3)	-4(4)	-8(3)
C(522)	54(5)	62(5)	58(5)	-15(4)	2(4)	-4(4)
C(523)	75(6)	88(7)	66(6)	5(5)	1(5)	-11(5)
C(524)	79(6)	110(8)	67(6)	-14(6)	5(6)	-24(6)
C(525)	80(7)	75(6)	69(6)	-14(5)	6(5)	-5(5)
C(526)	54(5)	56(4)	56(5)	-13(4)	-2(4)	-3(4)
C(531)	53(5)	30(3)	65(5)	-12(3)	3(4)	7(3)
C(532)	57(5)	42(4)	74(6)	-8(4)	-6(5)	0(4)
C(533)	61(5)	64(5)	94(7)	-6(5)	-5(5)	-2(5)
C(534)	78(6)	63(6)	103(8)	-19(5)	1(6)	-21(5)
C(535)	98(7)	35(4)	86(6)	4(4)	-8(6)	-12(4)
C(536)	56(4)	46(4)	71(5)	-3(4)	4(4)	1(4)
C(541)	58(5)	38(4)	53(4)	-7(3)	-7(4)	4(3)
C(542)	55(5)	36(4)	83(6)	6(4)	17(4)	7(3)
C(543)	60(6)	67(6)	115(8)	-5(5)	10(6)	23(5)
C(544)	91(7)	40(4)	102(7)	-1(4)	4(6)	22(4)
C(545)	88(6)	40(4)	89(6)	4(4)	-11(5)	2(4)
C(546)	57(4)	37(3)	61(5)	-3(3)	1(4)	-8(3)
B(6)	43(4)	31(4)	44(5)	-3(3)	5(4)	-2(3)
C(611)	53(4)	43(4)	60(5)	7(4)	5(4)	-4(3)
C(612)	75(5)	47(5)	106(7)	1(5)	11(5)	-3(4)
C(613)	111(8)	53(5)	140(10)	-20(6)	15(7)	-7(5)
C(614)	91(8)	53(6)	142(10)	4(6)	23(7)	13(5)
C(615)	73(6)	81(7)	124(8)	36(7)	16(6)	17(6)
C(616)	67(6)	48(5)	81(6)	10(4)	2(5)	-2(4)
C(621)	56(4)	40(4)	57(5)	-1(3)	2(4)	5(3)
C(622)	80(6)	59(5)	61(6)	10(4)	15(5)	5(4)
C(623)	91(7)	86(7)	98(8)	15(6)	35(7)	5(5)
C(624)	168(11)	113(9)	66(7)	4(6)	32(8)	-11(8)
C(625)	123(8)	77(6)	81(7)	-5(6)	-6(7)	15(6)
C(626)	69(5)	54(5)	60(5)	-2(4)	2(4)	10(4)
C(631)	49(4)	48(4)	51(4)	19(3)	-5(4)	-12(3)
C(632)	82(6)	66(5)	46(5)	11(4)	-2(4)	-24(4)
C(633)	141(10)	93(7)	55(5)	5(5)	1(7)	-52(7)
C(634)	89(8)	128(9)	117(10)	63(8)	-34(8)	-33(7)
C(635)	59(5)	114(8)	104(8)	51(7)	-8(6)	-14(5)
C(636)	50(4)	68(5)	68(5)	25(4)	-2(4)	-4(4)
C(641)	59(5)	37(4)	52(4)	-3(3)	-10(4)	-5(3)
C(642)	66(5)	41(4)	72(5)	-3(4)	6(4)	-4(3)
C(643)	95(7)	41(4)	90(6)	5(4)	-2(6)	-22(4)
C(644)	86(6)	61(5)	92(7)	-4(5)	10(6)	-26(5)
C(645)	68(5)	76(6)	86(6)	5(5)	18(5)	-17(4)
C(646)	59(5)	54(4)	72(5)	-1(4)	5(4)	-14(4)
B(7)	58(5)	45(5)	63(6)	6(4)	-14(5)	3(4)
C(711)	65(5)	39(4)	52(5)	13(3)	-2(4)	3(3)
C(712)	72(6)	53(5)	54(5)	9(4)	5(5)	-4(4)

C(713)	64(6)	74(6)	94(8)	18(6)	13(6)	0(5)
C(714)	93(7)	85(7)	77(7)	18(6)	31(6)	31(6)
C(715)	86(7)	83(7)	60(6)	-7(5)	0(5)	23(5)
C(716)	68(6)	67(6)	76(6)	-1(5)	-3(5)	18(5)
C(721)	56(5)	44(4)	66(5)	17(4)	-12(4)	-6(3)
C(722)	76(5)	54(5)	99(7)	25(5)	-5(5)	-10(4)
C(723)	105(7)	48(5)	132(9)	6(5)	4(7)	-3(5)
C(724)	90(7)	82(7)	114(8)	24(6)	4(7)	-19(6)
C(725)	59(6)	69(6)	114(8)	25(6)	3(6)	-1(5)
