SUPPORTING INFORMATION

FOR

Neutral and dianionic Iron and Ruthenium 1,4-Diphosphabutadiene Complexes.

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X-ray data for complex 2.

X-ray data for complex 5.

Table 1. Crystal data for complex **2.**

Compound	**2**
Molecular formula	$C_{212}H_{296}Fe_2N_8Na_4O_{33}P_8$
Molecular weight	3935.99
Crystal habit	brown needle
Crystal dimensions(mm)	0.22x0.12x0.12
Crystal system	monoclinic
Space group	C2/c
a(Å)	52.6790(10)
b(Å)	13.7220(10)
c(Å)	30.6390(10)
α(°)	90.00
β(°)	113.1900(10)
γ(°)	90.00
V(Å^3)	20358.3(17)
Z	4
d(g-cm^{-3})	1.284
F000	8416
μ(cm^{-1})	0.286
Absorption corrections	multiple scans ; 0.9397 min, 0.9664 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(10)
Scan mode	phi and omega scans
Maximum θ	20.81
HKL ranges	-52 52 ; -13 13 ; -30 30
Reflections measured	17520
Unique data	10501
Rint	0.0666
Reflections used	6551
Criterion	>2sigma(I)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	1203
Reflections / parameter	5
wR2	0.2125
R1	0.0737
Weights a, b	0.0909 ; 85.088
GoF	1.045
difference peak / hole (e Å^{-3})	0.444(0.058) / -0.296(0.058)

TABLE 2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**

atom	x	y	z	U(eq)
Fe(1)	1270(1)	749(1)	7413(1)	53(1)
P(1)	1575(1)	628(1)	8161(1)	56(1)
P(2)	1066(1)	-417(1)	7659(1)	54(1)
P(3)	1299(1)	2315(1)	7219(1)	54(1)
P(4)	1120(1)	523(1)	6624(1)	54(1)
Na(1)	2399(1)	-2818(1)	7915(1)	67(1)
Na(2)	-301(1)	1627(1)	6085(1)	60(1)
O(1)	2651(1)	-4388(1)	8132(1)	72(1)
O(2)	2383(1)	-3538(1)	8650(1)	79(1)
O(3)	2181(1)	-1237(1)	7818(1)	69(1)
O(4)	2685(1)	-1584(1)	8536(1)	73(1)
O(5)	2389(1)	-2285(1)	7134(1)	75(1)
O(6)	2106(1)	-3906(1)	7225(1)	70(1)
O(7)	117(1)	2041(1)	6771(1)	73(1)
O(8)	-324(1)	3301(1)	6372(1)	77(1)
O(9)	-340(1)	480(1)	6698(1)	102(1)
O(10)	-224(1)	-108(1)	5963(1)	84(1)
O(11)	-297(1)	2573(1)	5371(1)	77(1)
O(12)	-703(1)	1349(1)	5361(1)	73(1)
N(1)	2916(1)	-2642(1)	7958(1)	69(1)
N(2)	1872(1)	-2986(1)	7855(1)	75(1)
N(3)	169(1)	1313(1)	5906(1)	60(1)
N(4)	-765(1)	1922(1)	6251(1)	72(1)
C(1)	1468(1)	-210(1)	8512(1)	53(1)
C(2)	1257(1)	-816(1)	8257(1)	52(1)
C(3)	1145(1)	2490(1)	6586(1)	48(1)
C(4)	1122(1)	1649(1)	6319(1)	49(1)
C(5)	1707(1)	1684(1)	8538(1)	54(1)
C(6)	1589(1)	2091(1)	8819(1)	72(1)
C(7)	1674(1)	2939(1)	9074(1)	85(1)
C(8)	1894(1)	3434(1)	9054(1)	85(1)
C(9)	2025(1)	3048(1)	8782(1)	97(1)
C(10)	1931(1)	2186(1)	8528(1)	76(1)
C(11)	1614(1)	-233(1)	9041(1)	54(1)
C(12)	1471(1)	-338(1)	9333(1)	55(1)
C(13)	1602(1)	-326(1)	9820(1)	64(1)
C(14)	1886(1)	-200(1)	10034(1)	76(1)
C(15)	2035(1)	-95(1)	9752(1)	69(1)
C(16)	1901(1)	-109(1)	9265(1)	59(1)
C(17)	1177(1)	-1687(1)	8457(1)	53(1)
C(18)	901(1)	-1890(1)	8357(1)	61(1)
C(19)	820(1)	-2719(1)	8537(1)	68(1)
C(20)	1013(1)	-3341(1)	8820(1)	70(1)
C(21)	1289(1)	-3181(1)	8926(1)	68(1)
C(22)	1367(1)	-2342(1)	8742(1)	58(1)
C(23)	902(1)	-1484(1)	7310(1)	52(1)
C(24)	996(1)	-2449(1)	7398(1)	61(1)
C(25)	861(1)	-3185(1)	7086(1)	69(1)
C(26)	635(1)	-3001(1)	6681(1)	80(1)
C(27)	534(1)	-2061(1)	6586(1)	75(1)
C(28)	669(1)	-1328(1)	6899(1)	64(1)
C(29)	1151(1)	3271(1)	7463(1)	55(1)
C(30)	1317(1)	3708(1)	7888(1)	68(1)
C(31)	1222(1)	4452(1)	8091(1)	79(1)

C(32)	956(1)	4767(1)	7869(1)	77(1)
C(33)	784(1)	4360(1)	7447(1)	69(1)
C(34)	882(1)	3603(1)	7248(1)	61(1)
C(35)	1060(1)	3456(1)	6376(1)	49(1)
C(36)	1203(1)	4285(1)	6592(1)	61(1)
C(37)	1112(1)	5214(1)	6428(1)	73(1)
C(38)	870(1)	5338(1)	6033(1)	82(1)
C(39)	726(1)	4524(1)	5805(1)	78(1)
C(40)	813(1)	3585(1)	5970(1)	60(1)
C(41)	1067(1)	1657(1)	5806(1)	49(1)
C(42)	1216(1)	2261(1)	5624(1)	60(1)
C(43)	1170(1)	2262(1)	5148(1)	70(1)
C(44)	970(1)	1668(1)	4833(1)	73(1)
C(45)	819(1)	1062(1)	5003(1)	67(1)
C(46)	873(1)	1046(1)	5487(1)	55(1)
C(47)	1273(1)	-405(1)	6372(1)	47(1)
C(48)	1221(1)	-1392(1)	6434(1)	59(1)
C(49)	1323(1)	-2112(1)	6243(1)	66(1)
C(50)	1480(1)	-1928(1)	5980(1)	64(1)
C(51)	1533(1)	-975(1)	5923(1)	57(1)
C(52)	1435(1)	-221(1)	6115(1)	56(1)
C(53)	2711(1)	-4662(1)	8607(1)	79(1)
C(54)	2458(1)	-4554(1)	8704(1)	83(1)
C(55)	2130(1)	-3329(1)	8710(1)	94(1)
C(56)	1876(1)	-3536(1)	8261(1)	89(1)
C(57)	1770(1)	-1964(1)	7846(1)	86(1)
C(58)	1891(1)	-1293(1)	7600(1)	76(1)
C(59)	2278(1)	-632(1)	8225(1)	78(1)
C(60)	2587(1)	-616(1)	8392(1)	81(1)
C(61)	2974(1)	-1684(1)	8666(1)	79(1)
C(62)	3051(1)	-1811(1)	8259(1)	79(1)
C(63)	2882(1)	-4433(1)	7996(1)	73(1)
C(64)	3066(1)	-3534(1)	8154(1)	73(1)
C(65)	2890(1)	-2482(1)	7466(1)	80(1)
C(66)	2645(1)	-1850(1)	7188(1)	80(1)
C(67)	2296(1)	-2999(1)	6770(1)	84(1)
C(68)	2042(1)	-3434(1)	6779(1)	80(1)
C(69)	1875(1)	-4282(1)	7289(1)	73(1)
C(70)	1710(1)	-3501(1)	7405(1)	81(1)
C(71)	399(1)	1745(1)	6310(1)	70(1)
C(72)	362(1)	1600(1)	6772(1)	67(1)
C(73)	142(1)	3050(1)	6868(1)	80(1)
C(74)	-124(1)	3396(1)	6854(1)	84(1)
C(75)	-599(1)	3594(1)	6289(1)	91(1)
C(76)	-752(1)	2895(1)	6456(1)	96(1)
C(77)	-793(1)	1142(1)	6555(1)	84(1)
C(78)	-516(1)	843(1)	6910(1)	80(1)
C(79)	-333(1)	-465(1)	6618(1)	107(1)
C(80)	-160(1)	-718(1)	6366(1)	76(1)
C(81)	-64(1)	-265(1)	5690(1)	72(1)
C(82)	206(1)	265(1)	5877(1)	71(1)
C(83)	136(1)	1777(1)	5461(1)	70(1)
C(84)	-23(1)	2716(1)	5389(1)	84(1)
C(85)	-485(1)	2161(1)	4934(1)	92(1)
C(86)	-753(1)	2006(1)	4984(1)	101(1)
C(87)	-940(1)	1143(1)	5456(1)	81(1)
C(88)	-987(1)	1892(1)	5773(1)	91(1)
C(89)	2651(1)	-1390(1)	9621(1)	145(1)
C(90)	2794(1)	-859(1)	10044(1)	127(1)
O(91)	3044(1)	-1286(1)	10317(1)	140(1)
C(92)	3053(1)	-2217(1)	10098(1)	151(1)

