Supplementary Information for:

Synthesis and structural studies of two pyridine-armed reinforced cyclen chelators and their transition metal complexes

Kevin R. Wilson[a], Desiray J. Cannon-Smith[a], Benjamin P. Burke[b], Orry C. Birdsong[a], Stephen J. Archibald[b] and Timothy J. Hubin[a]*

Table 1. Crystal data and structure refinement for sja3_12.

Identification code	shelxl	
Empirical formula	C17 H29 Cl F6 N5 P Zn	
Formula weight	549.24	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 11.584(2) Å	α= 90°.
	b = 11.729 (3)Å	β= 96.95(2)°.
	c = 15.730(3) Å	γ = 90°.
Volume	2121.6(9) $Å^3$	
Z	4	
Density (calculated)	1.720 Mg/m^3	
Absorption coefficient	1.427 mm^{-1}	
F(000)	1128	
Crystal size	0.20 x 0.18 x 0.16 mm^3	
Theta range for data collection	2.48 to 25.00°.	
Index ranges	-13<=h<=13, 0<=k<=13, 0<=l<=18	
Reflections collected	3733	
Independent reflections	3733 [R(int) = 0.0000]	
Completeness to theta = 25.00°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3733 / 0 / 282	
Goodness-of-fit on F^2	0.712	
Final R indices [I>2sigma(I)]	R1 = 0.0288, wR2 = 0.0623	
R indices (all data)	R1 = 0.0598, wR2 = 0.0660	
Extinction coefficient	0.00086(14)	
Largest diff. peak and hole	0.276 and -0.512 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sja3_12. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	8137(1)	2526(1)	574(1)	23(1)
Cl(1)	9348(1)	2555(1)	-550(1)	31(1)
N(1)	9042(2)	1260(2)	1507(2)	24(1)
N(2)	6990(2)	2603(3)	1579(2)	25(1)
N(3)	7176(3)	4114(2)	234(2)	27(1)
N(4)	9176(3)	3604(2)	1460(2)	25(1)
N(5)	7445(3)	964(2)	64(2)	26(1)
C(1)	8248(3)	1034(3)	2167(2)	28(1)
C(2)	7004(3)	1438(3)	1901(2)	27(1)
C(3)	5883(3)	2935(3)	1075(2)	31(1)
C(4)	6014(3)	4031(3)	561(2)	30(1)
C(5)	7927(3)	5036(3)	677(2)	32(1)
C(6)	9172(3)	4660(3)	962(2)	29(1)
C(7)	10310(3)	3014(3)	1575(2)	31(1)
C(8)	10172(3)	1775(3)	1868(2)	29(1)
C(9)	7388(3)	3453(3)	2242(2)	31(1)
C(10)	8697(3)	3740(3)	2283(2)	30(1)
C(11)	9169(3)	264(3)	962(2)	28(1)
C(12)	8111(3)	66(3)	312(2)	25(1)
C(13)	7899(3)	-1001(3)	-46(2)	30(1)
C(14)	6977(3)	-1134(3)	-685(2)	34(1)
C(15)	6295(3)	-206(3)	-939(2)	36(1)
C(16)	6552(3)	819(3)	-554(2)	31(1)
C(17)	7014(4)	4342(3)	-706(2)	36(1)
P(1)	3624(1)	2634(1)	3146(1)	29(1)
F(1)	3793(2)	3884(2)	3534(1)	45(1)
F(2)	3454(2)	1388(2)	2760(2)	56(1)
F(3)	2296(2)	2644(2)	3307(1)	50(1)
F(4)	3273(2)	3158(2)	2211(1)	45(1)
F(5)	4960(2)	2613(2)	2987(1)	49(1)
F(6)	3984(2)	2122(2)	4081(1)	42(1)

Table 3. Bond lengths [Å] and angles [°] for sja3_12.

Zn(1)-N(5)	2.118(3)
Zn(1)-N(4)	2.142(3)
Zn(1)-N(2)	2.185(2)
Zn(1)-N(3)	2.202(3)
Zn(1)-N(1)	2.255(3)
Zn(1)-Cl(1)	2.3870(8)
N(1)-C(11)	1.467(4)
N(1)-C(8)	1.489(4)
N(1)-C(1)	1.492(4)
N(2)-C(2)	1.457(4)
N(2)-C(3)	1.476(4)
N(2)-C(9)	1.476(4)
N(3)-C(17)	1.493(4)
N(3)-C(4)	1.501(4)
N(3)-C(5)	1.505(4)
N(4)-C(6)	1.466(4)
N(4)-C(10)	1.477(4)
N(4)-C(7)	1.476(4)
N(5)-C(12)	1.335(4)
N(5)-C(16)	1.342(4)
C(1)-C(2)	1.526(5)
C(3)-C(4)	1.536(5)
C(5)-C(6)	1.523(5)
C(7)-C(8)	1.539(5)
C(9)-C(10)	1.546(5)
C(11)-C(12)	1.516(5)
C(12)-C(13)	1.383(5)
C(13)-C(14)	1.384(5)
C(14)-C(15)	1.375(5)
C(15)-C(16)	1.364(5)
P(1)-F(2)	1.586(2)
P(1)-F(1)	1.590(2)
P(1)-F(3)	1.589(2)