C(726)	72(6)	52(5)	88(6)	16(4)	-13(5)	-1(4)
C(731)	67(5)	73(6)	63(5)	29(5)	-5(5)	-23(4)
C(732)	75(6)	106(8)	120(8)	76(7)	-6(6)	-10(5)
C(733)	81(7)	126(9)	121(9)	70(8)	-15(7)	-6(6)
C(734)	96(9)	157(11)	103(9)	66(9)	-18(8)	-48(8)
C(735)	105(8)	136(9)	71(7)	36(6)	-14(7)	-35(7)
C(736)	89(7)	85(7)	98(8)	44(6)	-11(6)	-38(5)
C(741)	58(5)	44(4)	38(4)	4(3)	-5(4)	-6(3)
C(742)	78(6)	67(6)	59(5)	2(4)	-3(5)	-16(4)
C(743)	105(7)	65(6)	82(7)	-7(5)	-5(6)	-17(5)
C(744)	116(8)	39(5)	102(8)	3(5)	44(7)	7(5)
C(745)	71(5)	52(5)	79(6)	13(4)	10(4)	13(5)
C(746)	66(6)	44(4)	57(5)	1(4)	0(4)	-2(4)
B(8)	56(5)	38(4)	65(6)	-2(4)	-13(5)	-6(4)
C(811)	49(4)	39(4)	56(5)	-6(3)	1(4)	-3(3)
C(812)	58(4)	37(4)	74(5)	-11(4)	-3(4)	-2(4)
C(813)	95(7)	49(5)	99(7)	-10(5)	6(6)	-13(5)
C(814)	90(7)	46(5)	105(7)	5(5)	9(6)	8(5)
C(815)	64(5)	53(5)	91(6)	12(5)	-1(5)	6(4)
C(816)	50(5)	48(4)	63(5)	-1(4)	-7(4)	1(4)
C(821)	53(4)	44(4)	60(5)	16(4)	-6(4)	-12(3)
C(822)	67(6)	61(5)	78(6)	19(4)	-13(5)	-3(4)
C(823)	76(6)	76(6)	90(7)	43(6)	-22(6)	-23(5)
C(824)	107(8)	89(7)	62(6)	23(6)	-15(6)	-36(6)
C(825)	91(7)	90(7)	76(7)	17(5)	10(6)	-40(5)
C(826)	92(7)	70(6)	72(6)	20(5)	-2(5)	-19(5)
C(831)	51(4)	38(4)	73(6)	2(4)	-3(4)	2(3)
C(832)	66(5)	48(5)	98(7)	11(5)	7(5)	4(4)
C(833)	68(6)	62(6)	138(9)	13(6)	3(6)	-10(5)
C(834)	73(6)	64(6)	138(9)	17(6)	-15(6)	-20(5)
C(835)	109(7)	45(5)	100(7)	10(5)	-26(6)	-2(5)
C(836)	74(5)	49(4)	66(5)	11(4)	-12(4)	-9(4)
C(841)	47(4)	49(4)	57(5)	10(3)	-2(4)	7(3)
C(842)	63(5)	60(5)	62(5)	0(4)	13(4)	-2(4)
C(843)	70(5)	77(6)	79(6)	-1(5)	2(5)	-11(4)
C(844)	79(6)	62(5)	84(7)	19(5)	25(5)	20(4)
C(845)	87(6)	59(5)	57(5)	9(4)	-5(5)	17(4)
C(846)	56(5)	49(4)	62(5)	4(4)	-11(4)	-1(3)
P(1)	83(2)	60(1)	154(3)	27(2)	-31(2)	-18(1)
F(11)	150(5)	105(4)	128(5)	9(4)	-12(4)	8(4)
F(12)	115(4)	82(3)	134(5)	25(3)	-2(4)	-34(3)
F(13)	140(5)	81(3)	171(6)	25(4)	-46(4)	-54(3)
F(14)	161(6)	152(6)	217(7)	89(5)	-80(5)	-44(5)
F(15)	110(4)	90(4)	208(7)	29(4)	-64(4)	-29(3)
F(16)	141(5)	107(5)	249(8)	-25(5)	32(5)	20(4)
P(2)	129(3)	80(2)	195(4)	-52(2)	43(3)	-24(2)
F(21)	181(6)	135(6)	180(7)	-43(5)	-44(6)	-26(5)
F(22)	135(6)	193(7)	261(9)	-28(7)	23(6)	-1(6)

F(23)	186(7)	152(7)	293(10)	31(7)	11(7)	-68(6)
F(24)	215(8)	155(7)	301(10)	-61(7)	75(8)	35(6)
F(25)	251(9)	142(6)	229(9)	-42(6)	92(7)	-68(6)
F(26)	291(10)	209(8)	177(7)	-87(7)	2(7)	-60(7)

Table S5. Bond lengths [\AA] and angles [$^\circ$] for **1**.