C(93)	2787(1)	-2389(1)	9718(1)	114(1)
C(94)	2596(1)	1317(2)	9325(1)	290(1)
C(95)	2624(1)	1989(1)	9644(1)	371(1)
O(96)	2728(1)	2796(1)	9724(1)	558(2)
C(97)	3015(1)	2333(2)	9584(1)	330(1)
C(98)	2857(1)	1352(1)	9331(1)	191(1)
C(99)	-185(1)	-4716(1)	5786(1)	291(1)
C(100)	-41(1)	-4362(1)	5626(1)	218(1)
O(101)	-89(1)	-3329(1)	5618(1)	233(1)
C(102)	-353(1)	-3245(1)	5563(1)	181(1)
C(104)	3779(1)	553(1)	10295(1)	275(1)
C(105)	3566(1)	603(2)	10039(1)	511(2)
C(106)	3872(1)	314(1)	9883(1)	299(1)
O(103)	3620(1)	89(1)	9463(1)	286(1)
C(108)	95(1)	-2738(1)	7365(1)	137(1)
C(109)	181(1)	-3774(1)	7417(1)	151(1)
O(110)	0	5701(1)	7500	298(1)
C(107)	-400(1)	-4052(1)	5797(1)	283(1)
C(103)	3408(1)	143(2)	9608(1)	415(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

TABLE 3. Bond lengths (A) and angles (deg) for **2**

Fe(1)-P(2)	2.2194(3	Fe(1)-P(1)	2.2292(2)
Fe(1)-P(4)	2.2471(2	Fe(1)-P(3)	2.2506(3)
P(1)-C(1)	1.8097(8	P(1)-C(5)	1.8122(7)
P(2)-C(2)	1.7938(6	P(2)-C(23)	1.8174(7)
P(3)-C(3)	1.8014(6	P(3)-C(29)	1.8309(8)
P(4)-C(4)	1.8078(7	P(4)-C(47)	1.8347(8)
Na(1)-O(3)	2.4180(6	Na(1)-O(1)	2.4811(6)
Na(1)-O(5)	2.4849(6	Na(1)-O(2)	2.4886(6)
Na(1)-O(4)	2.5488(5	Na(1)-O(6)	2.5507(5)
Na(1)-N(1)	2.6857(8	Na(1)-N(2)	2.7174(8)
Na(2)-O(12)	2.4201(5	Na(2)-O(7)	2.4378(5)
Na(2)-O(10)	2.4676(6	Na(2)-O(8)	2.4793(6)
Na(2)-O(9)	2.5212(7	Na(2)-O(11)	2.5508(6)
Na(2)-N(4)	2.7154(8	Na(2)-N(3)	2.7705(7)
O(1)-C(53)	1.413(1)	O(1)-C(63)	1.436(1)
O(2)-C(55)	1.441(1)	O(2)-C(54)	1.441(1)
O(3)-C(58)	1.408(1)	O(3)-C(59)	1.414(1)
O(4)-C(61)	1.421(1)	O(4)-C(60)	1.430(1)
O(5)-C(67)	1.420(1)	O(5)-C(66)	1.423(1)
O(6)-C(69)	1.406(1)	O(6)-C(68)	1.427(1)
O(7)-C(73)	1.410(1)	O(7)-C(72)	1.423(1)
O(8)-C(75)	1.429(1)	O(8)-C(74)	1.4449(8)
O(9)-C(79)	1.322(1)	O(9)-C(78)	1.417(1)
O(10)-C(80)	1.419(1)	O(10)-C(81)	1.419(1)
O(11)-C(85)	1.4314(8	O(11)-C(84)	1.434(1)
O(12)-C(86)	1.406(1)	O(12)-C(87)	1.417(1)
N(1)-C(64)	1.454(1)	N(1)-C(62)	1.464(1)
N(1)-C(65)	1.476(1)	N(2)-C(56)	1.449(1)
N(2)-C(70)	1.482(1)	N(2)-C(57)	1.498(1)
N(3)-C(83)	1.453(1)	N(3)-C(82)	1.458(1)
N(3)-C(71)	1.4728(8	N(4)-C(77)	1.464(1)
N(4)-C(76)	1.466(1)	N(4)-C(88)	1.474(1)
C(1)-C(2)	1.362(1)	C(1)-C(11)	1.4958(8)
C(2)-C(17)	1.478(1)	C(3)-C(4)	1.391(1)
C(3)-C(35)	1.464(1)	C(4)-C(41)	1.483(1)
C(5)-C(6)	1.365(1)	C(5)-C(10)	1.378(1)
C(6)-C(7)	1.374(1)	C(7)-C(8)	1.369(1)
C(8)-C(9)	1.378(2)	C(9)-C(10)	1.395(1)
C(11)-C(12)	1.385(1)	C(11)-C(16)	1.405(1)
C(12)-C(13)	1.373(1)	C(13)-C(14)	1.384(1)
C(14)-C(15)	1.383(1)	C(15)-C(16)	1.378(1)
C(17)-C(22)	1.372(1)	C(17)-C(18)	1.388(1)
C(18)-C(19)	1.403(1)	C(19)-C(20)	1.350(1)
C(20)-C(21)	1.378(1)	C(21)-C(22)	1.412(1)
C(23)-C(28)	1.3870(8	C(23)-C(24)	1.403(1)
C(24)-C(25)	1.382(1)	C(25)-C(26)	1.360(1)
C(26)-C(27)	1.383(1)	C(27)-C(28)	1.379(1)
C(29)-C(34)	1.383(1)	C(29)-C(30)	1.386(1)
C(30)-C(31)	1.389(1)	C(31)-C(32)	1.363(1)
C(32)-C(33)	1.371(1)	C(33)-C(34)	1.402(1)
C(35)-C(36)	1.381(1)	C(35)-C(40)	1.4121(8)
C(36)-C(37)	1.384(1)	C(37)-C(38)	1.381(1)
C(38)-C(39)	1.375(1)	C(39)-C(40)	1.395(1)
C(41)-C(46)	1.383(1)	C(41)-C(42)	1.399(1)
C(42)-C(43)	1.382(1)	C(43)-C(44)	1.379(1)
C(44)-C(45)	1.387(1)	C(45)-C(46)	1.398(1)
C(47)-C(52)	1.393(1)	C(47)-C(48)	1.411(1)
C(48)-C(49)	1.362(1)	C(49)-C(50)	1.385(1)
C(50)-C(51)	1.364(1)	C(51)-C(52)	1.384(1)
C(53)-C(54)	1.482(1)	C(55)-C(56)	1.519(1)
C(57)-C(58)	1.482(1)	C(59)-C(60)	1.502(1)
C(61)-C(62)	1.467(1)	C(63)-C(64)	1.526(1)
C(65)-C(66)	1.510(1)	C(67)-C(68)	1.476(1)
C(69)-C(70)	1.510(1)	C(71)-C(72)	1.519(1)
C(73)-C(74)	1.461(1)	C(75)-C(76)	1.468(1)
C(77)-C(78)	1.491(1)	C(79)-C(80)	1.448(1)
C(81)-C(82)	1.493(1)	C(83)-C(84)	1.505(1)
C(85)-C(86)	1.495(1)	C(87)-C(88)	1.499(1)
C(89)-C(90)	1.419(1)	C(89)-C(93)	1.520(2)
C(90)-O(91)	1.384(1)	O(91)-C(92)	1.453(2)
C(92)-C(93)	1.448(1)	C(94)-C(95)	1.311(3)
C(94)-C(98)	1.366(2)	C(95)-O(96)	1.217(2)

C(95)-C(98)	2.029(3)	O(96)-C(97)	1.839(3)
C(97)-C(98)	1.611(3)	C(99)-C(100)	1.160(2)
C(99)-C(107)	1.468(2)	C(100)-O(101)	1.438(2)
O(101)-C(102)	1.337(2)	C(102)-C(107)	1.395(2)
C(104)-C(105)	1.087(3)	C(104)-C(106)	1.561(3)
C(105)-C(103)	1.405(2)	C(105)-C(106)	1.897(4)
C(106)-O(103)	1.473(2)	O(103)-C(103)	1.354(2)
C(108)-C(109)	1.481(2)	C(108)-C(108)#2	1.536(3)
C(109)-O(110)#1	1.297(2)	O(110)-C(109)#1	1.297(2)
O(110)-C(109)#2	1.297(2)		

