Electronic Supplementary Material (ESI) for Dalton Transactions.

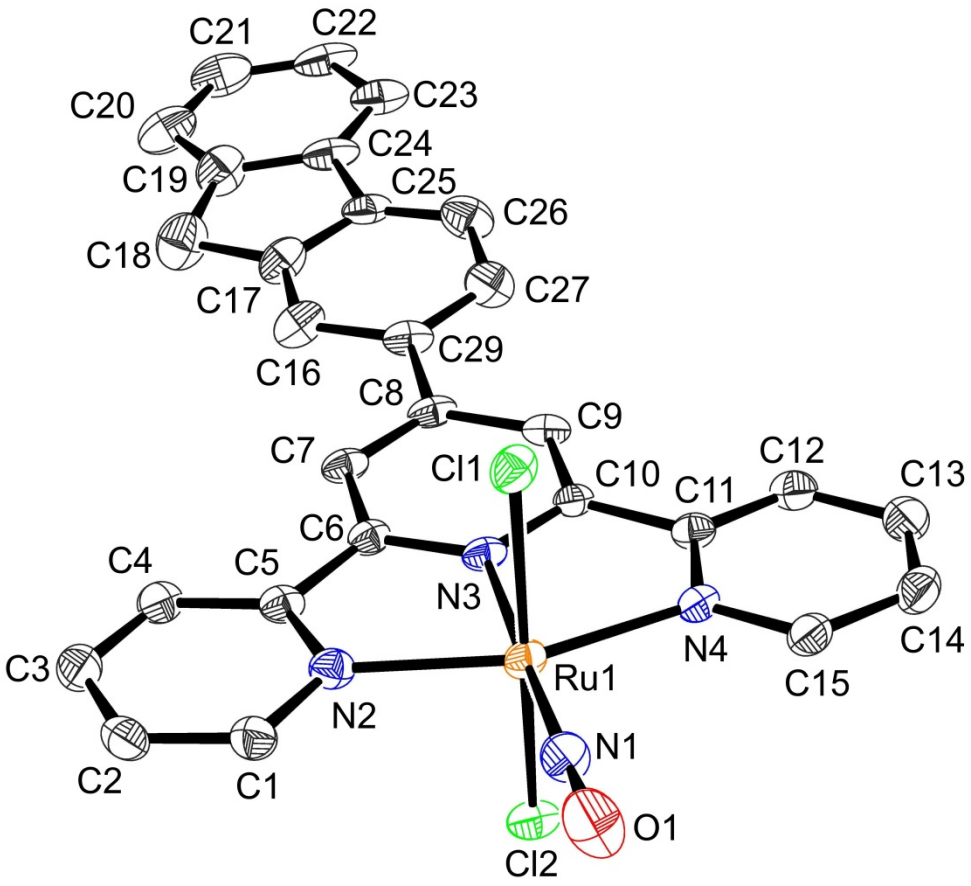

Table 1. Crystal data and structure refinement for transrunocl.

Identification code	TransRuNOCl
Empirical formula	C28 H19 Cl2 N4 O Ru, F6 P, C H4 O
Formula weight	776.45
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	triclinic, P -1
Unit cell dimensions	a = 10.3340(5) A alpha = 72.680(2) deg. b = 13.0961(6) A beta = 70.488(2) deg. c = 13.2279(6) A gamma = 67.090(2) deg.
Volume	1525.02(13) A^3
Z, Calculated density	2, 1.691 Mg/m^3
Absorption coefficient	0.816 mm^-1
F(000)	776