Ru(1)-N(28)	1.938(7)	C(22)-C(23)	1.37(1)
Ru(1)-N(18)	2.038(5)	C(23)-C(24)	1.435(13)
Ru(1)-N(214)	2.063(6)	C(24)-C(25)	1.389(10)
Ru(1)-N(114)	2.069(7)	C(25)-C(26)	1.374(9)
Ru(1)-N(21)	2.076(5)	C(26)-C(27)	1.493(9)
Ru(1)-N(11)	2.083(6)	C(27)-C(212)	1.339(10)
N(11)-C(12)	1.313(8)	C(27)-N(28)	1.373(8)
N(11)-C(16)	1.392(8)	N(28)-C(29)	1.384(8)
		C(29)-C(210)	1.335(11)
		C(29)-C(213)	1.483(10)
		C(210)-C(211)	1.388(10)
C(12)-C(13)	1.371(10)	C(211)-C(212)	1.406(10)
C(13)-C(14)	1.387(11)	C(213)-N(214)	1.365(8)
C(14)-C(15)	1.392(10)	C(213)-C(218)	1.392(10)
C(15)-C(16)	1.364(10)	N(214)-C(215)	1.346(8)
C(16)-C(17)	1.467(9)	C(215)-C(216)	1.368(10)
C(17)-N(18)	1.307(8)	C(216)-C(217)	1.409(12)
C(17)-C(112)	1.417(8)	C(217)-C(218)	1.371(11)
N(18)-C(19)	1.288(8)	Ru(3)-N(48)	1.930(8)
C(19)-C(110)	1.426(9)	Ru(3)-N(38)	2.035(6)
C(19)-C(113)	1.456(9)	Ru(3)-N(31)	2.055(6)
C(110)-C(111)	1.377(9)	Ru(3)-N(414)	2.070(7)
C(111)-C(112)	1.387(9)	Ru(3)-N(314)	2.090(5)
C(111)-C(119)	1.475(10)	Ru(3)-N(41)	2.100(6)
C(113)-C(118)	1.372(9)	N(31)-C(32)	1.332(7)
C(113)-N(114)	1.394(8)	N(31)-C(36)	1.350(8)
N(114)-C(115)	1.305(9)	C(32)-C(33)	1.365(9)
C(115)-C(116)	1.421(11)	C(33)-C(34)	1.356(11)
C(116)-C(117)	1.401(11)	C(34)-C(35)	1.383(10)
C(117)-C(118)	1.405(10)	C(35)-C(36)	1.412(9)
C(119)-C(124)	1.381(9)	C(36)-C(37)	1.424(9)
C(119)-C(120)	1.418(10)	C(37)-N(38)	1.320(8)
C(120)-C(121)	1.365(9)	C(37)-C(312)	1.426(9)
C(121)-C(122)	1.411(11)	N(38)-C(39)	1.311(8)
C(122)-C(123)	1.383(10)	C(39)-C(310)	1.431(9)
C(122)-C(125)	1.548(11)	C(39)-C(313)	1.448(9)
C(123)-C(124)	1.364(9)	C(310)-C(311)	1.408(9)
C(125)-N(126)	1.313(8)	C(311)-C(312)	1.405(9)
C(125)-N(130)	1.318(8)	C(311)-C(319)	1.483(10)
N(126)-C(127)	1.449(7)	C(313)-N(314)	1.370(8)
C(127)-C(128)	1.446(8)	C(313)-C(318)	1.390(9)
C(128)-C(129)	1.536(7)	N(314)-C(315)	1.336(8)
N(130)-C(131)	1.439(7)	C(315)-C(316)	1.409(9)
C(131)-C(132)	1.459(9)	C(316)-C(317)	1.316(11)
C(132)-C(133)	1.585(9)	C(317)-C(318)	1.36(1)
N(21)-C(22)	1.344(8)	C(319)-C(324)	1.374(9)
N(21)-C(26)	1.366(8)	C(319)-C(320)	1.398(9)

C (320) -C (321)	1.384 (9)	C (542) -C (543)	1.383 (11)
C (321) -C (322)	1.381 (10)	C (543) -C (544)	1.389 (12)
C (322) -C (323)	1.375 (11)	C (544) -C (545)	1.410 (12)
C (322) -C (325)	1.501 (10)	C (545) -C (546)	1.40 (1)
C (323) -C (324)	1.402 (10)	B (6) -C (621)	1.615 (11)
C (325) -N (326)	1.314 (8)	B (6) -C (611)	1.64 (1)
C (325) -N (330)	1.327 (9)	B (6) -C (641)	1.65 (1)
N (326) -C (327)	1.445 (8)	B (6) -C (631)	1.69 (1)
C (327) -C (328)	1.474 (9)	C (611) -C (612)	1.376 (11)
C (328) -C (329)	1.586 (10)	C (611) -C (616)	1.406 (11)
N (330) -C (331)	1.446 (7)	C (612) -C (613)	1.420 (13)
C (331) -C (332)	1.432 (9)	C (613) -C (614)	1.355 (14)
C (332) -C (333)	1.546 (10)	C (614) -C (615)	1.381 (14)
N (41) -C (42)	1.314 (10)	C (615) -C (616)	1.375 (12)
N (41) -C (46)	1.341 (9)	C (621) -C (622)	1.389 (10)
C (42) -C (43)	1.318 (12)	C (621) -C (626)	1.428 (10)
C (43) -C (44)	1.435 (15)	C (622) -C (623)	1.394 (12)
C (44) -C (45)	1.358 (13)	C (623) -C (624)	1.373 (14)
C (45) -C (46)	1.366 (11)	C (624) -C (625)	1.406 (14)