P(2)-Fe(1)-P(1)	81.139(8)	P(2)-Fe(1)-P(4)	104.721(8)
P(1)-Fe(1)-P(4)	154.35(1)	P(2)-Fe(1)-P(3)	150.54(1)
P(1)-Fe(1)-P(3)	104.179(8	P(4)-Fe(1)-P(3)	83.137(8)
C(1)-P(1)-C(5)	105.11(3)	C(1)-P(1)-Fe(1)	113.01(2)
C(5)-P(1)-Fe(1)	122.43(2)	C(2)-P(2)-C(23)	107.44(3)
C(2)-P(2)-Fe(1)	114.59(2)	C(23)-P(2)-Fe(1)	124.12(3)
C(3)-P(3)-C(29)	104.96(3)	C(3)-P(3)-Fe(1)	111.24(2)
C(29)-P(3)-Fe(1)	119.47(3)	C(4)-P(4)-C(47)	106.36(3)
C(4)-P(4)-Fe(1)	111.49(2)	C(47)-P(4)-Fe(1)	121.51(2)
O(3)-Na(1)-O(1)	172.24(2)	O(3)-Na(1)-O(5)	77.80(2)
O(1)-Na(1)-O(5)	108.57(2)	O(3)-Na(1)-O(2)	106.54(2)
O(1)-Na(1)-O(2)	67.58(2)	O(5)-Na(1)-O(2)	173.11(2)
O(3)-Na(1)-O(4)	66.96(2)	O(1)-Na(1)-O(4)	106.29(2)
O(5)-Na(1)-O(4)	107.72(2)	O(2)-Na(1)-O(4)	79.06(2)
O(3)-Na(1)-O(6)	108.69(2)	O(1)-Na(1)-O(6)	78.37(2)
O(5)-Na(1)-O(6)	66.24(2)	O(2)-Na(1)-O(6)	107.03(2)
O(4)-Na(1)-O(6)	173.58(2)	O(3)-Na(1)-N(1)	110.40(2)
O(1)-Na(1)-N(1)	68.84(2)	O(5)-Na(1)-N(1)	69.81(2)
O(2)-Na(1)-N(1)	112.75(2)	O(4)-Na(1)-N(1)	67.28(2)
O(6)-Na(1)-N(1)	111.22(2)	O(3)-Na(1)-N(2)	69.21(2)
O(1)-Na(1)-N(2)	111.70(2)	O(5)-Na(1)-N(2)	109.08(2)
O(2)-Na(1)-N(2)	68.35(2)	O(4)-Na(1)-N(2)	113.31(2)
O(6)-Na(1)-N(2)	68.08(2)	N(1)-Na(1)-N(2)	178.88(2)
O(12)-Na(2)-O(7)	174.15(2)	O(12)-Na(2)-O(10)	81.16(2)
O(7)-Na(2)-O(10)	102.05(2)	O(12)-Na(2)-O(8)	108.88(2)
O(7)-Na(2)-O(8)	68.39(2)	O(10)-Na(2)-O(8)	168.85(2)
O(12)-Na(2)-O(9)	106.59(2)	O(7)-Na(2)-O(9)	79.25(2)
O(10)-Na(2)-O(9)	64.97(2)	O(8)-Na(2)-O(9)	106.51(2)
O(12)-Na(2)-O(11)	66.09(2)	O(7)-Na(2)-O(11)	108.14(2)
O(10)-Na(2)-O(11)	107.70(2)	O(8)-Na(2)-O(11)	81.42(2)
O(9)-Na(2)-O(11)	170.98(2)	O(12)-Na(2)-N(4)	70.59(2)
O(7)-Na(2)-N(4)	112.10(2)	O(10)-Na(2)-N(4)	112.71(2)
O(8)-Na(2)-N(4)	67.78(2)	O(9)-Na(2)-N(4)	67.01(2)
O(11)-Na(2)-N(4)	113.43(2)	O(12)-Na(2)-N(3)	108.85(2)
O(7)-Na(2)-N(3)	68.48(2)	O(10)-Na(2)-N(3)	66.86(2)
O(8)-Na(2)-N(3)	112.74(2)	O(9)-Na(2)-N(3)	113.02(2)
O(11)-Na(2)-N(3)	66.44(2)	N(4)-Na(2)-N(3)	179.38(2)
C(53)-O(1)-C(63)	114.64(5)	C(53)-O(1)-Na(1)	112.63(5)
C(63)-O(1)-Na(1)	112.73(4)	C(55)-O(2)-C(54)	113.77(7)
C(55)-O(2)-Na(1)	113.42(4)	C(54)-O(2)-Na(1)	112.51(5)
C(58)-O(3)-C(59)	113.60(6)	C(58)-O(3)-Na(1)	112.53(4)
C(59)-O(3)-Na(1)	115.29(4)	C(61)-O(4)-C(60)	113.05(6)
C(61)-O(4)-Na(1)	113.48(5)	C(60)-O(4)-Na(1)	110.59(4)
C(67)-O(5)-C(66)	113.57(7)	C(67)-O(5)-Na(1)	115.06(5)
C(66)-O(5)-Na(1)	110.70(4)	C(69)-O(6)-C(68)	113.98(5)
C(69)-O(6)-Na(1)	111.94(4)	C(68)-O(6)-Na(1)	111.51(4)
C(73)-O(7)-C(72)	114.09(6)	C(73)-O(7)-Na(2)	112.82(4)
C(72)-O(7)-Na(2)	114.36(4)	C(75)-O(8)-C(74)	115.92(7)
C(75)-O(8)-Na(2)	112.76(4)	C(74)-O(8)-Na(2)	109.18(4)
C(79)-O(9)-C(78)	120.07(8)	C(79)-O(9)-Na(2)	117.20(6)
C(78)-O(9)-Na(2)	112.43(5)	C(80)-O(10)-C(81)	115.60(6)
C(80)-O(10)-Na(2)	115.77(5)	C(81)-O(10)-Na(2)	114.04(5)
C(85)-O(11)-C(84)	113.97(6)	C(85)-O(11)-Na(2)	111.37(5)
C(84)-O(11)-Na(2)	112.54(4)	C(86)-O(12)-C(87)	113.76(6)
C(86)-O(12)-Na(2)	117.63(5)	C(87)-O(12)-Na(2)	111.50(4)
C(64)-N(1)-C(62)	110.04(5)	C(64)-N(1)-C(65)	111.26(7)
C(62)-N(1)-C(65)	110.71(7)	C(64)-N(1)-Na(1)	108.78(5)
C(62)-N(1)-Na(1)	109.54(5)	C(65)-N(1)-Na(1)	106.42(4)
C(56)-N(2)-C(70)	111.05(6)	C(56)-N(2)-C(57)	112.84(7)
C(70)-N(2)-C(57)	110.95(5)	C(56)-N(2)-Na(1)	108.30(4)
C(70)-N(2)-Na(1)	107.67(5)	C(57)-N(2)-Na(1)	105.72(5)
C(83)-N(3)-C(82)	110.21(6)	C(83)-N(3)-C(71)	111.46(6)
C(82)-N(3)-C(71)	111.31(5)	C(83)-N(3)-Na(2)	109.36(4)
C(82)-N(3)-Na(2)	108.35(5)	C(71)-N(3)-Na(2)	106.00(5)
C(77)-N(4)-C(76)	113.09(7)	C(77)-N(4)-C(88)	111.88(6)

C(76)-N(4)-C(88)	109.55(6)	C(77)-N(4)-Na(2)	109.61(5)
C(76)-N(4)-Na(2)	108.90(5)	C(88)-N(4)-Na(2)	103.34(5)
C(2)-C(1)-C(11)	124.36(7)	C(2)-C(1)-P(1)	115.05(5)
C(11)-C(1)-P(1)	120.55(5)	C(1)-C(2)-C(17)	123.95(5)
C(1)-C(2)-P(2)	113.67(5)	C(17)-C(2)-P(2)	122.25(4)
C(4)-C(3)-C(35)	123.58(6)	C(4)-C(3)-P(3)	114.76(5)
C(35)-C(3)-P(3)	121.62(5)	C(3)-C(4)-C(41)	123.44(6)
C(3)-C(4)-P(4)	115.03(5)	C(41)-C(4)-P(4)	121.10(5)
C(6)-C(5)-C(10)	114.66(7)	C(6)-C(5)-P(1)	125.03(6)
C(10)-C(5)-P(1)	120.13(6)	C(5)-C(6)-C(7)	125.27(8)
C(8)-C(7)-C(6)	119.2(1)	C(7)-C(8)-C(9)	118.11(8)
C(8)-C(9)-C(10)	120.7(1)	C(5)-C(10)-C(9)	122.0(1)
C(12)-C(11)-C(16)	116.85(6)	C(12)-C(11)-C(1)	121.58(6)
C(16)-C(11)-C(1)	121.52(7)	C(13)-C(12)-C(11)	122.06(7)
C(12)-C(13)-C(14)	120.31(8)	C(15)-C(14)-C(13)	119.13(7)
C(16)-C(15)-C(14)	120.19(7)	C(15)-C(16)-C(11)	121.46(8)
C(22)-C(17)-C(18)	116.57(7)	C(22)-C(17)-C(2)	122.46(6)
C(18)-C(17)-C(2)	120.96(6)	C(17)-C(18)-C(19)	122.03(6)
C(20)-C(19)-C(18)	119.67(7)	C(19)-C(20)-C(21)	120.68(8)
C(20)-C(21)-C(22)	118.73(6)	C(17)-C(22)-C(21)	122.29(7)
C(28)-C(23)-C(24)	116.10(6)	C(28)-C(23)-P(2)	117.08(5)
C(24)-C(23)-P(2)	126.71(4)	C(25)-C(24)-C(23)	120.67(6)
C(26)-C(25)-C(24)	121.55(7)	C(25)-C(26)-C(27)	119.45(7)
C(28)-C(27)-C(26)	118.90(6)	C(27)-C(28)-C(23)	123.30(7)
C(34)-C(29)-C(30)	116.97(7)	C(34)-C(29)-P(3)	124.32(5)
C(30)-C(29)-P(3)	118.71(6)	C(29)-C(30)-C(31)	122.33(7)
C(32)-C(31)-C(30)	119.30(7)	C(31)-C(32)-C(33)	120.56(8)
C(32)-C(33)-C(34)	119.54(7)	C(29)-C(34)-C(33)	121.28(6)
C(36)-C(35)-C(40)	117.26(6)	C(36)-C(35)-C(3)	121.44(5)
C(40)-C(35)-C(3)	121.03(6)	C(35)-C(36)-C(37)	122.65(6)
C(38)-C(37)-C(36)	119.96(7)	C(39)-C(38)-C(37)	118.65(7)
C(38)-C(39)-C(40)	121.98(6)	C(39)-C(40)-C(35)	119.47(6)
C(46)-C(41)-C(42)	116.79(6)	C(46)-C(41)-C(4)	121.69(7)
C(42)-C(41)-C(4)	121.49(5)	C(43)-C(42)-C(41)	121.89(6)
C(44)-C(43)-C(42)	120.55(8)	C(43)-C(44)-C(45)	118.89(7)
C(44)-C(45)-C(46)	120.05(6)	C(41)-C(46)-C(45)	121.76(7)
C(52)-C(47)-C(48)	116.53(7)	C(52)-C(47)-P(4)	125.69(5)
C(48)-C(47)-P(4)	117.78(6)	C(49)-C(48)-C(47)	120.41(8)
C(48)-C(49)-C(50)	123.03(7)	C(51)-C(50)-C(49)	116.64(7)
C(50)-C(51)-C(52)	122.22(8)	C(51)-C(52)-C(47)	121.15(7)
O(1)-C(53)-C(54)	109.07(6)	O(2)-C(54)-C(53)	107.52(7)
O(2)-C(55)-C(56)	112.04(7)	N(2)-C(56)-C(55)	113.01(7)
C(58)-C(57)-N(2)	111.61(8)	O(3)-C(58)-C(57)	113.37(6)
O(3)-C(59)-C(60)	106.17(7)	O(4)-C(60)-C(59)	107.52(7)
O(4)-C(61)-C(62)	113.53(6)	N(1)-C(62)-C(61)	113.47(7)
O(1)-C(63)-C(64)	112.23(7)	N(1)-C(64)-C(63)	112.04(6)
N(1)-C(65)-C(66)	111.92(7)	O(5)-C(66)-C(65)	112.64(7)
O(5)-C(67)-C(68)	107.43(7)	O(6)-C(68)-C(67)	109.07(6)
O(6)-C(69)-C(70)	112.61(7)	N(2)-C(70)-C(69)	112.51(6)
N(3)-C(71)-C(72)	111.34(7)	O(7)-C(72)-C(71)	113.08(5)
O(7)-C(73)-C(74)	107.74(7)	O(8)-C(74)-C(73)	107.75(7)
O(8)-C(75)-C(76)	114.26(7)	N(4)-C(76)-C(75)	112.68(8)
N(4)-C(77)-C(78)	110.43(7)	O(9)-C(78)-C(77)	113.16(6)
O(9)-C(79)-C(80)	113.77(8)	O(10)-C(80)-C(79)	109.83(7)
O(10)-C(81)-C(82)	113.16(6)	N(3)-C(82)-C(81)	112.05(6)
N(3)-C(83)-C(84)	111.44(7)	O(11)-C(84)-C(83)	112.51(7)
O(11)-C(85)-C(86)	107.11(7)	O(12)-C(86)-C(85)	107.31(7)
O(12)-C(87)-C(88)	112.38(7)	N(4)-C(88)-C(87)	113.13(7)
C(90)-C(89)-C(93)	104.20(8)	O(91)-C(90)-C(89)	111.7(1)
C(90)-O(91)-C(92)	106.90(7)	C(93)-C(92)-O(91)	108.4(1)
C(92)-C(93)-C(89)	104.1(1)	C(95)-C(94)-C(98)	98.6(2)
O(96)-C(95)-C(94)	134.3(3)	O(96)-C(95)-C(98)	100.2(2)
C(94)-C(95)-C(98)	41.7(1)	C(95)-O(96)-C(97)	89.2(2)
C(98)-C(97)-O(96)	94.8(1)	C(94)-C(98)-C(97)	111.3(2)
C(94)-C(98)-C(95)	39.7(1)	C(97)-C(98)-C(95)	73.0(1)
C(100)-C(99)-C(107)	113.0(1)	C(99)-C(100)-O(101)	106.2(1)
C(102)-O(101)-C(100)	104.8(1)	O(101)-C(102)-C(107)	104.8(1)
C(105)-C(104)-C(106)	89.7(2)	C(104)-C(105)-C(103)	135.2(3)
C(104)-C(105)-C(106)	55.4(2)	C(103)-C(105)-C(106)	85.1(2)
O(103)-C(106)-C(104)	106.6(2)	O(103)-C(106)-C(105)	72.5(1)
C(104)-C(106)-C(105)	35.0(1)	C(103)-O(103)-C(106)	106.2(1)
C(109)-C(108)-C(108)#2	100.21(8)	O(110)-C(109)#1-C(108)	109.8(1)
C(109)-O(110)#1-C(109)#2	112.5(2)	C(102)-C(107)-C(99)	100.6(1)
O(103)-C(103)-C(105)	94.3(2)		