Crystal size	0.10 x 0.06 x 0.04 mm
Theta range for data collection	2.15 to 23.85 deg.
Limiting indices	-11<=h<=11, -14<=k<=14, -14<=l<=15
Reflections collected / unique	16406 / 4680 [R(int) = 0.0470]
Completeness to theta = 23.85	99.6 %
Max. and min. transmission	0.9681 and 0.9430
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4680 / 27 / 428
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0594, wR2 = 0.1613
R indices (all data)	R1 = 0.0809, wR2 = 0.1780
Largest diff. peak and hole	1.229 and -0.994 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for transrunocl.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	6312(1)	6571(1)	6880(1)	33(1)
Cl(1)	3907(2)	6521(2)	7555(1)	43(1)
Cl(2)	8792(2)	6372(2)	6312(2)	47(1)
P(1)	3850(4)	9060(3)	3292(3)	94(1)
N(3)	6872(6)	4996(4)	7744(4)	33(1)
C(6)	6908(7)	4841(5)	8794(5)	33(2)
C(5)	6586(7)	5897(6)	9143(5)	35(2)
N(4)	6616(6)	5634(4)	5754(4)	34(1)
C(29)	7792(7)	1667(6)	9627(6)	40(2)
F(2)	4681(7)	7861(4)	2921(5)	86(2)
C(24)	8683(8)	-1600(6)	11605(7)	54(2)
N(2)	6238(6)	6839(5)	8375(5)	37(1)
C(2)	5884(8)	7952(6)	9639(6)	45(2)
C(10)	7120(7)	4130(5)	7276(5)	32(2)
C(9)	7432(7)	3051(5)	7878(6)	37(2)
C(14)	6659(8)	5332(7)	4048(6)	50(2)
C(11)	7028(7)	4494(5)	6128(5)	35(2)
C(8)	7490(7)	2836(6)	8974(6)	36(2)
C(4)	6585(8)	5949(7)	10161(6)	43(2)
C(7)	7225(7)	3758(6)	9412(6)	37(2)
C(1)	5908(8)	7858(6)	8630(6)	42(2)
C(15)	6434(8)	6053(6)	4734(6)	42(2)
C(12)	7280(8)	3764(6)	5483(6)	44(2)
C(13)	7108(8)	4179(7)	4431(6)	49(2)
C(3)	6206(8)	6999(7)	10419(6)	49(2)
C(19)	8736(10)	-1365(8)	12584(8)	67(2)
C(21)	9307(10)	-3317(8)	13363(10)	77(3)
C(23)	8941(8)	-2698(7)	11540(8)	63(2)
C(22)	9292(9)	-3581(8)	12409(9)	69(3)
C(20)	9029(10)	-2204(8)	13463(8)	75(3)
F(4)	3019(8)	10267(5)	3639(7)	119(2)
F(5)	2277(6)	8985(5)	3392(6)	94(2)
F(1)	3671(7)	8416(6)	4566(5)	106(2)
F(6)	5371(7)	9120(6)	3249(5)	105(2)
F(3)	4166(13)	9601(7)	2005(6)	164(4)
N(1)	5795(7)	7952(5)	6117(5)	45(2)
O(1)	5458(8)	8837(5)	5622(5)	78(2)
C(16)	7907(8)	1443(6)	10716(6)	52(2)
C(26)	8221(10)	-338(7)	9829(8)	62(2)
C(17)	8183(9)	361(7)	11304(6)	53(2)
C(27)	7937(9)	802(6)	9204(7)	55(2)
C(25)	8319(8)	-502(7)	10843(7)	47(2)
C(18)	8425(12)	-70(8)	12430(8)	76(3)
O(2)	9990(20)	2070(20)	2660(20)	121(6)
C(28)	9620(30)	1540(20)	3630(30)	128(8)
O(2')	9900(20)	2820(20)	1780(20)	121(6)
C(28')	9670(30)	3740(30)	1070(30)	123(8)

Table 3. Bond lengths [A] and angles [deg] for transrunocl.

Ru(1)-N(1)	1.759(6)
Ru(1)-N(3)	2.001(5)
Ru(1)-N(4)	2.073(6)
Ru(1)-N(2)	2.081(6)
Ru(1)-Cl(2)	2.3478(18)
Ru(1)-Cl(1)	2.3642(18)
P(1)-F(6)	1.585(7)
P(1)-F(4)	1.599(7)
P(1)-F(2)	1.604(6)
P(1)-F(3)	1.612(8)
P(1)-F(5)	1.626(7)
P(1)-F(1)	1.629(7)
N(3)-C(10)	1.350(8)
N(3)-C(6)	1.353(8)
C(6)-C(7)	1.384(9)
C(6)-C(5)	1.468(10)
C(5)-N(2)	1.355(8)
C(5)-C(4)	1.368(10)
N(4)-C(15)	1.344(8)
N(4)-C(11)	1.363(8)
C(29)-C(27)	1.345(11)
C(29)-C(16)	1.418(11)
C(29)-C(8)	1.487(9)
C(24)-C(23)	1.382(12)
C(24)-C(19)	1.440(13)
C(24)-C(25)	1.482(10)
N(2)-C(1)	1.360(9)
C(2)-C(1)	1.368(10)
C(2)-C(3)	1.369(11)
C(2)-H(2)	0.9500
C(10)-C(9)	1.372(9)
C(10)-C(11)	1.473(9)
C(9)-C(8)	1.409(10)
C(9)-H(9)	0.9500
C(14)-C(13)	1.381(11)
C(14)-C(15)	1.403(11)
C(14)-H(14)	0.9500
C(11)-C(12)	1.362(10)
C(8)-C(7)	1.386(10)
C(4)-C(3)	1.389(11)
C(4)-H(4)	0.9500
C(7)-H(7)	0.9500
C(1)-H(1)	0.9500
C(15)-H(15)	0.9500
C(12)-C(13)	1.380(10)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(3)-H(3)	0.9500
C(19)-C(20)	1.366(13)
C(19)-C(18)	1.559(13)
C(21)-C(22)	1.409(15)
C(21)-C(20)	1.410(14)
C(21)-H(21)	0.9500
C(23)-C(22)	1.397(11)
C(23)-H(23)	0.9500