C (46) -C (47)	1.445 (11)	C (625) -C (626)	1.307 (12)
C (47) -C (412)	1.341 (12)	C (631) -C (636)	1.357 (10)
C (47) -N (48)	1.413 (10)	C (631) -C (632)	1.36 (1)
N (48) -C (49)	1.374 (9)	C (632) -C (633)	1.461 (12)
C (49) -C (410)	1.338 (11)	C (633) -C (634)	1.400 (15)
C (49) -C (413)	1.479 (11)	C (634) -C (635)	1.345 (15)
C (410) -C (411)	1.325 (13)	C (635) -C (636)	1.391 (11)
C (411) -C (412)	1.409 (13)	C (641) -C (646)	1.381 (10)
C (413) -C (418)	1.346 (11)	C (641) -C (642)	1.397 (9)
C (413) -N (414)	1.362 (9)	C (642) -C (643)	1.394 (10)
N (414) -C (415)	1.321 (10)	C (643) -C (644)	1.355 (12)
C (415) -C (416)	1.362 (11)	C (644) -C (645)	1.392 (12)
C (416) -C (417)	1.417 (13)	C (645) -C (646)	1.402 (10)
C (417) -C (418)	1.383 (12)	B (7) -C (711)	1.606 (12)
B (5) -C (521)	1.629 (11)	B (7) -C (731)	1.633 (11)
B (5) -C (541)	1.656 (10)	B (7) -C (721)	1.635 (11)
B (5) -C (531)	1.667 (10)	B (7) -C (741)	1.683 (11)
B (5) -C (511)	1.667 (10)	C (711) -C (716)	1.328 (11)
C (511) -C (516)	1.359 (9)	C (711) -C (712)	1.375 (10)
C (511) -C (512)	1.406 (9)	C (712) -C (713)	1.392 (11)
C (512) -C (513)	1.383 (10)	C (713) -C (714)	1.360 (13)
C (513) -C (514)	1.426 (11)	C (714) -C (715)	1.280 (12)
C (514) -C (515)	1.355 (11)	C (715) -C (716)	1.410 (12)
C (515) -C (516)	1.454 (10)	C (721) -C (726)	1.391 (12)
C (521) -C (526)	1.417 (10)	C (721) -C (722)	1.400 (11)
C (521) -C (522)	1.471 (10)	C (722) -C (723)	1.415 (11)
C (522) -C (523)	1.338 (11)	C (723) -C (724)	1.354 (14)
C (523) -C (524)	1.408 (12)	C (724) -C (725)	1.363 (14)
C (524) -C (525)	1.398 (12)	C (725) -C (726)	1.416 (12)
C (525) -C (526)	1.385 (11)	C (731) -C (736)	1.365 (13)
C (531) -C (532)	1.37 (1)	C (731) -C (732)	1.397 (12)
C (531) -C (536)	1.378 (10)	C (732) -C (733)	1.401 (12)
C (532) -C (533)	1.363 (11)	C (733) -C (734)	1.382 (16)
C (533) -C (534)	1.420 (13)	C (734) -C (735)	1.338 (16)
C (534) -C (535)	1.339 (12)	C (735) -C (736)	1.418 (12)
C (535) -C (536)	1.411 (11)	C (741) -C (746)	1.384 (10)
C (541) -C (542)	1.395 (10)	C (741) -C (742)	1.411 (10)
C (541) -C (546)	1.401 (9)	C (742) -C (743)	1.353 (12)

C (743) -C (744)	1.412 (13)	N (21) -RU1-N (11)	96.1 (2)
C (744) -C (745)	1.363 (13)	C (12) -N (11) -C (16)	119.0 (7)
C (745) -C (746)	1.414 (11)	C (12) -N (11) -RU1	128.1 (5)
B (8) -C (821)	1.595 (11)	C (16) -N (11) -RU1	112.8 (5)
B (8) -C (841)	1.632 (12)	N (11) -C (12) -C (13)	122.4 (7)
B (8) -C (811)	1.641 (11)	C (12) -C (13) -C (14)	120.0 (8)
B (8) -C (831)	1.674 (11)	C (13) -C (14) -C (15)	118.0 (8)
C (811) -C (816)	1.393 (10)	C (16) -C (15) -C (14)	119.8 (7)
C (811) -C (812)	1.396 (10)	C (15) -C (16) -N (11)	120.7 (7)
C (812) -C (813)	1.384 (11)	C (15) -C (16) -C (17)	125.4 (6)
C (813) -C (814)	1.404 (13)	N (11) -C (16) -C (17)	113.9 (7)
C (814) -C (815)	1.335 (13)	N (18) -C (17) -C (112)	117.5 (6)
C (815) -C (816)	1.386 (11)	N (18) -C (17) -C (16)	117.9 (6)
C (821) -C (822)	1.414 (10)	C (112) -C (17) -C (16)	124.6 (7)
C (821) -C (826)	1.430 (12)	C (19) -N (18) -C (17)	127.3 (6)
C (822) -C (823)	1.407 (11)	C (19) -N (18) -RU1	117.3 (5)
C (823) -C (824)	1.312 (13)	C (17) -N (18) -RU1	115.4 (4)