Estimated standard deviations are given in the parenthesis.

```
Symmetry operators ::
   1: x, y, z              2: -x, y, -z+1/2        3: x+1/2, y+1/2, z
   4: -x+1/2, y+1/2, -z+1/ 5: -x, -y, -z           6: x, -y, z-1/2
   7: -x+1/2, -y+1/2, -z   8: x+1/2, -y+1/2, z-1/2
```

TABLE 4. Anisotropic displacement parameters (A^2 x 10^3) for **2**

atom	U11	U22	U33	U23	U13	U12
Fe(1)	62(1)	42(1)	56(1)	-1(1)	23(1)	0(1)
P(1)	62(1)	46(1)	58(1)	-1(1)	22(1)	-1(1)
P(2)	61(1)	43(1)	56(1)	0(1)	22(1)	0(1)
P(3)	63(1)	42(1)	56(1)	-2(1)	22(1)	0(1)
P(4)	67(1)	39(1)	57(1)	-1(1)	25(1)	-2(1)
Na(1)	65(1)	59(1)	77(1)	-5(1)	28(1)	-4(1)
Na(2)	62(1)	54(1)	65(1)	-3(1)	25(1)	1(1)
O(1)	79(1)	66(1)	67(1)	4(1)	23(1)	-2(1)
O(2)	96(1)	69(1)	70(1)	-5(1)	31(1)	-15(1)
O(3)	58(1)	57(1)	89(1)	-9(1)	25(1)	-4(1)
O(4)	75(1)	52(1)	88(1)	-6(1)	26(1)	-5(1)
O(5)	64(1)	74(1)	82(1)	4(1)	25(1)	8(1)
O(6)	64(1)	67(1)	78(1)	-8(1)	26(1)	3(1)
O(7)	75(1)	74(1)	72(1)	-16(1)	30(1)	-12(1)
O(8)	78(1)	63(1)	101(1)	-11(1)	47(1)	-6(1)
O(9)	164(1)	74(1)	110(1)	13(1)	98(1)	14(1)
O(10)	97(1)	69(1)	103(1)	12(1)	59(1)	6(1)
O(11)	76(1)	81(1)	76(1)	17(1)	32(1)	12(1)
O(12)	67(1)	76(1)	70(1)	6(1)	19(1)	6(1)
N(1)	68(1)	63(1)	67(1)	5(1)	18(1)	4(1)
N(2)	81(1)	58(1)	96(1)	-17(1)	46(1)	-11(1)
N(3)	58(1)	54(1)	66(1)	7(1)	20(1)	5(1)
N(4)	64(1)	68(1)	81(1)	-2(1)	27(1)	-6(1)
C(1)	56(1)	55(1)	51(1)	2(1)	22(1)	11(1)
C(2)	53(1)	45(1)	57(1)	-3(1)	21(1)	-1(1)
C(3)	45(1)	30(1)	69(1)	2(1)	24(1)	-4(1)
C(4)	51(1)	41(1)	51(1)	8(1)	15(1)	1(1)
C(5)	54(1)	57(1)	48(1)	3(1)	17(1)	0(1)
C(6)	82(1)	59(1)	83(1)	-7(1)	41(1)	-12(1)
C(7)	116(1)	60(1)	91(1)	-20(1)	52(1)	-13(1)
C(8)	96(1)	62(1)	75(1)	-12(1)	9(1)	-17(1)
C(9)	96(1)	81(1)	125(1)	-29(1)	55(1)	-37(1)
C(10)	79(1)	75(1)	81(1)	-19(1)	41(1)	-17(1)
C(11)	69(1)	39(1)	58(1)	0(1)	29(1)	3(1)
C(12)	63(1)	43(1)	55(1)	0(1)	19(1)	8(1)
C(13)	87(1)	50(1)	59(1)	-7(1)	33(1)	-2(1)
C(14)	93(1)	77(1)	54(1)	-7(1)	22(1)	-2(1)
C(15)	73(1)	64(1)	63(1)	0(1)	18(1)	8(1)
C(16)	71(1)	38(1)	67(1)	2(1)	26(1)	0(1)
C(17)	63(1)	50(1)	52(1)	-3(1)	30(1)	3(1)
C(18)	62(1)	62(1)	64(1)	-6(1)	31(1)	-1(1)
C(19)	70(1)	70(1)	71(1)	1(1)	33(1)	-4(1)
C(20)	96(1)	60(1)	61(1)	-5(1)	38(1)	-22(1)
C(21)	92(1)	48(1)	64(1)	-4(1)	30(1)	-2(1)
C(22)	58(1)	56(1)	60(1)	-2(1)	21(1)	-3(1)
C(23)	57(1)	48(1)	52(1)	1(1)	24(1)	-2(1)
C(24)	67(1)	46(1)	71(1)	0(1)	29(1)	1(1)
C(25)	89(1)	49(1)	74(1)	-1(1)	36(1)	1(1)
C(26)	91(1)	59(1)	91(1)	-23(1)	36(1)	-18(1)
C(27)	63(1)	77(1)	75(1)	-19(1)	15(1)	10(1)
C(28)	64(1)	51(1)	72(1)	-2(1)	22(1)	4(1)
C(29)	73(1)	34(1)	59(1)	-1(1)	27(1)	-6(1)
C(30)	82(1)	52(1)	59(1)	-3(1)	17(1)	5(1)
C(31)	105(1)	59(1)	60(1)	-3(1)	18(1)	10(1)