C(22)-H(22)	0.9500
C(20)-H(20)	0.9500
N(1)-O(1)	1.132(7)
C(16)-C(17)	1.368(10)
C(16)-H(16)	0.9500
C(26)-C(25)	1.326(11)
C(26)-C(27)	1.443(11)
C(26)-H(26)	0.9500
C(17)-C(25)	1.377(12)
C(17)-C(18)	1.496(12)
C(27)-H(27)	0.9500
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
O(2)-C(28)	1.27(2)
O(2)-H(2A)	0.8400
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
O(2')-C(28')	1.28(2)
O(2')-H(2')	0.8400
C(28')-H(28D)	0.9800
C(28')-H(28E)	0.9800
C(28')-H(28F)	0.9800

N(1)-Ru(1)-N(3)	179.0(2)
N(1)-Ru(1)-N(4)	100.8(2)
N(3)-Ru(1)-N(4)	78.7(2)
N(1)-Ru(1)-N(2)	102.9(2)
N(3)-Ru(1)-N(2)	77.6(2)
N(4)-Ru(1)-N(2)	156.4(2)
N(1)-Ru(1)-Cl(2)	93.9(2)
N(3)-Ru(1)-Cl(2)	86.93(16)
N(4)-Ru(1)-Cl(2)	89.69(15)
N(2)-Ru(1)-Cl(2)	89.27(16)
N(1)-Ru(1)-Cl(1)	93.4(2)
N(3)-Ru(1)-Cl(1)	85.73(15)
N(4)-Ru(1)-Cl(1)	87.88(15)
N(2)-Ru(1)-Cl(1)	90.15(16)
Cl(2)-Ru(1)-Cl(1)	172.58(6)
F(6)-P(1)-F(4)	91.6(4)
F(6)-P(1)-F(2)	88.6(4)
F(4)-P(1)-F(2)	178.9(4)
F(6)-P(1)-F(3)	86.5(5)
F(4)-P(1)-F(3)	93.2(5)
F(2)-P(1)-F(3)	85.7(5)
F(6)-P(1)-F(5)	177.6(4)
F(4)-P(1)-F(5)	87.9(4)
F(2)-P(1)-F(5)	91.9(3)
F(3)-P(1)-F(5)	95.9(4)
F(6)-P(1)-F(1)	90.7(4)
F(4)-P(1)-F(1)	91.5(4)
F(2)-P(1)-F(1)	89.6(4)
F(3)-P(1)-F(1)	174.6(6)
F(5)-P(1)-F(1)	87.0(4)
C(10)-N(3)-C(6)	122.4(5)
C(10)-N(3)-Ru(1)	118.5(4)
C(6)-N(3)-Ru(1)	119.0(4)
N(3)-C(6)-C(7)	119.2(6)