C (824) -C (825)	1.408 (13)	N (18) -C (19) -C (110)	116.9 (7)
C (825) -C (826)	1.408 (12)	N (18) -C (19) -C (113)	116.4 (6)
C (831) -C (832)	1.376 (11)	C (110) -C (19) -C (113)	126.7 (7)
C (831) -C (836)	1.418 (10)	C (111) -C (110) -C (19)	120.8 (7)
C (832) -C (833)	1.399 (11)	C (110) -C (111) -C (112)	117.7 (7)
C (833) -C (834)	1.348 (14)	C (110) -C (111) -C (119)	121.7 (7)
C (834) -C (835)	1.338 (14)	C (112) -C (111) -C (119)	120.6 (7)
C (835) -C (836)	1.407 (11)	C (111) -C (112) -C (17)	119.9 (7)
C (841) -C (842)	1.363 (10)	C (118) -C (113) -N (114)	120.9 (7)
C (841) -C (846)	1.402 (10)	C (118) -C (113) -C (19)	124.9 (7)
C (842) -C (843)	1.373 (11)	N (114) -C (113) -C (19)	114.0 (7)
C (843) -C (844)	1.417 (12)	C (115) -N (114) -C (113)	118.5 (7)
C (844) -C (845)	1.361 (12)	C (115) -N (114) -RU1	127.5 (6)
C (845) -C (846)	1.397 (11)	C (113) -N (114) -RU1	113.3 (5)
P (1) -F (16)	1.539 (7)	N (114) -C (115) -C (116)	123.7 (8)
P (1) -F (14)	1.582 (7)	C (117) -C (116) -C (115)	118.4 (8)
P (1) -F (12)	1.583 (6)	C (116) -C (117) -C (118)	117.3 (8)
P (1) -F (15)	1.587 (5)	C (113) -C (118) -C (117)	121.1 (7)
P (1) -F (13)	1.596 (5)	C (124) -C (119) -C (120)	116.8 (7)
P (1) -F (11)	1.622 (7)	C (124) -C (119) -C (111)	122.6 (7)
P (2) -F (24)	1.561 (9)	C (120) -C (119) -C (111)	120.4 (7)
P (2) -F (25)	1.569 (8)	C (121) -C (120) -C (119)	122.9 (8)
P (2) -F (21)	1.578 (7)	C (120) -C (121) -C (122)	117.2 (8)
P (2) -F (23)	1.594 (8)	C (123) -C (122) -C (121)	121.2 (8)
P (2) -F (22)	1.594 (8)	C (123) -C (122) -C (125)	119.0 (8)
P (2) -F (26)	1.625 (8)	C (121) -C (122) -C (125)	119.7 (8)
N (28) -RU1-N (18)	177.0 (2)	C (124) -C (123) -C (122)	119.4 (8)
N (28) -RU1-N (214)	79.1 (2)	C (123) -C (124) -C (119)	122.3 (8)
N (18) -RU1-N (214)	98.8 (2)	N (126) -C (125) -N (130)	123.4 (8)
N (28) -RU1-N (114)	103.7 (2)	N (126) -C (125) -C (122)	115.9 (7)
N (18) -RU1-N (114)	78.6 (2)	N (130) -C (125) -C (122)	120.7 (8)
N (214) -RU1-N (114)	96.0 (2)	C (125) -N (126) -C (127)	124.7 (7)
N (28) -RU1-N (21)	78.4 (2)	C (128) -C (127) -N (126)	112.8 (7)
N (18) -RU1-N (21)	103.6 (2)	C (127) -C (128) -C (129)	115.0 (7)
N (214) -RU1-N (21)	157.5 (2)	C (125) -N (130) -C (131)	128.3 (8)
N (114) -RU1-N (21)	87.8 (2)	N (130) -C (131) -C (132)	113.3 (7)
N (28) -RU1-N (11)	97.8 (2)	C (131) -C (132) -C (133)	108.6 (8)
N (18) -RU1-N (11)	79.9 (2)	C (22) -N (21) -C (26)	118.4 (6)
N (214) -RU1-N (11)	88.6 (2)	C (22) -N (21) -RU1	126.9 (5)
N (114) -RU1-N (11)	158.5 (2)	C (26) -N (21) -RU1	114.3 (4)

N(21)-C(22)-C(23)	123.6(8)	C(39)-N(38)-C(37)	129.4(7)
C(22)-C(23)-C(24)	118.2(8)	C(39)-N(38)-RU3	115.6(5)
C(25)-C(24)-C(23)	117.7(7)	C(37)-N(38)-RU3	114.9(4)
C(26)-C(25)-C(24)	120.4(7)	N(38)-C(39)-C(310)	117.1(6)
N(21)-C(26)-C(25)	121.7(7)	N(38)-C(39)-C(313)	117.8(7)
N(21)-C(26)-C(27)	115.3(6)	C(310)-C(39)-C(313)	125.0(7)
C(25)-C(26)-C(27)	123.0(7)	C(311)-C(310)-C(39)	118.2(7)
C(212)-C(27)-N(28)	122.8(7)	C(312)-C(311)-C(310)	119.7(8)
C(212)-C(27)-C(26)	127.6(7)	C(312)-C(311)-C(319)	120.5(6)
N(28)-C(27)-C(26)	109.5(7)	C(310)-C(311)-C(319)	119.7(7)