P(1)-F(6)	1.596(2)
P(1)-F(5)	1.598(2)
P(1)-F(4)	1.601(2)
N(5)-Zn(1)-N(4)	156.13(11)
N(5)-Zn(1)-N(2)	94.28(11)
N(4)-Zn(1)-N(2)	81.26(11)
N(5)-Zn(1)-N(3)	118.85(10)
N(4)-Zn(1)-N(3)	83.49(11)
N(2)-Zn(1)-N(3)	78.88(11)
N(5)-Zn(1)-N(1)	78.58(11)
N(4)-Zn(1)-N(1)	77.55(9)
N(2)-Zn(1)-N(1)	80.34(10)
N(3)-Zn(1)-N(1)	153.69(10)
N(5)-Zn(1)-Cl(1)	87.75(8)
N(4)-Zn(1)-Cl(1)	98.00(8)
N(2)-Zn(1)-Cl(1)	176.51(9)
N(3)-Zn(1)-Cl(1)	97.66(8)
N(1)-Zn(1)-Cl(1)	102.86(8)
C(11)-N(1)-C(8)	113.6(3)
C(11)-N(1)-C(1)	112.2(3)
C(8)-N(1)-C(1)	113.2(3)
C(11)-N(1)-Zn(1)	102.5(2)
C(8)-N(1)-Zn(1)	107.4(2)
C(1)-N(1)-Zn(1)	107.0(2)
C(2)-N(2)-C(3)	114.0(3)
C(2)-N(2)-C(9)	113.5(3)
C(3)-N(2)-C(9)	112.2(3)
C(2)-N(2)-Zn(1)	103.3(2)
C(3)-N(2)-Zn(1)	100.80(19)
C(9)-N(2)-Zn(1)	111.9(2)
C(17)-N(3)-C(4)	109.9(3)
C(17)-N(3)-C(5)	109.0(3)
C(4)-N(3)-C(5)	112.3(3)
C(17)-N(3)-Zn(1)	113.1(2)

C(4)-N(3)-Zn(1)	108.1(2)
C(5)-N(3)-Zn(1)	104.4(2)
C(6)-N(4)-C(10)	113.6(3)
C(6)-N(4)-C(7)	114.0(3)
C(10)-N(4)-C(7)	111.5(3)
C(6)-N(4)-Zn(1)	100.7(2)
C(10)-N(4)-Zn(1)	113.1(2)
C(7)-N(4)-Zn(1)	103.0(2)
C(12)-N(5)-C(16)	118.7(3)
C(12)-N(5)-Zn(1)	113.1(2)
C(16)-N(5)-Zn(1)	127.4(2)
N(1)-C(1)-C(2)	113.3(3)
N(2)-C(2)-C(1)	110.9(3)
N(2)-C(3)-C(4)	111.6(3)
N(3)-C(4)-C(3)	112.6(3)
N(3)-C(5)-C(6)	113.7(3)
N(4)-C(6)-C(5)	110.1(3)
N(4)-C(7)-C(8)	110.9(3)
N(1)-C(8)-C(7)	112.8(3)
N(2)-C(9)-C(10)	113.4(3)
N(4)-C(10)-C(9)	114.2(3)
N(1)-C(11)-C(12)	112.7(3)
N(5)-C(12)-C(13)	121.8(3)
N(5)-C(12)-C(11)	117.9(3)
C(13)-C(12)-C(11)	120.2(3)
C(12)-C(13)-C(14)	118.7(3)
C(15)-C(14)-C(13)	119.2(3)
C(16)-C(15)-C(14)	118.8(3)
N(5)-C(16)-C(15)	122.7(3)
F(2)-P(1)-F(1)	179.96(16)
F(2)-P(1)-F(3)	89.44(15)
F(1)-P(1)-F(3)	90.57(14)
F(2)-P(1)-F(6)	90.71(13)
F(1)-P(1)-F(6)	89.33(12)
F(3)-P(1)-F(6)	90.37(12)