C(32)	121(1)	42(1)	79(1)	-10(1)	51(1)	-2(1)
C(33)	72(1)	59(1)	79(1)	-6(1)	34(1)	3(1)
C(34)	73(1)	42(1)	75(1)	-10(1)	37(1)	-5(1)
C(35)	59(1)	40(1)	51(1)	0(1)	24(1)	-2(1)
C(36)	70(1)	42(1)	64(1)	3(1)	21(1)	-2(1)
C(37)	96(1)	44(1)	69(1)	-8(1)	22(1)	-9(1)
C(38)	106(1)	40(1)	94(1)	2(1)	32(1)	7(1)
C(39)	82(1)	74(1)	72(1)	10(1)	25(1)	11(1)
C(40)	59(1)	58(1)	64(1)	2(1)	23(1)	3(1)
C(41)	43(1)	47(1)	55(1)	-1(1)	16(1)	9(1)
C(42)	72(1)	46(1)	64(1)	1(1)	27(1)	-8(1)
C(43)	81(1)	66(1)	73(1)	8(1)	40(1)	3(1)
C(44)	89(1)	71(1)	64(1)	-2(1)	34(1)	7(1)
C(45)	61(1)	66(1)	67(1)	-12(1)	16(1)	-2(1)
C(46)	61(1)	50(1)	56(1)	1(1)	24(1)	4(1)
C(47)	48(1)	46(1)	42(1)	1(1)	13(1)	4(1)
C(48)	74(1)	53(1)	54(1)	3(1)	30(1)	7(1)
C(49)	82(1)	42(1)	68(1)	8(1)	23(1)	-5(1)
C(50)	82(1)	50(1)	65(1)	3(1)	33(1)	18(1)
C(51)	60(1)	51(1)	60(1)	7(1)	23(1)	10(1)
C(52)	55(1)	50(1)	60(1)	0(1)	20(1)	-7(1)
C(53)	85(1)	76(1)	65(1)	16(1)	17(1)	-8(1)
C(54)	97(1)	70(1)	74(1)	16(1)	26(1)	-10(1)
C(55)	120(1)	84(1)	101(1)	-18(1)	69(1)	-17(1)
C(56)	88(1)	86(1)	114(1)	-18(1)	61(1)	-23(1)
C(57)	64(1)	70(1)	128(1)	-26(1)	43(1)	-4(1)
C(58)	69(1)	58(1)	102(1)	-11(1)	34(1)	1(1)
C(59)	77(1)	61(1)	91(1)	-9(1)	29(1)	-4(1)
C(60)	84(1)	57(1)	97(1)	-11(1)	32(1)	-12(1)
C(61)	73(1)	68(1)	82(1)	-4(1)	15(1)	-2(1)
C(62)	61(1)	82(1)	87(1)	6(1)	22(1)	-1(1)
C(63)	77(1)	79(1)	60(1)	10(1)	25(1)	19(1)
C(64)	65(1)	75(1)	73(1)	14(1)	19(1)	7(1)
C(65)	65(1)	88(1)	81(1)	17(1)	23(1)	-1(1)
C(66)	65(1)	90(1)	85(1)	15(1)	29(1)	-5(1)
C(67)	77(1)	103(1)	71(1)	-4(1)	28(1)	4(1)
C(68)	73(1)	82(1)	75(1)	-8(1)	17(1)	10(1)
C(69)	70(1)	56(1)	90(1)	-16(1)	30(1)	-4(1)
C(70)	58(1)	75(1)	105(1)	-20(1)	25(1)	-9(1)
C(71)	60(1)	78(1)	66(1)	-1(1)	20(1)	-7(1)
C(72)	59(1)	67(1)	67(1)	-6(1)	16(1)	-8(1)
C(73)	59(1)	99(1)	84(1)	-30(1)	32(1)	-15(1)
C(74)	92(1)	74(1)	100(1)	-27(1)	52(1)	-19(1)
C(75)	85(1)	64(1)	136(1)	-16(1)	56(1)	9(1)
C(76)	79(1)	92(1)	139(1)	-26(1)	66(1)	-10(1)
C(77)	86(1)	85(1)	89(1)	-2(1)	42(1)	-18(1)
C(78)	102(1)	72(1)	79(1)	-6(1)	51(1)	-14(1)
C(79)	142(1)	74(1)	141(1)	34(1)	96(1)	11(1)
C(80)	91(1)	56(1)	91(1)	12(1)	45(1)	1(1)
C(81)	84(1)	73(1)	71(1)	-12(1)	42(1)	0(1)
C(82)	63(1)	68(1)	79(1)	-7(1)	26(1)	-4(1)
C(83)	61(1)	72(1)	78(1)	4(1)	30(1)	3(1)
C(84)	88(1)	90(1)	89(1)	16(1)	51(1)	0(1)
C(85)	85(1)	118(1)	72(1)	34(1)	30(1)	23(1)
C(86)	81(1)	136(1)	82(1)	31(1)	26(1)	18(1)
C(87)	70(1)	87(1)	84(1)	-11(1)	27(1)	-15(1)
C(88)	71(1)	86(1)	131(1)	8(1)	55(1)	11(1)
C(89)	200(1)	117(1)	92(1)	3(1)	31(1)	58(1)
C(90)	159(1)	82(1)	96(1)	3(1)	1(1)	31(1)
O(91)	119(1)	143(1)	138(1)	-39(1)	28(1)	-1(1)
C(92)	109(1)	116(1)	182(1)	-76(1)	9(1)	13(1)

C(93)	134(1)	98(1)	97(1)	-2(1)	33(1)	-4(1)
C(94)	270(1)	265(2)	414(2)	141(2)	220(1)	114(1)
C(95)	667(3)	270(2)	120(1)	-16(1)	94(1)	257(2)
O(96)	491(2)	153(1)	621(3)	74(2)	-221(2)	-121(1)
C(97)	167(1)	623(3)	150(1)	98(2)	8(1)	-151(2)
C(98)	171(1)	246(2)	148(1)	29(1)	55(1)	84(1)
C(99)	351(1)	132(1)	540(1)	172(1)	338(1)	116(1)
C(100)	268(1)	141(1)	359(1)	-18(1)	247(1)	25(1)
O(101)	238(1)	179(1)	335(1)	90(1)	170(1)	16(1)
C(102)	190(1)	112(1)	275(1)	28(1)	128(1)	43(1)
C(104)	614(2)	135(1)	79(1)	-59(1)	139(1)	-26(1)
C(105)	869(3)	599(4)	159(1)	-84(1)	306(1)	65(3)
C(106)	319(2)	298(2)	294(2)	-179(1)	137(1)	-167(2)
O(103)	356(1)	268(1)	300(1)	-109(1)	200(1)	-101(1)
C(108)	175(1)	109(1)	115(1)	33(1)	44(1)	-38(1)
C(109)	140(1)	134(1)	187(1)	-5(1)	72(1)	7(1)
O(110)	441(2)	126(1)	450(2)	0	309(1)	0
C(107)	345(1)	166(1)	522(1)	34(1)	369(1)	32(1)
C(103)	413(1)	473(2)	599(1)	-404(1)	459(1)	-327(1)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

TABLE 5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**

atom	x	y	z	U(eq)
H(6)	1435	1763	8840	87
H(7)	1581	3177	9263	103
H(8)	1956	4028	9222	102
H(9)	2180	3371	8767	116
H(10)	2024	1936	8343	91
H(12)	1277	-420	9193	66
H(13)	1498	-406.0000	10009	77
H(14)	1976	-186	10369	92
H(15)	2229	-12.0000	9896	83
H(16)	2006	-34	9076	71
H(18)	763	-1453	8161	73
H(19)	629	-2841	8461	82
H(20)	958	-3895	8947	84
H(21)	1425	-3626.9998	9119	82
H(22)	1557	-2226	8818	70
H(24)	1155	-2597.9998	7676	73
H(25)	927	-3835	7155	83
H(26)	548	-3515	6466	96
H(27)	374	-1923.0001	6309	91
H(28)	599	-683	6829	76
H(30)	1502	3491	8045	81
H(31)	1340	4738	8382	95
H(32)	889	5273	8008	92
H(33)	600	4589	7291	82
H(34)	761	3313	6959	73
H(36)	1371	4215	6863	73
H(37)	1217	5766	6587	88
H(38)	804	5972	5921	99
H(39)	563	4605	5527	93
H(40)	708	3036	5809	72
H(42)	1353	2682	5834	73
H(43)	1276	2675	5036	84
H(44)	937	1673	4505	88
H(45)	678	658	4789	81
H(46)	774	604	5601	66
H(48)	1114	-1556	6610	70
H(49)	1284	-2770	6291	79
H(50)	1547	-2441	5847	77
H(51)	1640	-822	5745	69
H(52)	1480	432	6071	67
H(53A)	2859	-4243	8826	95
H(53B)	2775	-5347	8658	95
H(54A)	2306	-4953	8478	99
H(54B)	2493	-4774	9030	99
H(55A)	2129	-2635	8797	113
H(55B)	2123	-3730	8973	113
H(56A)	1870	-4241	8187	107
H(56B)	1709	-3378	8319	107
H(57A)	1566	-1955	7681	103
H(57B)	1817	-1736	8175	103
H(58A)	1835	-1514	7268	91
H(58B)	1813	-634	7592	91
H(59A)	2223	-897	8475	93

H(59B)	2202	35	8144	93
H(60A)	2640	-400	8132	97
H(60B)	2667	-160	8662	97
H(61A)	3040	-2254	8879	95
H(61B)	3068	-1098	8846	95
H(62A)	3004	-1210	8065	95
H(62B)	3254	-1900	8378	95
H(63A)	2814	-4496	7647	87
H(63B)	2992	-5021	8139	87
H(64A)	3143	-3494.0002	8505	88
H(64B)	3222	-3598	8052	88
H(65A)	2870	-3120	7304	96
H(65B)	3061	-2168	7472	96
H(66A)	2664	-1216	7353	96
H(66B)	2645	-1720.9999	6870	96
H(67A)	2439	-3507	6825	101
H(67B)	2257	-2694.9998	6457	101
H(68A)	1902	-2919	6735	96
H(68B)	1965	-3912	6518	96
H(69A)	1937	-4767	7548	87
H(69B)	1755	-4621	6995	87
H(70A)	1644	-3021	7143	98
H(70B)	1544	-3801	7431	98
H(71A)	410	2451	6251	84
H(71B)	575	1441	6335	84
H(72A)	356	893	6832	80
H(72B)	523	1878	7036	80
H(73A)	190	3396	6627	95
H(73B)	289	3172	7185	95
H(74A)	-181.0000	3003	7070	101
H(74B)	-109	4084	6955	101
H(75A)	-702.0001	3697	5944	110
H(75B)	-592	4227	6449	110
H(76A)	-662	2848	6806	115
H(76B)	-942	3138	6372	115
H(77A)	-886	575	6358	101
H(77B)	-908	1372	6723	101
H(78A)	-427	1411	7110	96
H(78B)	-541	334	7118	96
H(79A)	-523	-693.0001	6431	128
H(79B)	-265	-814	6925	128
H(80A)	37	-640	6579	92
H(80B)	-191.0000	-1408	6264	92
H(81A)	-171	-52	5359	87
H(81B)	-28.0000	-972	5683	87
H(82A)	320	12	6197	85
H(82B)	305	138	5668	85
H(83A)	38	1329	5195	84
H(83B)	320	1912	5459	84
H(84A)	78	3168	5653	101
H(84B)	-35	3023	5090	101
H(85A)	-413	1534	4871	110
H(85B)	-511	2609	4666	110
H(86A)	-823	2632	5053	122
H(86B)	-892	1736	4686	122
H(87A)	-917.9999	496	5608	98
H(87B)	-1104	1116	5153	98
H(88A)	-1003	2542	5624	109
H(88B)	-1164	1751	5802	109
H(89A)	2672	-1076	9346	173
H(89B)	2452	-1439.9999	9555	173