C(27)-N(28)-C(29)	116.7(7)	C(311)-C(312)-C(37)	119.8(7)
C(27)-N(28)-RU1	122.2(5)	N(314)-C(313)-C(318)	120.7(7)
C(29)-N(28)-RU1	121.1(5)	N(314)-C(313)-C(39)	114.1(6)
C(210)-C(29)-N(28)	122.1(8)	C(318)-C(313)-C(39)	125.1(7)
C(210)-C(29)-C(213)	128.2(7)	C(315)-N(314)-C(313)	118.3(6)
N(28)-C(29)-C(213)	109.7(7)	C(315)-N(314)-RU3	128.1(5)
C(29)-C(210)-C(211)	121.2(7)	C(313)-N(314)-RU3	113.5(5)
C(210)-C(211)-C(212)	117.1(7)	N(314)-C(315)-C(316)	121.0(7)
C(27)-C(212)-C(211)	120.1(7)	C(317)-C(316)-C(315)	119.8(7)
N(214)-C(213)-C(218)	120.4(7)	C(316)-C(317)-C(318)	120.9(8)
N(214)-C(213)-C(29)	116.1(6)	C(317)-C(318)-C(313)	119.1(7)
C(218)-C(213)-C(29)	123.5(7)	C(324)-C(319)-C(320)	120.6(6)
C(215)-N(214)-C(213)	118.9(6)	C(324)-C(319)-C(311)	122.0(7)
C(215)-N(214)-RU1	127.2(5)	C(320)-C(319)-C(311)	117.4(6)
C(213)-N(214)-RU1	113.7(5)	C(321)-C(320)-C(319)	120.3(7)
N(214)-C(215)-C(216)	122.8(7)	C(322)-C(321)-C(320)	119.1(8)
C(215)-C(216)-C(217)	118.9(8)	C(323)-C(322)-C(321)	120.6(7)
C(218)-C(217)-C(216)	118.3(8)	C(323)-C(322)-C(325)	120.6(8)
C(217)-C(218)-C(213)	120.6(8)	C(321)-C(322)-C(325)	118.7(8)
N(48)-RU3-N(38)	178.2(2)	C(322)-C(323)-C(324)	120.8(8)
N(48)-RU3-N(31)	99.6(2)	C(319)-C(324)-C(323)	118.4(7)
N(38)-RU3-N(31)	79.1(2)	N(326)-C(325)-N(330)	121.7(8)
N(48)-RU3-N(414)	78.7(3)	N(326)-C(325)-C(322)	116.7(7)
N(38)-RU3-N(414)	102.6(2)	N(330)-C(325)-C(322)	121.1(8)
N(31)-RU3-N(414)	91.8(2)	C(325)-N(326)-C(327)	125.5(8)
N(48)-RU3-N(314)	102.3(2)	N(326)-C(327)-C(328)	108.3(9)
N(38)-RU3-N(314)	78.9(2)	C(327)-C(328)-C(329)	105.1(9)
N(31)-RU3-N(314)	158.0(3)	C(325)-N(330)-C(331)	126.3(8)
N(414)-RU3-N(314)	92.2(2)	C(332)-C(331)-N(330)	117.4(9)
N(48)-RU3-N(41)	79.1(3)	C(331)-C(332)-C(333)	117.40(11)
N(38)-RU3-N(41)	99.6(2)	C(42)-N(41)-C(46)	121.4(8)
N(31)-RU3-N(41)	91.9(2)	C(42)-N(41)-RU3	125.7(6)
N(414)-RU3-N(41)	157.9(3)	C(46)-N(41)-RU3	112.7(6)
N(314)-RU3-N(41)	92.5(2)	N(41)-C(42)-C(43)	122.4(9)
C(32)-N(31)-C(36)	118.5(6)	C(42)-C(43)-C(44)	119.00(11)
C(32)-N(31)-RU3	128.0(5)	C(45)-C(44)-C(43)	116.9(1)
C(36)-N(31)-RU3	113.5(5)	C(44)-C(45)-C(46)	121.3(9)
N(31)-C(32)-C(33)	122.2(7)	N(41)-C(46)-C(45)	118.9(9)
C(34)-C(33)-C(32)	120.7(7)	N(41)-C(46)-C(47)	117.9(8)
C(33)-C(34)-C(35)	118.9(7)	C(45)-C(46)-C(47)	123.2(8)
C(34)-C(35)-C(36)	118.2(7)	C(412)-C(47)-N(48)	119.5(1)
N(31)-C(36)-C(35)	121.3(7)	C(412)-C(47)-C(46)	130.1(1)
N(31)-C(36)-C(37)	115.8(6)	N(48)-C(47)-C(46)	110.4(8)
C(35)-C(36)-C(37)	122.7(7)	C(49)-N(48)-C(47)	118.2(9)
N(38)-C(37)-C(36)	116.6(6)	C(49)-N(48)-RU3	121.9(6)
N(38)-C(37)-C(312)	115.6(6)	C(47)-N(48)-RU3	119.9(6)
C(36)-C(37)-C(312)	127.8(6)	C(410)-C(49)-N(48)	122.6(1)

C (410) -C (49) -C (413)	127.8 (9)	C (611) -B (6) -C (631)	113.5 (6)
N (48) -C (49) -C (413)	109.5 (7)	C (641) -B (6) -C (631)	102.7 (6)
C (411) -C (410) -C (49)	118.40 (11)	C (612) -C (611) -C (616)	115.2 (8)
C (410) -C (411) -C (412)	122.70 (12)	C (612) -C (611) -B (6)	125.3 (7)
C (47) -C (412) -C (411)	118.50 (11)	C (616) -C (611) -B (6)	119.4 (7)
C (418) -C (413) -N (414)	121.7 (9)	C (611) -C (612) -C (613)	121.4 (9)
C (418) -C (413) -C (49)	122.1 (8)	C (614) -C (613) -C (612)	121.10 (11)