F(2)-P(1)-F(5)	90.18(15)
F(1)-P(1)-F(5)	89.81(14)
F(3)-P(1)-F(5)	179.50(18)
F(6)-P(1)-F(5)	89.31(12)
F(2)-P(1)-F(4)	89.74(13)
F(1)-P(1)-F(4)	90.22(13)
F(3)-P(1)-F(4)	90.03(12)
F(6)-P(1)-F(4)	179.40(14)
F(5)-P(1)-F(4)	90.29(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sja3_12. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	26(1)	23(1)	21(1)	0(1)	3(1)	1(1)
Cl(1)	36(1)	34(1)	26(1)	2(1)	9(1)	3(1)
N(1)	23(2)	23(2)	25(2)	-1(1)	2(1)	-1(1)
N(2)	27(1)	25(2)	24(1)	0(1)	5(1)	2(2)
N(3)	33(2)	27(2)	21(2)	1(1)	2(1)	3(1)
N(4)	30(2)	24(2)	23(2)	1(1)	8(1)	0(1)
N(5)	27(2)	27(2)	24(2)	0(1)	6(1)	1(1)
C(1)	36(2)	24(2)	24(2)	3(2)	7(2)	0(2)
C(2)	32(2)	27(2)	22(2)	3(2)	9(2)	1(2)
C(3)	30(2)	31(2)	34(2)	1(2)	9(2)	2(2)
C(4)	30(2)	33(2)	28(2)	0(2)	5(2)	6(2)
C(5)	44(2)	23(2)	29(2)	2(2)	9(2)	-2(2)
C(6)	35(3)	25(2)	26(2)	1(2)	4(2)	-4(2)
C(7)	27(2)	34(2)	32(2)	2(2)	-2(2)	-2(2)
C(8)	30(2)	30(2)	27(2)	-1(2)	-1(2)	-1(2)
C(9)	39(2)	30(2)	25(2)	-3(2)	6(2)	1(2)
C(10)	40(2)	23(2)	26(2)	-5(2)	5(2)	-6(2)
C(11)	28(2)	26(2)	29(2)	-4(2)	3(2)	3(2)
C(12)	28(2)	27(2)	21(2)	-1(2)	5(2)	0(2)
C(13)	32(2)	26(2)	33(2)	-1(2)	7(2)	1(2)
C(14)	38(2)	33(2)	31(2)	-8(2)	5(2)	-5(2)
C(15)	34(2)	40(2)	32(2)	-6(2)	0(2)	0(2)
C(16)	32(2)	30(2)	29(2)	-2(2)	0(2)	1(2)
C(17)	48(3)	38(2)	22(2)	7(2)	5(2)	8(2)
P(1)	30(1)	30(1)	27(1)	-1(1)	4(1)	-1(1)
F(1)	59(1)	31(1)	48(1)	-7(1)	12(1)	-4(1)
F(2)	92(2)	36(1)	41(1)	-13(1)	14(1)	-14(1)
F(3)	29(1)	80(2)	40(1)	-1(1)	7(1)	-6(1)
F(4)	52(1)	54(1)	29(1)	9(1)	2(1)	3(1)
F(5)	32(1)	68(2)	49(1)	-3(1)	12(1)	4(1)
F(6)	52(1)	49(1)	25(1)	9(1)	3(1)	5(1)

Table 1. Crystal data and structure refinement for sja4_12.

Identification code	shelxl	
Empirical formula	C17 H29 Cl F6 N5 Ni P	
Formula weight	542.58	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 11.6458(10) Å	α= 90°.
	b = 11.6930(12) Å	β= 97.680(7)°.
	c = 15.6867(13) Å	γ = 90°.
Volume	2117.0(3) $Å^3$	
Z	4	
Density (calculated)	1.702 Mg/m^3	
Absorption coefficient	1.186 mm^{-1}	
F(000)	1120	
Crystal size	0.18 x 0.15 x 0.15 mm^3	
Theta range for data collection	2.48 to 27.50°.	
Index ranges	-15<=h<=14, 0<=k<=15, 0<=l<=19	
Reflections collected	4710	
Independent reflections	4710 [R(int) = 0.0000]	
Completeness to theta = 27.50°	96.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4710 / 0 / 280	
Goodness-of-fit on F^2	0.810	
Final R indices [I>2sigma(I)]	R1 = 0.0639, wR2 = 0.1760	
R indices (all data)	R1 = 0.1144, wR2 = 0.1980	
Largest diff. peak and hole	0.925 and -0.877 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sja4_12. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5182(5)	8147(5)	1837(5)	42(2)
C(2)	5258(5)	6895(5)	1612(5)	49(2)
C(3)	4119(6)	5295(5)	929(4)	42(2)
C(4)	2869(6)	4963(5)	610(5)	54(2)
C(5)	999(6)	6022(6)	480(5)	55(2)
C(6)	891(6)	7108(6)	1038(5)	50(2)
C(7)	2043(5)	8545(5)	1915(5)	43(2)
C(8)	3300(6)	8914(5)	2167(4)	43(2)
C(9)	3597(6)	6183(5)	2266(4)	47(2)
C(10)	2337(6)	6504(5)	2198(5)	52(2)
C(11)	4164(5)	9667(4)	931(4)	38(2)
C(12)	3087(5)	9859(5)	300(4)	43(2)
C(13)	2858(6)	10922(5)	-56(5)	45(2)
C(14)	1950(6)	11043(6)	-696(5)	57(2)
C(15)	1275(6)	10104(6)	-949(5)	56(2)
C(16)	1564(6)	9070(6)	-565(5)	54(2)
C(17)	2006(7)	5783(6)	-755(5)	60(2)
N(1)	4037(4)	8670(4)	1487(3)	32(1)
N(2)	4109(4)	6346(4)	1452(3)	34(1)
N(3)	2210(5)	5950(4)	172(4)	44(1)
N(4)	1991(4)	7398(4)	1538(3)	38(1)
N(5)	2427(4)	8953(4)	57(3)	37(1)
Cl(1)	4404(1)	7469(1)	-480(1)	42(1)
P(1)	1421(1)	2380(2)	1897(1)	42(1)
F(1)	1238(5)	1098(4)	1549(4)	88(2)
F(2)	1618(6)	3611(4)	2253(4)	104(2)
F(3)	1036(4)	2799(4)	956(3)	63(1)
F(4)	127(3)	2405(4)	2093(3)	73(1)
F(5)	1800(4)	1862(4)	2831(3)	71(1)
F(6)	2719(4)	2359(5)	1696(3)	90(2)