H(90A)	2825	-185	9962	153
H(90B)	2678	-823	10231	153
H(92A)	3199	-2205	9969	181
H(92B)	3097	-2745.0002	10336	181
H(93A)	2676	-2856	9818	137
H(93B)	2808	-2648	9432	137
H(94A)	2454	1493	9010	348
H(94B)	2552	671	9422	348
H(95A)	2432	2104	9615	445
H(95B)	2716	1641	9949	445
H(97A)	3059	2764	9364	396
H(97B)	3183	2201	9871	396
H(98A)	2846	1326	9002	229
H(98B)	2963	778	9504	229
H(99A)	-72	-4935	6114	349
H(99B)	-273	-5299	5597	349
H(10A)	-84	-4609	5301	261
H(10B)	155	-4511	5824	261
H(10A)	-477	-3252	5223	217
H(10B)	-382.0000	-2632.0002	5707	217
H(10C)	3811	16	10526	330
H(10D)	3853	1176	10459	330
H(10E)	3543	1305	9958	613
H(10F)	3458	491	10235	613
H(10C)	3969	879	9818	359
H(10D)	3999	-252	9967	359
H(10E)	-5	-2555	7027	165
H(10F)	255	-2297	7514	165
H(10G)	197	-4002	7122	181
H(10H)	364	-3844	7682	181
H(10G)	-587	-4326	5625	339
H(10H)	-376	-3892	6127	339
H(10I)	3339	-505.0000	9651	497
H(10J)	3254	552	9397	497

Figure S1. Ortep view of complex **2** structure**.**

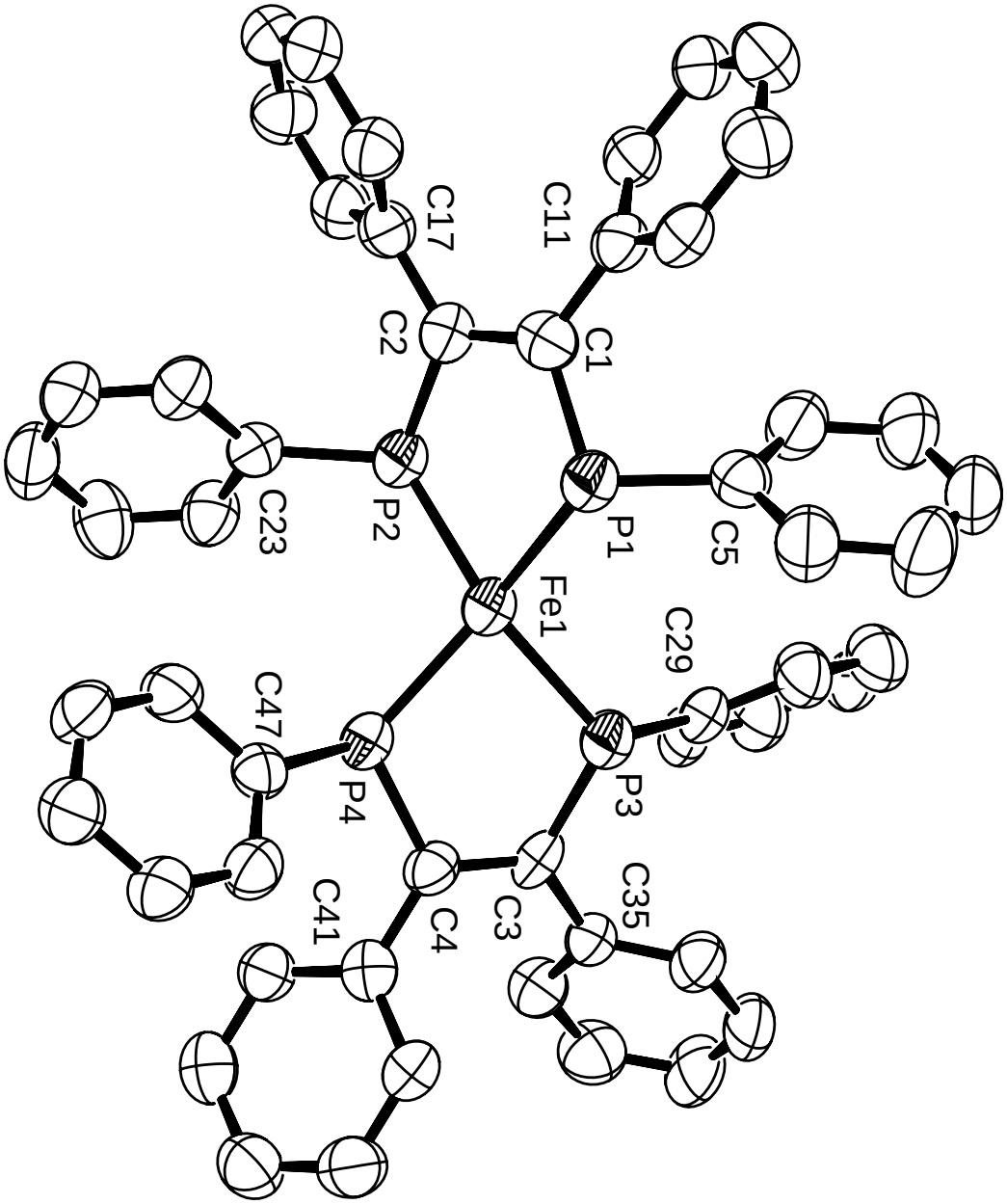

Table 6. Crystal data for complex **5.**

Compound	**5**
Molecular formula	$C_{89}H_{71}Cl_3P_4RuSn_2$
Molecular weight	1709.18
Crystal habit	green cube
Crystal dimensions(mm)	0.16x0.16x0.16
Crystal system	monoclinic
Space group	P21/c
a(Å)	13.36690(10)
b(Å)	52.3062(3)
c(Å)	12.59120(10)
α(°)	90.00
β(°)	115.8570(10)
γ(°)	90.00
V(Å^3)	7922.06(10)
Z	4
d(g-cm^{-3})	1.433
F000	3440
μ(cm^{-1})	1.040
Absorption corrections	multiple scans ; 0.8512 min, 0.8512 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(10)
Scan mode	phi and omega scans
Maximum θ	28.70
HKL ranges	-18 18 ; -69 70 ; -17 17
Reflections measured	32603
Unique data	18771
Rint	0.0302
Reflections used	13381
Criterion	>2sigma(I)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	963
Reflections / parameter	13
wR2	0.1237
R1	0.0454
Weights a, b	0.0701 ; 0.0000
GoF	1.015
difference peak / hole (e Å^{-3})	1.721(0.113) / -0.976(0.113)