N(3)-C(6)-C(5)	113.5(5)
C(7)-C(6)-C(5)	127.3(6)
N(2)-C(5)-C(4)	122.0(7)
N(2)-C(5)-C(6)	114.0(6)
C(4)-C(5)-C(6)	123.9(6)
C(15)-N(4)-C(11)	119.7(6)
C(15)-N(4)-Ru(1)	125.9(5)
C(11)-N(4)-Ru(1)	114.3(4)
C(27)-C(29)-C(16)	118.6(7)
C(27)-C(29)-C(8)	120.7(7)
C(16)-C(29)-C(8)	120.7(7)
C(23)-C(24)-C(19)	119.8(8)
C(23)-C(24)-C(25)	133.4(9)
C(19)-C(24)-C(25)	106.8(7)
C(5)-N(2)-C(1)	118.2(6)
C(5)-N(2)-Ru(1)	115.8(5)
C(1)-N(2)-Ru(1)	126.0(5)
C(1)-C(2)-C(3)	119.6(7)
C(1)-C(2)-H(2)	120.2
C(3)-C(2)-H(2)	120.2
N(3)-C(10)-C(9)	119.1(6)
N(3)-C(10)-C(11)	113.1(5)
C(9)-C(10)-C(11)	127.8(6)
C(10)-C(9)-C(8)	121.1(6)
C(10)-C(9)-H(9)	119.4
C(8)-C(9)-H(9)	119.4
C(13)-C(14)-C(15)	118.7(7)
C(13)-C(14)-H(14)	120.6
C(15)-C(14)-H(14)	120.6
C(12)-C(11)-N(4)	121.3(6)
C(12)-C(11)-C(10)	123.4(6)
N(4)-C(11)-C(10)	115.2(6)
C(7)-C(8)-C(9)	117.2(6)
C(7)-C(8)-C(29)	122.1(6)
C(9)-C(8)-C(29)	120.6(7)
C(5)-C(4)-C(3)	119.1(7)
C(5)-C(4)-H(4)	120.5
C(3)-C(4)-H(4)	120.5
C(6)-C(7)-C(8)	120.9(6)
C(6)-C(7)-H(7)	119.5
C(8)-C(7)-H(7)	119.5
N(2)-C(1)-C(2)	121.9(7)
N(2)-C(1)-H(1)	119.0
C(2)-C(1)-H(1)	119.0
N(4)-C(15)-C(14)	120.8(7)
N(4)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(11)-C(12)-C(13)	119.7(7)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(12)-C(13)-C(14)	119.7(7)
C(12)-C(13)-H(13)	120.2
C(14)-C(13)-H(13)	120.2
C(2)-C(3)-C(4)	119.2(7)
C(2)-C(3)-H(3)	120.4
C(4)-C(3)-H(3)	120.4
C(20)-C(19)-C(24)	121.6(10)
C(20)-C(19)-C(18)	129.4(10)