Ni(1)	3143(1)	7464(1)	636(1)	31(1)

Table 3. Bond lengths [Å] and angles [°] for sja4_12.

C(1)-N(1)	1.503(7)
C(1)-C(2)	1.511(8)
C(2)-N(2)	1.475(7)
C(3)-N(2)	1.478(7)
C(3)-C(4)	1.525(9)
C(4)-N(3)	1.500(8)
C(5)-N(3)	1.553(9)
C(5)-C(6)	1.557(10)
C(6)-N(4)	1.450(8)
C(7)-N(4)	1.464(7)
C(7)-C(8)	1.526(9)
C(8)-N(1)	1.484(8)
C(9)-N(2)	1.492(8)
C(9)-C(10)	1.505(9)
C(10)-N(4)	1.488(8)
C(11)-N(1)	1.476(7)
C(11)-C(12)	1.507(8)
C(12)-N(5)	1.333(7)
C(12)-C(13)	1.375(8)
C(13)-C(14)	1.364(9)
C(14)-C(15)	1.377(9)
C(15)-C(16)	1.372(9)
C(16)-N(5)	1.311(8)
C(17)-N(3)	1.456(9)
N(1)-Ni(1)	2.117(4)
N(2)-Ni(1)	2.057(4)
N(3)-Ni(1)	2.153(5)
N(4)-Ni(1)	2.077(5)
N(5)-Ni(1)	2.085(5)
Cl(1)-Ni(1)	2.4302(16)
P(1)-F(2)	1.550(5)
P(1)-F(3)	1.561(4)
P(1)-F(4)	1.578(4)

P(1)-F(6)	1.585(5)
P(1)-F(5)	1.593(5)
P(1)-F(1)	1.600(5)

N(1)-C(1)-C(2)	112.6(5)
N(2)-C(2)-C(1)	112.5(5)
N(2)-C(3)-C(4)	108.4(5)
N(3)-C(4)-C(3)	111.3(5)
N(3)-C(5)-C(6)	111.4(5)
N(4)-C(6)-C(5)	111.3(5)
N(4)-C(7)-C(8)	110.5(5)
N(1)-C(8)-C(7)	112.7(5)
N(2)-C(9)-C(10)	113.9(5)
N(4)-C(10)-C(9)	113.3(5)
N(1)-C(11)-C(12)	111.4(4)
N(5)-C(12)-C(13)	121.9(6)
N(5)-C(12)-C(11)	117.9(5)
C(13)-C(12)-C(11)	120.0(5)
C(14)-C(13)-C(12)	118.8(6)
C(13)-C(14)-C(15)	119.1(6)
C(16)-C(15)-C(14)	118.6(6)
N(5)-C(16)-C(15)	122.5(7)
C(11)-N(1)-C(8)	112.7(4)
C(11)-N(1)-C(1)	112.5(5)
C(8)-N(1)-C(1)	112.7(5)
C(11)-N(1)-Ni(1)	103.5(3)
C(8)-N(1)-Ni(1)	107.4(3)
C(1)-N(1)-Ni(1)	107.3(3)
C(2)-N(2)-C(3)	112.5(5)
C(2)-N(2)-C(9)	111.5(5)
C(3)-N(2)-C(9)	113.8(5)
C(2)-N(2)-Ni(1)	103.7(3)
C(3)-N(2)-Ni(1)	103.2(4)
C(9)-N(2)-Ni(1)	111.4(4)
C(17)-N(3)-C(4)	111.1(5)