Table 7. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**

atom	x	y	z	U(eq)
Cl(1)	4606(1)	-2273(1)	3503(2)	94(1)
Cl(2)	3352(2)	-2233(1)	4838(2)	114(1)
Cl(3)	2277(1)	-2208(1)	2289(2)	118(1)
C(89)	3460(4)	-2128(1)	3561(5)	74(2)
Sn(1)	9654(1)	-1129(1)	2927(1)	23(1)
Sn(2)	6812(1)	-1325(1)	4780(1)	25(1)
Ru(1)	8373(1)	-1249(1)	4016(1)	20(1)
P(1)	9750(1)	-1396(1)	5721(1)	23(1)
P(2)	8524(1)	-1668(1)	3553(1)	24(1)
P(3)	6975(1)	-1076(1)	2361(1)	24(1)
P(4)	8468(1)	-834(1)	4532(1)	23(1)
C(1)	10181(3)	-1704(1)	5732(3)	24(1)
C(2)	9559(3)	-1842(1)	4651(3)	25(1)
C(3)	6778(3)	-753(1)	2446(3)	26(1)
C(4)	7505(3)	-629(1)	3531(3)	25(1)
C(5)	10594(3)	-1248(1)	7121(3)	25(1)
C(6)	10087(3)	-1148(1)	7783(3)	31(1)
C(7)	10720(4)	-1041(1)	8885(3)	44(1)
C(8)	11841(4)	-1035(1)	9295(3)	44(1)
C(9)	12363(3)	-1130(1)	8670(3)	42(1)
C(10)	11750(3)	-1237(1)	7576(3)	32(1)
C(11)	11110(3)	-1828(1)	6750(3)	27(1)
C(12)	11995(3)	-1941(1)	6603(3)	33(1)
C(13)	12867(3)	-2053(1)	7548(4)	42(1)
C(14)	12874(3)	-2060(1)	8637(3)	43(1)
C(15)	12004(3)	-1953(1)	8807(3)	40(1)
C(16)	11123(3)	-1840(1)	7855(3)	32(1)
C(17)	9732(3)	-2115(1)	4518(3)	26(1)
C(18)	10098(3)	-2202(1)	3698(3)	33(1)
C(19)	10265(3)	-2458(1)	3576(3)	39(1)
C(20)	10042(3)	-2639(1)	4264(4)	39(1)
C(21)	9690(3)	-2558(1)	5092(4)	41(1)
C(22)	9547(3)	-2298(1)	5230(3)	37(1)
C(23)	7706(3)	-1899(1)	2421(3)	28(1)
C(24)	7846(3)	-1931(1)	1414(3)	40(1)
C(25)	7215(4)	-2106(1)	564(4)	56(1)
C(26)	6432(4)	-2248(1)	727(5)	65(2)
C(27)	6276(4)	-2218(1)	1732(5)	57(1)
C(28)	6928(3)	-2047(1)	2597(4)	41(1)
C(29)	6114(3)	-1204(1)	904(3)	27(1)
C(30)	5785(3)	-1455(1)	846(3)	36(1)
C(31)	5165(3)	-1571(1)	-233(4)	47(1)
C(32)	4887(3)	-1435(1)	-1257(3)	45(1)
C(33)	5227(3)	-1185(1)	-1221(3)	38(1)
C(34)	5851(3)	-1068(1)	-142(3)	34(1)
C(35)	5971(3)	-603(1)	1419(3)	27(1)
C(36)	4840(3)	-654(1)	952(3)	36(1)
C(37)	4112(3)	-524(1)	-65(4)	44(1)
C(38)	4507(4)	-348(1)	-606(4)	52(1)
C(39)	5634(3)	-293(1)	-123(3)	45(1)
C(40)	6376(3)	-421(1)	894(3)	34(1)
C(41)	7372(3)	-355(1)	3746(3)	27(1)
C(42)	6326(3)	-259(1)	3524(3)	38(1)
C(43)	6181(4)	-7(1)	3729(4)	52(1)
C(44)	7090(5)	159(1)	4146(4)	58(1)
C(45)	8127(4)	68(1)	4369(4)	44(1)
C(46)	8269(3)	-186(1)	4172(3)	33(1)
C(47)	9385(3)	-666(1)	5857(3)	25(1)
C(48)	9009(3)	-527(1)	6550(3)	31(1)
C(49)	9758(3)	-398(1)	7531(3)	35(1)
C(50)	10870(4)	-408(1)	7821(3)	41(1)
C(51)	11267(3)	-551(1)	7168(3)	35(1)
C(52)	10527(3)	-681(1)	6188(3)	28(1)

C(53)	9484(3)	-750(1)	2156(3)	26(1)
C(54)	9743(3)	-528(1)	2831(3)	30(1)
C(55)	9651(3)	-289(1)	2309(3)	36(1)
C(56)	9296(3)	-267(1)	1104(4)	42(1)
C(57)	9043(4)	-487(1)	438(3)	44(1)
C(58)	9131(3)	-721(1)	944(3)	37(1)
C(59)	11406(3)	-1155(1)	4110(3)	28(1)
C(60)	12082(3)	-941(1)	4431(3)	34(1)
C(61)	13218(3)	-965(1)	5192(3)	42(1)
C(62)	13680(3)	-1197(1)	5599(3)	38(1)
C(63)	13018(3)	-1414(1)	5284(3)	40(1)
C(64)	11893(3)	-1394(1)	4558(3)	34(1)
C(65)	9442(3)	-1371(1)	1442(3)	28(1)
C(66)	10273(3)	-1534(1)	1470(3)	34(1)
C(67)	10108(3)	-1692(1)	526(4)	44(1)
C(68)	9111(3)	-1689(1)	-487(3)	43(1)
C(69)	8274(3)	-1526(1)	-540(3)	41(1)
C(70)	8444(3)	-1368(1)	418(3)	32(1)
C(71)	6906(3)	-1660(1)	5842(3)	28(1)
C(72)	7656(3)	-1859(1)	6071(3)	38(1)
C(73)	7618(4)	-2073(1)	6702(4)	46(1)
C(74)	6824(3)	-2090(1)	7125(3)	41(1)
C(75)	6073(4)	-1896(1)	6910(4)	45(1)
C(76)	6102(3)	-1684(1)	6267(4)	41(1)
C(77)	5121(3)	-1378(1)	3430(3)	29(1)
C(78)	4856(3)	-1601(1)	2805(4)	45(1)
C(79)	3801(4)	-1647(1)	1902(4)	55(1)
C(80)	2984(3)	-1464(1)	1634(3)	47(1)
C(81)	3225(4)	-1245(1)	2273(4)	52(1)
C(82)	4289(3)	-1196(1)	3149(3)	39(1)
C(83)	6644(3)	-1013(1)	5825(3)	29(1)
C(84)	7013(3)	-1037(1)	7043(3)	35(1)
C(85)	6886(3)	-843(1)	7708(3)	45(1)
C(86)	6366(3)	-616(1)	7185(4)	48(1)
C(87)	6002(3)	-586(1)	5997(4)	41(1)
C(88)	6136(3)	-780(1)	5316(3)	35(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 8. Bond lengths (A) and angles (deg) for **5**

Cl(1)-C(89)	1.740(6)	Cl(2)-C(89)	1.764(6)
Cl(3)-C(89)	1.742(6)	Sn(1)-C(59)	2.163(3)
Sn(1)-C(65)	2.169(3)	Sn(1)-C(53)	2.176(3)
Sn(1)-Ru(1)	2.6929(3	Sn(2)-C(83)	2.169(4)
Sn(2)-C(71)	2.172(4)	Sn(2)-C(77)	2.174(3)
Sn(2)-Ru(1)	2.6814(3	Ru(1)-P(4)	2.255(1)
Ru(1)-P(1)	2.267(1)	Ru(1)-P(3)	2.293(1)
Ru(1)-P(2)	2.301(1)	P(1)-C(1)	1.711(4)
P(1)-C(5)	1.801(3)	P(2)-C(2)	1.728(3)
P(2)-C(23)	1.822(4)	P(3)-C(3)	1.719(4)
P(3)-C(29)	1.817(3)	P(4)-C(4)	1.724(3)
P(4)-C(47)	1.809(3)	C(1)-C(2)	1.441(5)
C(1)-C(11)	1.488(4)	C(2)-C(17)	1.466(5)
C(3)-C(4)	1.439(5)	C(3)-C(35)	1.494(4)
C(4)-C(41)	1.488(5)	C(5)-C(6)	1.386(5)
C(5)-C(10)	1.395(5)	C(6)-C(7)	1.389(5)
C(7)-C(8)	1.356(6)	C(8)-C(9)	1.355(6)
C(9)-C(10)	1.376(5)	C(11)-C(16)	1.385(5)
C(11)-C(12)	1.403(5)	C(12)-C(13)	1.381(5)
C(13)-C(14)	1.367(6)	C(14)-C(15)	1.390(6)
C(15)-C(16)	1.392(5)	C(17)-C(18)	1.397(5)
C(17)-C(22)	1.404(5)	C(18)-C(19)	1.380(5)
C(19)-C(20)	1.398(6)	C(20)-C(21)	1.384(6)
C(21)-C(22)	1.395(6)	C(23)-C(24)	1.371(5)
C(23)-C(28)	1.390(5)	C(24)-C(25)	1.384(5)
C(25)-C(26)	1.370(7)	C(26)-C(27)	1.378(7)
C(27)-C(28)	1.384(6)	C(29)-C(30)	1.375(5)
C(29)-C(34)	1.400(5)	C(30)-C(31)	1.385(5)
C(31)-C(32)	1.375(6)	C(32)-C(33)	1.378(6)
C(33)-C(34)	1.388(5)	C(35)-C(36)	1.388(5)
C(35)-C(40)	1.394(5)	C(36)-C(37)	1.402(5)
C(37)-C(38)	1.379(6)	C(38)-C(39)	1.386(6)
C(39)-C(40)	1.403(5)	C(41)-C(46)	1.392(5)
C(41)-C(42)	1.395(5)	C(42)-C(43)	1.372(6)
C(43)-C(44)	1.395(7)	C(44)-C(45)	1.374(6)
C(45)-C(46)	1.380(6)	C(47)-C(48)	1.390(5)
C(47)-C(52)	1.397(5)	C(48)-C(49)	1.381(5)
C(49)-C(50)	1.368(6)	C(50)-C(51)	1.379(6)
C(51)-C(52)	1.378(5)	C(53)-C(54)	1.391(5)
C(53)-C(58)	1.396(5)	C(54)-C(55)	1.396(5)
C(55)-C(56)	1.382(5)	C(56)-C(57)	1.377(6)
C(57)-C(58)	1.357(5)	C(59)-C(60)	1.386(5)
C(59)-C(64)	1.406(5)	C(60)-C(61)	1.404(5)
C(61)-C(62)	1.357(6)	C(62)-C(63)	1.386(6)
C(63)-C(64)	1.382(5)	C(65)-C(66)	1.388(5)
C(65)-C(70)	1.394(5)	C(66)-C(67)	1.386(5)
C(67)-C(68)	1.386(6)	C(68)-C(69)	1.383(6)
C(69)-C(70)	1.397(5)	C(71)-C(72)	1.386(5)
C(71)-C(76)	1.400(5)	C(72)-C(73)	1.388(6)
C(73)-C(74)	1.382(6)	C(74)-C(75)	1.370(6)
C(75)-C(76)	1.387(6)	C(77)-C(78)	1.366(6)
C(77)-C(82)	1.388(5)	C(78)-C(79)	1.393(6)
C(79)-C(80)	1.380(6)	C(80)-C(81)	1.354(6)
C(81)-C(82)	1.392(6)	C(83)-C(84)	1.397(5)
C(83)-C(88)	1.406(5)	C(84)-C(85)	1.372(6)
C(85)-C(86)	1.386(6)	C(86)-C(87)	1.366(6)
C(87)-C(88)	1.392(5)		