C(24)-C(19)-C(18)	109.0(7)
C(22)-C(21)-C(20)	122.8(10)
C(22)-C(21)-H(21)	118.6
C(20)-C(21)-H(21)	118.6
C(24)-C(23)-C(22)	120.1(10)
C(24)-C(23)-H(23)	120.0
C(22)-C(23)-H(23)	120.0
C(23)-C(22)-C(21)	118.5(10)
C(23)-C(22)-H(22)	120.7
C(21)-C(22)-H(22)	120.7
C(19)-C(20)-C(21)	117.1(11)
C(19)-C(20)-H(20)	121.4
C(21)-C(20)-H(20)	121.4
O(1)-N(1)-Ru(1)	179.5(6)
C(17)-C(16)-C(29)	119.8(8)
C(17)-C(16)-H(16)	120.1
C(29)-C(16)-H(16)	120.1
C(25)-C(26)-C(27)	117.5(8)
C(25)-C(26)-H(26)	121.2
C(27)-C(26)-H(26)	121.2
C(16)-C(17)-C(25)	119.8(8)
C(16)-C(17)-C(18)	128.6(9)
C(25)-C(17)-C(18)	111.5(7)
C(29)-C(27)-C(26)	121.5(8)
C(29)-C(27)-H(27)	119.3
C(26)-C(27)-H(27)	119.3
C(26)-C(25)-C(17)	122.8(7)
C(26)-C(25)-C(24)	126.7(8)
C(17)-C(25)-C(24)	110.4(7)
C(17)-C(18)-C(19)	102.3(8)
C(17)-C(18)-H(18A)	111.3
C(19)-C(18)-H(18A)	111.3
C(17)-C(18)-H(18B)	111.3
C(19)-C(18)-H(18B)	111.3
H(18A)-C(18)-H(18B)	109.2
O(2)-C(28)-H(28A)	109.5
O(2)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
O(2)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(28')-O(2')-H(2')	109.5
O(2')-C(28')-H(28D)	109.5
O(2')-C(28')-H(28E)	109.5
H(28D)-C(28')-H(28E)	109.5
O(2')-C(28')-H(28F)	109.5
H(28D)-C(28')-H(28F)	109.5
H(28E)-C(28')-H(28F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for transrunocl.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ru(1)	37(1)	26(1)	31(1)	4(1)	-12(1)	-10(1)
Cl(1)	36(1)	52(1)	36(1)	-4(1)	-10(1)	-12(1)
Cl(2)	43(1)	45(1)	50(1)	4(1)	-11(1)	-21(1)
P(1)	131(3)	67(2)	112(3)	1(2)	-69(2)	-43(2)
N(3)	32(3)	28(3)	35(3)	5(2)	-9(2)	-13(2)
C(6)	26(3)	38(4)	33(4)	2(3)	-10(3)	-12(3)
C(5)	22(3)	40(4)	40(4)	-2(3)	-11(3)	-10(3)
N(4)	32(3)	35(3)	30(3)	-1(2)	-5(2)	-13(2)
C(29)	25(4)	32(4)	55(5)	6(3)	-15(3)	-7(3)
F(2)	107(5)	58(3)	89(4)	-21(3)	-25(3)	-18(3)
C(24)	33(4)	38(4)	74(6)	14(4)	-11(4)	-14(3)
N(2)	38(3)	37(3)	39(3)	0(3)	-14(3)	-15(3)
C(2)	38(4)	46(4)	56(5)	-21(4)	-6(4)	-17(4)
C(10)	29(4)	34(4)	32(4)	0(3)	-7(3)	-15(3)
C(9)	28(4)	28(4)	51(4)	-3(3)	-6(3)	-12(3)
C(14)	40(4)	74(6)	34(4)	-6(4)	-6(3)	-23(4)
C(11)	28(4)	34(4)	39(4)	-7(3)	-3(3)	-11(3)
C(8)	23(3)	35(4)	42(4)	11(3)	-11(3)	-11(3)
C(4)	39(4)	57(5)	37(4)	3(3)	-18(3)	-22(4)
C(7)	29(4)	37(4)	38(4)	8(3)	-11(3)	-13(3)
C(1)	45(4)	39(4)	43(4)	-6(3)	-11(3)	-17(3)
C(15)	41(4)	46(4)	35(4)	-1(3)	-8(3)	-18(3)
C(12)	40(4)	44(4)	48(5)	-9(4)	-5(3)	-18(3)
C(13)	40(4)	60(5)	48(5)	-21(4)	-1(4)	-19(4)
C(3)	42(4)	72(6)	42(4)	-12(4)	-11(4)	-26(4)
C(19)	64(6)	68(6)	60(6)	0(5)	-22(5)	-14(5)
C(21)	59(6)	58(6)	88(8)	12(5)	-11(5)	-17(5)
C(23)	39(5)	58(6)	80(6)	9(5)	-12(4)	-21(4)
C(22)	36(5)	55(5)	86(7)	29(5)	-13(5)	-19(4)
C(20)	56(6)	64(6)	72(6)	6(5)	-4(5)	-10(5)
F(4)	123(6)	65(4)	184(7)	-45(4)	-46(5)	-22(4)
F(5)	86(4)	68(4)	145(6)	-26(4)	-52(4)	-21(3)
F(1)	111(5)	111(5)	88(4)	-8(4)	-36(4)	-28(4)
F(6)	85(4)	154(6)	109(5)	-51(5)	-15(4)	-60(4)
F(3)	332(13)	136(6)	113(6)	63(5)	-131(7)	-168(8)
N(1)	61(4)	33(4)	45(4)	5(3)	-27(3)	-15(3)
O(1)	135(6)	34(3)	81(4)	13(3)	-70(5)	-25(4)
C(16)	44(5)	39(4)	50(5)	3(4)	-8(4)	-2(3)
C(26)	67(6)	45(5)	80(7)	-4(4)	-27(5)	-23(4)
C(17)	46(5)	51(5)	44(5)	3(4)	-11(4)	-7(4)
C(27)	66(6)	42(5)	60(5)	8(4)	-33(4)	-18(4)
C(25)	31(4)	55(5)	53(5)	9(4)	-11(4)	-24(4)
C(18)	89(7)	63(6)	64(6)	-3(5)	-21(5)	-15(5)
O(2)	112(8)	126(10)	147(10)	-57(8)	-29(8)	-40(7)
C(28)	106(15)	124(16)	155(15)	-68(12)	-16(14)	-23(13)

O(2')	86(10)	146(14)	164(16)	-68(12)	-15(11)	-58(11)
C(28')	77(13)	157(19)	170(20)	-57(14)	-22(14)	-65(15)