C(17)-N(3)-C(5)	106.5(5)
C(4)-N(3)-C(5)	109.3(6)
C(17)-N(3)-Ni(1)	117.1(4)
C(4)-N(3)-Ni(1)	105.9(4)
C(5)-N(3)-Ni(1)	106.8(4)
C(6)-N(4)-C(7)	114.7(5)
C(6)-N(4)-C(10)	110.5(5)
C(7)-N(4)-C(10)	111.7(5)
C(6)-N(4)-Ni(1)	104.2(4)
C(7)-N(4)-Ni(1)	104.2(4)
C(10)-N(4)-Ni(1)	111.1(4)
C(16)-N(5)-C(12)	119.0(5)
C(16)-N(5)-Ni(1)	129.3(4)
C(12)-N(5)-Ni(1)	110.9(4)
F(2)-P(1)-F(3)	93.4(3)
F(2)-P(1)-F(4)	90.7(3)
F(3)-P(1)-F(4)	91.0(2)
F(2)-P(1)-F(6)	89.2(3)
F(3)-P(1)-F(6)	88.8(3)
F(4)-P(1)-F(6)	179.8(4)
F(2)-P(1)-F(5)	90.7(3)
F(3)-P(1)-F(5)	175.9(3)
F(4)-P(1)-F(5)	88.9(3)
F(6)-P(1)-F(5)	91.3(3)
F(2)-P(1)-F(1)	178.6(3)
F(3)-P(1)-F(1)	87.9(3)
F(4)-P(1)-F(1)	89.8(3)
F(6)-P(1)-F(1)	90.3(3)
F(5)-P(1)-F(1)	88.0(3)
N(2)-Ni(1)-N(4)	84.4(2)
N(2)-Ni(1)-N(5)	162.85(18)
N(4)-Ni(1)-N(5)	94.1(2)
N(2)-Ni(1)-N(1)	81.32(16)
N(4)-Ni(1)-N(1)	84.46(19)
N(5)-Ni(1)-N(1)	81.54(17)

N(2)-Ni(1)-N(3)	84.06(18)
N(4)-Ni(1)-N(3)	81.8(2)
N(5)-Ni(1)-N(3)	112.67(18)
N(1)-Ni(1)-N(3)	160.8(2)
N(2)-Ni(1)-Cl(1)	96.69(15)
N(4)-Ni(1)-Cl(1)	176.36(13)
N(5)-Ni(1)-Cl(1)	85.95(15)
N(1)-Ni(1)-Cl(1)	99.13(14)
N(3)-Ni(1)-Cl(1)	94.86(17)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sja4_12. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	36(3)	39(3)	48(4)	-4(3)	-11(3)	1(2)
C(2)	37(3)	39(3)	67(5)	-1(3)	-8(3)	7(3)
C(3)	54(4)	28(3)	43(4)	-4(3)	6(3)	8(2)
C(4)	73(5)	30(3)	55(5)	-5(3)	-11(4)	4(3)
C(5)	47(4)	44(3)	74(5)	4(3)	2(3)	-12(3)
C(6)	43(3)	55(4)	54(5)	-2(3)	10(3)	-4(3)
C(7)	52(4)	30(3)	52(4)	-1(3)	21(3)	0(2)
C(8)	60(4)	30(3)	38(4)	-4(3)	7(3)	0(3)
C(9)	74(5)	30(3)	40(4)	5(3)	16(3)	5(3)
C(10)	70(5)	36(3)	54(5)	-1(3)	23(4)	-3(3)
C(11)	37(3)	27(3)	46(4)	4(2)	-5(3)	-6(2)
C(12)	48(3)	33(3)	45(4)	6(3)	-2(3)	-7(3)
C(13)	52(4)	37(3)	48(4)	0(3)	6(3)	1(3)
C(14)	58(4)	41(3)	70(5)	13(3)	2(4)	7(3)
C(15)	62(4)	54(4)	46(4)	9(3)	-12(3)	-2(3)
C(16)	56(4)	46(4)	55(5)	11(3)	-13(3)	4(3)
C(17)	94(6)	49(4)	35(4)	-6(3)	1(4)	-20(4)
N(1)	35(2)	26(2)	32(3)	2(2)	-5(2)	-1(2)
N(2)	39(3)	29(2)	33(3)	1(2)	1(2)	2(2)
N(3)	62(3)	33(2)	34(3)	-5(2)	-9(2)	2(2)
N(4)	40(2)	44(3)	29(3)	-8(2)	6(2)	-6(2)
N(5)	45(3)	33(2)	31(3)	2(2)	-3(2)	-6(2)
Cl(1)	47(1)	40(1)	41(1)	-1(1)	11(1)	-2(1)
P(1)	39(1)	45(1)	39(1)	-2(1)	2(1)	-2(1)
F(1)	125(4)	42(2)	95(4)	-10(2)	7(3)	-4(3)
F(2)	170(6)	52(3)	94(4)	-26(3)	36(4)	-34(3)
F(3)	59(2)	85(3)	42(3)	5(2)	-1(2)	5(2)
F(4)	47(2)	104(4)	71(3)	9(3)	20(2)	10(2)
F(5)	75(3)	77(3)	59(3)	18(2)	-1(2)	4(2)
F(6)	43(2)	160(5)	68(3)	-7(3)	3(2)	-6(3)
Ni(1)	32(1)	29(1)	30(1)	-1(1)	0(1)	-1(1)