N (414) -C (413) -C (49)	116.2 (7)	C (613) -C (614) -C (615)	119.0 (1)
C (415) -N (414) -C (413)	118.5 (8)	C (616) -C (615) -C (614)	119.5 (1)
C (415) -N (414) -RU3	127.9 (5)	C (615) -C (616) -C (611)	123.8 (9)
C (413) -N (414) -RU3	113.6 (6)	C (622) -C (621) -C (626)	113.2 (8)
N (414) -C (415) -C (416)	122.7 (9)	C (622) -C (621) -B (6)	123.0 (7)
C (415) -C (416) -C (417)	119.9 (1)	C (626) -C (621) -B (6)	123.4 (7)
C (418) -C (417) -C (416)	115.9 (9)	C (621) -C (622) -C (623)	124.2 (9)
C (413) -C (418) -C (417)	121.4 (9)	C (624) -C (623) -C (622)	118.50 (11)
C (521) -B (5) -C (541)	114.6 (6)	C (623) -C (624) -C (625)	119.10 (11)
C (521) -B (5) -C (531)	104.8 (6)	C (626) -C (625) -C (624)	120.60 (11)
C (541) -B (5) -C (531)	109.1 (6)	C (625) -C (626) -C (621)	124.3 (9)
C (521) -B (5) -C (511)	111.5 (6)	C (636) -C (631) -C (632)	118.6 (8)
C (541) -B (5) -C (511)	103.6 (6)	C (636) -C (631) -B (6)	120.8 (7)
C (531) -B (5) -C (511)	113.5 (6)	C (632) -C (631) -B (6)	120.4 (7)
C (516) -C (511) -C (512)	117.0 (7)	C (631) -C (632) -C (633)	120.2 (9)
C (516) -C (511) -B (5)	122.1 (6)	C (634) -C (633) -C (632)	117.10 (11)
C (512) -C (511) -B (5)	120.5 (7)	C (635) -C (634) -C (633)	121.70 (11)
C (513) -C (512) -C (511)	122.6 (8)	C (634) -C (635) -C (636)	118.50 (11)
C (512) -C (513) -C (514)	119.2 (8)	C (631) -C (636) -C (635)	123.6 (1)
C (515) -C (514) -C (513)	120.0 (8)	C (646) -C (641) -C (642)	114.7 (7)
C (514) -C (515) -C (516)	118.7 (8)	C (646) -C (641) -B (6)	121.7 (7)
C (511) -C (516) -C (515)	122.5 (8)	C (642) -C (641) -B (6)	123.3 (7)
C (526) -C (521) -C (522)	116.2 (8)	C (643) -C (642) -C (641)	123.0 (8)
C (526) -C (521) -B (5)	121.8 (7)	C (644) -C (643) -C (642)	121.1 (8)
C (522) -C (521) -B (5)	121.6 (7)	C (643) -C (644) -C (645)	117.9 (9)
C (523) -C (522) -C (521)	119.2 (8)	C (644) -C (645) -C (646)	120.3 (9)
C (522) -C (523) -C (524)	125.8 (1)	C (641) -C (646) -C (645)	122.8 (8)
C (525) -C (524) -C (523)	114.3 (1)	C (711) -B (7) -C (731)	112.5 (7)
C (526) -C (525) -C (524)	123.8 (1)	C (711) -B (7) -C (721)	115.8 (7)
C (525) -C (526) -C (521)	120.5 (9)	C (731) -B (7) -C (721)	104.7 (7)
C (532) -C (531) -C (536)	114.8 (7)	C (711) -B (7) -C (741)	103.7 (6)
C (532) -C (531) -B (5)	119.9 (7)	C (731) -B (7) -C (741)	111.3 (7)
C (536) -C (531) -B (5)	125.2 (7)	C (721) -B (7) -C (741)	108.9 (7)
C (533) -C (532) -C (531)	123.3 (8)	C (716) -C (711) -C (712)	112.3 (9)
C (532) -C (533) -C (534)	120.7 (9)	C (716) -C (711) -B (7)	126.4 (8)
C (535) -C (534) -C (533)	117.8 (9)	C (712) -C (711) -B (7)	121.0 (8)
C (534) -C (535) -C (536)	119.6 (9)	C (711) -C (712) -C (713)	125.1 (9)
C (531) -C (536) -C (535)	123.9 (8)	C (714) -C (713) -C (712)	116.4 (1)
C (542) -C (541) -C (546)	116.1 (7)	C (715) -C (714) -C (713)	122.20 (11)
C (542) -C (541) -B (5)	122.8 (7)	C (714) -C (715) -C (716)	118.5 (1)
C (546) -C (541) -B (5)	120.8 (7)	C (711) -C (716) -C (715)	125.3 (1)
C (543) -C (542) -C (541)	121.9 (8)	C (726) -C (721) -C (722)	113.6 (8)
C (542) -C (543) -C (544)	122.8 (1)	C (726) -C (721) -B (7)	123.4 (8)