Table 1. Crystal data and structure refinement for sja26_12.

Identification code	shelxl	
Empirical formula	C17 H29 Cu F12 N5 P2	
Formula weight	656.93	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 11.4577(9) Å	α= 90°.
	b = 12.2495(14) Å	β= 95.837(6)°.
	c = 17.1539(14) Å	γ = 90°.
Volume	2395.1(4) $Å^3$	
Z	4	
Density (calculated)	1.822 Mg/m^3	
Absorption coefficient	1.157 mm^{-1}	
F(000)	1332	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.64 to 25.00°.	
Index ranges	-13<=h<=13, 0<=k<=14, 0<=l<=20	
Reflections collected	4213	
Independent reflections	4213 [R(int) = 0.0000]	
Completeness to theta = 25.00°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4213 / 0 / 334	
Goodness-of-fit on F^2	0.716	
Final R indices [I>2sigma(I)]	R1 = 0.0574, wR2 = 0.1289	
R indices (all data)	R1 = 0.1125, wR2 = 0.1389	
Largest diff. peak and hole	0.956 and -0.526 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sja26_12. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7936(7)	2084(8)	9436(4)	60(2)
C(2)	6689(6)	1897(6)	9099(4)	44(2)
C(3)	5078(7)	2812(9)	8248(5)	75(3)
C(4)	5018(8)	3245(14)	7530(6)	138(6)
C(5)	5964(10)	4973(9)	7369(6)	96(4)
C(6)	6924(9)	5539(9)	7875(5)	82(3)
C(7)	8565(7)	4931(8)	8879(5)	62(3)
C(8)	9010(6)	3860(7)	9296(4)	49(2)
C(9)	6096(8)	3742(7)	9377(5)	65(3)
C(10)	6495(7)	4855(8)	9196(5)	58(2)
C(11)	9490(6)	2248(7)	8541(4)	47(2)
C(12)	9725(5)	2803(6)	7783(4)	39(2)
C(13)	10795(6)	2705(8)	7484(4)	56(2)
C(14)	10909(7)	3189(8)	6768(4)	58(2)
C(15)	10016(6)	3782(7)	6397(4)	46(2)
C(16)	8976(6)	3840(7)	6737(4)	49(2)
C(17)	6049(8)	3551(8)	6419(4)	70(3)
N(1)	8560(5)	2844(5)	8905(3)	39(2)
N(2)	6181(4)	2909(5)	8758(3)	39(2)
N(3)	6042(5)	3792(6)	7259(3)	45(2)
N(4)	7329(5)	4890(6)	8589(4)	50(2)
N(5)	8816(4)	3369(6)	7415(3)	40(2)
P(1)	7715(2)	471(2)	6666(1)	38(1)
P(2)	12810(2)	3560(2)	4883(1)	49(1)
F(1)	7279(4)	1257(4)	7329(2)	53(1)
F(2)	6437(3)	521(4)	6196(2)	53(1)
F(3)	8087(4)	1506(4)	6198(2)	55(1)
F(4)	8146(4)	-288(4)	6000(3)	75(2)
F(5)	8981(3)	419(4)	7134(2)	56(1)
F(6)	7307(4)	-547(4)	7135(3)	72(1)

F(7)	13083(5)	3812(7)	5773(3)	129(3)
F(8)	11795(5)	2772(6)	5040(3)	104(2)
F(9)	11905(8)	4511(7)	4820(5)	180(4)
F(10)	12519(4)	3406(6)	3982(2)	88(2)
F(11)	13882(6)	4255(8)	4734(3)	152(4)
F(12)	13694(8)	2642(8)	4931(5)	162(3)
Cu(1)	7402(1)	3318(1)	8020(1)	33(1)

Table 3. Bond lengths [Å] and angles [°] for sja26_12.

C(1)-C(2)	1.504(10)
C(1)-N(1)	1.530(9)
C(2)-N(2)	1.466(9)
C(3)-C(4)	1.337(12)
C(3)-N(2)	1.466(9)
C(4)-N(3)	1.467(11)
C(5)-N(3)	1.463(12)
C(5)-C(6)	1.500(13)
C(6)-N(4)	1.494(11)
C(7)-N(4)	1.452(10)
C(7)-C(8)	1.555(12)
C(8)-N(1)	1.481(10)
C(9)-C(10)	1.481(12)
C(9)-N(2)	1.484(9)
C(10)-N(4)	1.484(9)
C(11)-N(1)	1.481(8)
C(11)-C(12)	1.515(9)
C(12)-N(5)	1.352(8)
C(12)-C(13)	1.383(9)
C(13)-C(14)	1.381(10)
C(14)-C(15)	1.359(11)
C(15)-C(16)	1.381(9)
C(16)-N(5)	1.328(8)
C(17)-N(3)	1.471(9)
N(1)-Cu(1)	1.998(6)
N(2)-Cu(1)	2.042(5)
N(3)-Cu(1)	2.014(6)
N(4)-Cu(1)	2.165(7)
N(5)-Cu(1)	2.012(5)
P(1)-F(6)	1.580(5)
P(1)-F(3)	1.582(5)
P(1)-F(5)	1.586(4)
P(1)-F(4)	1.590(5)

P(1)-F(2)	1.598(4)
P(1)-F(1)	1.608(4)
P(2)-F(12)	1.510(8)
P(2)-F(11)	1.537(6)
P(2)-F(9)	1.556(7)
P(2)-F(8)	1.557(5)
P(2)-F(7)	1.558(5)
P(2)-F(10)	1.559(5)

C(2)-C(1)-N(1)	110.3(6)
N(2)-C(2)-C(1)	110.4(6)
C(4)-C(3)-N(2)	118.6(8)
C(3)-C(4)-N(3)	120.3(8)
N(3)-C(5)-C(6)	118.8(8)
N(4)-C(6)-C(5)	112.2(9)
N(4)-C(7)-C(8)	113.0(7)
N(1)-C(8)-C(7)	114.7(6)
C(10)-C(9)-N(2)	116.0(6)
C(9)-C(10)-N(4)	114.1(7)
N(1)-C(11)-C(12)	109.8(6)
N(5)-C(12)-C(13)	122.7(7)
N(5)-C(12)-C(11)	115.8(5)
C(13)-C(12)-C(11)	121.4(7)
C(14)-C(13)-C(12)	117.4(7)
C(15)-C(14)-C(13)	120.8(7)
C(14)-C(15)-C(16)	118.1(7)
N(5)-C(16)-C(15)	123.3(7)
C(8)-N(1)-C(11)	111.9(6)
C(8)-N(1)-C(1)	113.8(5)
C(11)-N(1)-C(1)	110.5(6)
C(8)-N(1)-Cu(1)	105.9(5)
C(11)-N(1)-Cu(1)	105.9(4)
C(1)-N(1)-Cu(1)	108.3(4)
C(2)-N(2)-C(3)	116.9(7)
C(2)-N(2)-C(9)	110.4(6)

C(3)-N(2)-C(9)	111.6(7)
C(2)-N(2)-Cu(1)	100.7(4)
C(3)-N(2)-Cu(1)	104.7(4)
C(9)-N(2)-Cu(1)	112.0(4)
C(5)-N(3)-C(4)	110.4(9)
C(5)-N(3)-C(17)	109.3(7)
C(4)-N(3)-C(17)	107.7(7)
C(5)-N(3)-Cu(1)	104.7(5)
C(4)-N(3)-Cu(1)	104.7(6)
C(17)-N(3)-Cu(1)	119.8(5)
C(7)-N(4)-C(10)	115.9(6)
C(7)-N(4)-C(6)	118.2(7)
C(10)-N(4)-C(6)	114.9(7)
C(7)-N(4)-Cu(1)	96.0(5)
C(10)-N(4)-Cu(1)	110.3(5)
C(6)-N(4)-Cu(1)	97.2(5)
C(16)-N(5)-C(12)	117.7(6)
C(16)-N(5)-Cu(1)	130.9(5)
C(12)-N(5)-Cu(1)	111.4(4)
F(6)-P(1)-F(3)	178.3(3)
F(6)-P(1)-F(5)	90.8(3)
F(3)-P(1)-F(5)	90.5(2)
F(6)-P(1)-F(4)	91.9(3)
F(3)-P(1)-F(4)	89.1(3)
F(5)-P(1)-F(4)	90.3(2)
F(6)-P(1)-F(2)	89.1(2)
F(3)-P(1)-F(2)	89.7(2)
F(5)-P(1)-F(2)	179.8(3)
F(4)-P(1)-F(2)	89.7(2)
F(6)-P(1)-F(1)	89.1(3)
F(3)-P(1)-F(1)	89.9(2)
F(5)-P(1)-F(1)	90.0(2)
F(4)-P(1)-F(1)	179.0(3)
F(2)-P(1)-F(1)	90.0(2)
F(12)-P(2)-F(11)	83.1(5)