C (543) -C (544) -C (545)	116.0 (8)	C (722) -C (721) -B (7)	122.7 (8)
C (546) -C (545) -C (544)	121.1 (7)	C (721) -C (722) -C (723)	122.7 (9)
C (545) -C (546) -C (541)	122.0 (8)	C (724) -C (723) -C (722)	119.8 (1)
C (621) -B (6) -C (611)	104.9 (6)	C (723) -C (724) -C (725)	121.30 (11)
C (621) -B (6) -C (641)	114.8 (6)	C (724) -C (725) -C (726)	117.50 (11)
C (611) -B (6) -C (641)	111.1 (6)	C (721) -C (726) -C (725)	125.0 (9)
C (621) -B (6) -C (631)	110.2 (6)	C (736) -C (731) -C (732)	113.5 (9)

C(736)-C(731)-B(7)	125.6(9)	C(834)-C(835)-C(836)	122.1(9)
C(732)-C(731)-B(7)	120.4(9)	C(835)-C(836)-C(831)	119.7(9)
C(731)-C(732)-C(733)	126.10(12)	C(842)-C(841)-C(846)	113.1(8)
C(734)-C(733)-C(732)	111.90(12)	C(842)-C(841)-B(8)	121.9(7)
C(735)-C(734)-C(733)	128.60(13)	C(846)-C(841)-B(8)	124.6(7)
C(734)-C(735)-C(736)	113.00(12)	C(841)-C(842)-C(843)	126.3(8)
C(731)-C(736)-C(735)	126.00(11)	C(842)-C(843)-C(844)	117.4(8)
C(746)-C(741)-C(742)	115.4(7)	C(845)-C(844)-C(843)	120.2(9)
C(746)-C(741)-B(7)	120.1(7)	C(844)-C(845)-C(846)	118.0(9)
C(742)-C(741)-B(7)	124.2(7)	C(845)-C(846)-C(841)	124.7(8)
C(743)-C(742)-C(741)	121.7(9)	F(16)-P(1)-F(14)	89.6(4)
C(742)-C(743)-C(744)	122.0(9)	F(16)-P(1)-F(12)	90.1(4)
C(745)-C(744)-C(743)	118.2(9)	F(14)-P(1)-F(12)	179.0(4)
C(744)-C(745)-C(746)	119.1(9)	F(16)-P(1)-F(15)	89.9(4)
C(741)-C(746)-C(745)	123.6(8)	F(14)-P(1)-F(15)	91.3(3)
C(821)-B(8)-C(841)	111.1(7)	F(12)-P(1)-F(15)	89.7(3)
C(821)-B(8)-C(811)	114.0(7)	F(16)-P(1)-F(13)	90.9(4)
C(841)-B(8)-C(811)	104.7(6)	F(14)-P(1)-F(13)	88.4(3)
C(821)-B(8)-C(831)	103.8(6)	F(12)-P(1)-F(13)	90.6(3)
C(841)-B(8)-C(831)	113.4(7)	F(15)-P(1)-F(13)	179.1(5)
C(811)-B(8)-C(831)	110.1(7)	F(16)-P(1)-F(11)	179.7(5)
C(816)-C(811)-C(812)	115.4(7)	F(14)-P(1)-F(11)	90.2(4)
C(816)-C(811)-B(8)	121.4(7)	F(12)-P(1)-F(11)	90.1(3)
C(812)-C(811)-B(8)	122.9(7)	F(15)-P(1)-F(11)	90.1(4)
C(813)-C(812)-C(811)	121.9(7)	F(13)-P(1)-F(11)	89.1(4)
C(812)-C(813)-C(814)	120.0(9)	F(24)-P(2)-F(25)	91.0(5)
C(815)-C(814)-C(813)	118.8(9)	F(24)-P(2)-F(21)	88.9(5)
C(814)-C(815)-C(816)	121.0(8)	F(25)-P(2)-F(21)	86.8(4)
C(815)-C(816)-C(811)	122.7(8)	F(24)-P(2)-F(23)	90.6(5)
C(822)-C(821)-C(826)	113.2(8)	F(25)-P(2)-F(23)	174.7(6)
C(822)-C(821)-B(8)	124.3(8)	F(21)-P(2)-F(23)	88.2(5)
C(826)-C(821)-B(8)	122.5(8)	F(24)-P(2)-F(22)	178.9(6)
C(823)-C(822)-C(821)	123.6(1)	F(25)-P(2)-F(22)	88.8(5)
C(824)-C(823)-C(822)	120.00(11)	F(21)-P(2)-F(22)	92.2(5)
C(823)-C(824)-C(825)	122.10(11)	F(23)-P(2)-F(22)	89.7(5)
C(824)-C(825)-C(826)	117.50(11)	F(24)-P(2)-F(26)	94.3(5)
C(825)-C(826)-C(821)	123.5(1)	F(25)-P(2)-F(26)	90.9(5)
C(832)-C(831)-C(836)	114.5(8)	F(21)-P(2)-F(26)	176.1(5)
C(832)-C(831)-B(8)	122.9(8)	F(23)-P(2)-F(26)	94.1(5)
C(836)-C(831)-B(8)	122.5(7)	F(22)-P(2)-F(26)	84.7(5)
C(831)-C(832)-C(833)	125.0(9)		
C(834)-C(833)-C(832)	118.1(1)		
C(835)-C(834)-C(833)	120.4(1)		

Table S6. Bond lengths [\AA] and angles [$^\circ$] related to the hydrogen bonding for **1**.

D-H	. . A	d(D-H)	d(H. . A)	d(D. . A)	<DHA
N(326)-H(326)	F(15) #1	0.87	1.98	2.845(9)	173.9
N(330)-H(330)	F(21) #2	0.87	2.26	3.055(11)	152.4
N(330)-H(330)	F(25) #2	0.87	2.36	3.004(11)	131.5