F(12)-P(2)-F(9)	179.1(5)
F(11)-P(2)-F(9)	96.5(6)
F(12)-P(2)-F(8)	92.1(5)
F(11)-P(2)-F(8)	175.2(5)
F(9)-P(2)-F(8)	88.4(5)
F(12)-P(2)-F(7)	91.6(4)
F(11)-P(2)-F(7)	88.3(3)
F(9)-P(2)-F(7)	89.2(4)
F(8)-P(2)-F(7)	91.8(3)
F(12)-P(2)-F(10)	92.2(4)
F(11)-P(2)-F(10)	89.8(3)
F(9)-P(2)-F(10)	87.0(4)
F(8)-P(2)-F(10)	90.4(3)
F(7)-P(2)-F(10)	175.5(5)
N(1)-Cu(1)-N(5)	83.9(2)
N(1)-Cu(1)-N(3)	170.6(2)
N(5)-Cu(1)-N(3)	105.5(2)
N(1)-Cu(1)-N(2)	84.4(2)
N(5)-Cu(1)-N(2)	164.9(3)
N(3)-Cu(1)-N(2)	86.5(2)
N(1)-Cu(1)-N(4)	88.2(2)
N(5)-Cu(1)-N(4)	106.0(2)
N(3)-Cu(1)-N(4)	88.5(2)
N(2)-Cu(1)-N(4)	83.0(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sja26_12. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	62(5)	79(7)	40(4)	24(4)	15(4)	-2(5)
C(2)	48(4)	53(6)	34(4)	4(4)	18(3)	0(4)
C(3)	59(6)	99(8)	63(6)	22(5)	-9(4)	-26(5)
C(4)	42(5)	284(19)	88(7)	69(10)	10(5)	-36(9)
C(5)	132(10)	73(8)	76(7)	-5(6)	-30(7)	55(7)
C(6)	79(7)	94(9)	72(6)	11(6)	1(5)	3(6)
C(7)	49(5)	81(7)	62(5)	-28(5)	27(4)	-21(5)
C(8)	38(4)	75(6)	35(4)	2(4)	10(3)	6(4)
C(9)	91(6)	57(6)	56(5)	-3(5)	45(5)	-6(5)
C(10)	38(4)	80(7)	59(5)	-25(5)	21(4)	-6(4)
C(11)	42(4)	67(6)	34(4)	1(4)	8(3)	13(4)
C(12)	26(4)	57(5)	35(4)	-8(4)	3(3)	3(4)
C(13)	33(4)	88(7)	48(4)	-11(5)	13(3)	5(4)
C(14)	54(5)	80(7)	46(4)	-20(5)	33(4)	-14(5)
C(15)	34(4)	69(6)	37(4)	-3(4)	13(3)	-12(4)
C(16)	48(4)	63(6)	38(4)	1(4)	10(3)	-8(4)
C(17)	74(6)	96(9)	38(4)	9(5)	0(4)	8(6)
N(1)	33(3)	61(5)	24(3)	-5(3)	10(2)	-8(3)
N(2)	28(3)	58(5)	34(3)	2(3)	15(2)	-7(3)
N(3)	42(3)	58(5)	36(3)	1(3)	10(3)	3(3)
N(4)	36(3)	59(5)	56(4)	8(3)	12(3)	1(3)
N(5)	32(3)	58(4)	31(3)	-1(3)	14(2)	2(3)
P(1)	32(1)	48(1)	37(1)	-2(1)	9(1)	0(1)
P(2)	37(1)	79(2)	34(1)	-5(1)	13(1)	-10(1)
F(1)	56(2)	73(3)	33(2)	-2(2)	21(2)	13(2)
F(2)	38(2)	71(3)	48(2)	12(2)	2(2)	2(2)
F(3)	66(3)	67(3)	34(2)	4(2)	20(2)	-17(2)
F(4)	63(3)	82(4)	81(3)	-45(3)	15(2)	5(3)
F(5)	38(2)	65(3)	64(3)	-5(2)	4(2)	0(2)
F(6)	58(3)	65(3)	90(4)	32(3)	0(2)	-12(3)

F(7)	75(4)	276(9)	39(3)	-30(4)	19(2)	-65(5)
F(8)	108(4)	146(6)	63(3)	-12(3)	30(3)	-68(4)
F(9)	227(10)	155(8)	151(7)	-41(6)	-6(6)	115(8)
F(10)	73(3)	152(6)	41(2)	-19(3)	13(2)	-29(4)
F(11)	130(5)	256(10)	75(4)	-14(5)	34(4)	-133(6)
F(12)	147(7)	188(9)	153(7)	30(6)	21(5)	82(7)
Cu(1)	25(1)	51(1)	24(1)	2(1)	10(1)	2(1)