Cl(1)-C(89)-Cl(3)	108.6(4)	Cl(1)-C(89)-Cl(2)	109.0(3)
Cl(3)-C(89)-Cl(2)	111.1(3)	C(59)-Sn(1)-C(65)	104.6(1)
C(59)-Sn(1)-C(53)	103.6(1)	C(65)-Sn(1)-C(53)	101.3(1)
C(59)-Sn(1)-Ru(1)	111.9(1)	C(65)-Sn(1)-Ru(1)	115.5(1)
C(53)-Sn(1)-Ru(1)	118.2(1)	C(83)-Sn(2)-C(71)	103.1(1)
C(83)-Sn(2)-C(77)	102.8(1)	C(71)-Sn(2)-C(77)	98.1(1)
C(83)-Sn(2)-Ru(1)	114.1(1)	C(71)-Sn(2)-Ru(1)	119.7(1)
C(77)-Sn(2)-Ru(1)	116.4(1)	P(4)-Ru(1)-P(1)	97.65(3)

P(4)-Ru(1)-P(3)	78.55(3)	P(1)-Ru(1)-P(3)	176.01(3)
P(4)-Ru(1)-P(2)	172.36(3)	P(1)-Ru(1)-P(2)	78.00(3)
P(3)-Ru(1)-P(2)	105.91(3)	P(4)-Ru(1)-Sn(2)	89.67(2)
P(1)-Ru(1)-Sn(2)	92.71(2)	P(3)-Ru(1)-Sn(2)	86.09(2)
P(2)-Ru(1)-Sn(2)	96.76(2)	P(4)-Ru(1)-Sn(1)	87.38(2)
P(1)-Ru(1)-Sn(1)	97.30(2)	P(3)-Ru(1)-Sn(1)	83.81(2)
P(2)-Ru(1)-Sn(1)	86.97(2)	Sn(2)-Ru(1)-Sn(1)	169.86(1)
C(1)-P(1)-C(5)	109.4(2)	C(1)-P(1)-Ru(1)	117.3(1)
C(5)-P(1)-Ru(1)	133.2(1)	C(2)-P(2)-C(23)	106.0(2)
C(2)-P(2)-Ru(1)	115.3(1)	C(23)-P(2)-Ru(1)	137.7(1)
C(3)-P(3)-C(29)	112.2(2)	C(3)-P(3)-Ru(1)	114.8(1)
C(29)-P(3)-Ru(1)	132.7(1)	C(4)-P(4)-C(47)	111.3(2)
C(4)-P(4)-Ru(1)	117.2(1)	C(47)-P(4)-Ru(1)	131.5(1)
C(2)-C(1)-C(11)	121.0(3)	C(2)-C(1)-P(1)	114.3(2)
C(11)-C(1)-P(1)	124.7(3)	C(1)-C(2)-C(17)	122.7(3)
C(1)-C(2)-P(2)	115.0(3)	C(17)-C(2)-P(2)	122.1(2)
C(4)-C(3)-C(35)	121.3(3)	C(4)-C(3)-P(3)	116.2(2)
C(35)-C(3)-P(3)	122.3(3)	C(3)-C(4)-C(41)	121.5(3)
C(3)-C(4)-P(4)	113.3(3)	C(41)-C(4)-P(4)	125.2(2)
C(6)-C(5)-C(10)	118.7(3)	C(6)-C(5)-P(1)	119.3(3)
C(10)-C(5)-P(1)	122.0(3)	C(5)-C(6)-C(7)	120.6(4)
C(8)-C(7)-C(6)	118.7(4)	C(9)-C(8)-C(7)	122.3(4)
C(8)-C(9)-C(10)	119.8(4)	C(9)-C(10)-C(5)	119.9(4)
C(16)-C(11)-C(12)	118.1(3)	C(16)-C(11)-C(1)	121.6(3)
C(12)-C(11)-C(1)	120.3(3)	C(13)-C(12)-C(11)	120.5(4)
C(14)-C(13)-C(12)	120.6(4)	C(13)-C(14)-C(15)	120.2(3)
C(14)-C(15)-C(16)	119.2(4)	C(11)-C(16)-C(15)	121.3(4)
C(18)-C(17)-C(22)	117.9(3)	C(18)-C(17)-C(2)	121.6(3)
C(22)-C(17)-C(2)	120.5(3)	C(19)-C(18)-C(17)	121.5(4)
C(18)-C(19)-C(20)	120.0(4)	C(21)-C(20)-C(19)	119.6(4)
C(20)-C(21)-C(22)	120.2(4)	C(21)-C(22)-C(17)	120.7(4)
C(24)-C(23)-C(28)	119.5(4)	C(24)-C(23)-P(2)	121.8(3)
C(28)-C(23)-P(2)	118.7(3)	C(23)-C(24)-C(25)	120.9(4)
C(26)-C(25)-C(24)	119.5(4)	C(25)-C(26)-C(27)	120.4(4)
C(26)-C(27)-C(28)	120.1(5)	C(27)-C(28)-C(23)	119.5(4)
C(30)-C(29)-C(34)	119.4(3)	C(30)-C(29)-P(3)	116.9(3)
C(34)-C(29)-P(3)	123.5(3)	C(29)-C(30)-C(31)	120.7(4)
C(32)-C(31)-C(30)	119.6(4)	C(31)-C(32)-C(33)	120.6(4)
C(32)-C(33)-C(34)	119.9(4)	C(33)-C(34)-C(29)	119.6(4)
C(36)-C(35)-C(40)	120.4(3)	C(36)-C(35)-C(3)	120.5(3)
C(40)-C(35)-C(3)	119.0(3)	C(35)-C(36)-C(37)	119.2(4)
C(38)-C(37)-C(36)	120.8(4)	C(37)-C(38)-C(39)	119.9(4)
C(38)-C(39)-C(40)	120.1(4)	C(35)-C(40)-C(39)	119.6(4)
C(46)-C(41)-C(42)	118.0(4)	C(46)-C(41)-C(4)	122.0(3)
C(42)-C(41)-C(4)	120.0(3)	C(43)-C(42)-C(41)	121.3(4)
C(42)-C(43)-C(44)	119.7(4)	C(45)-C(44)-C(43)	119.9(4)
C(44)-C(45)-C(46)	120.1(4)	C(45)-C(46)-C(41)	121.1(4)
C(48)-C(47)-C(52)	119.3(3)	C(48)-C(47)-P(4)	123.2(3)
C(52)-C(47)-P(4)	117.5(3)	C(49)-C(48)-C(47)	119.9(3)
C(50)-C(49)-C(48)	120.0(4)	C(49)-C(50)-C(51)	121.2(4)
C(52)-C(51)-C(50)	119.3(4)	C(51)-C(52)-C(47)	120.3(3)
C(54)-C(53)-C(58)	116.8(3)	C(54)-C(53)-Sn(1)	122.6(2)
C(58)-C(53)-Sn(1)	120.6(3)	C(53)-C(54)-C(55)	121.0(3)
C(56)-C(55)-C(54)	120.4(4)	C(57)-C(56)-C(55)	118.5(4)
C(58)-C(57)-C(56)	121.1(4)	C(57)-C(58)-C(53)	122.2(4)
C(60)-C(59)-C(64)	118.2(3)	C(60)-C(59)-Sn(1)	121.6(3)
C(64)-C(59)-Sn(1)	120.3(3)	C(59)-C(60)-C(61)	119.9(4)
C(62)-C(61)-C(60)	121.2(4)	C(61)-C(62)-C(63)	119.7(4)
C(64)-C(63)-C(62)	120.0(4)	C(63)-C(64)-C(59)	120.9(4)
C(66)-C(65)-C(70)	117.5(3)	C(66)-C(65)-Sn(1)	122.2(3)
C(70)-C(65)-Sn(1)	120.3(3)	C(67)-C(66)-C(65)	121.3(3)
C(68)-C(67)-C(66)	120.6(4)	C(69)-C(68)-C(67)	119.1(4)
C(68)-C(69)-C(70)	119.9(4)	C(65)-C(70)-C(69)	121.5(4)
C(72)-C(71)-C(76)	117.4(3)	C(72)-C(71)-Sn(2)	125.2(3)
C(76)-C(71)-Sn(2)	117.3(3)	C(71)-C(72)-C(73)	121.5(4)
C(74)-C(73)-C(72)	119.9(4)	C(75)-C(74)-C(73)	119.7(4)
C(74)-C(75)-C(76)	120.3(4)	C(75)-C(76)-C(71)	121.1(4)
C(78)-C(77)-C(82)	117.6(3)	C(78)-C(77)-Sn(2)	118.6(3)
C(82)-C(77)-Sn(2)	123.8(3)	C(77)-C(78)-C(79)	122.2(4)
C(80)-C(79)-C(78)	119.4(5)	C(81)-C(80)-C(79)	118.9(4)

C(80)-C(81)-C(82)	121.7(4)	C(77)-C(82)-C(81)	120.1(4)
C(84)-C(83)-C(88)	116.6(3)	C(84)-C(83)-Sn(2)	121.2(3)
C(88)-C(83)-Sn(2)	122.2(3)	C(85)-C(84)-C(83)	121.7(4)
C(84)-C(85)-C(86)	120.8(4)	C(87)-C(86)-C(85)	119.2(4)
C(86)-C(87)-C(88)	120.5(4)	C(87)-C(88)-C(83)	121.3(4)

Table 9. Anisotropic displacement parameters (A^2 x 10^3) for **5**

atom	U11	U22	U33	U23	U13	U12
Cl(1)	81(1)	87(1)	127(1)	45(1)	58(1)	35(1)
Cl(2)	132(2)	119(2)	117(1)	-41(1)	79(1)	-41(1)
Cl(3)	78(1)	123(2)	113(1)	48(1)	3(1)	-11(1)
C(89)	60(3)	62(4)	91(4)	6(3)	25(3)	5(3)
Sn(1)	23(1)	22(1)	24(1)	-1(1)	9(1)	0(1)
Sn(2)	24(1)	24(1)	26(1)	2(1)	10(1)	0(1)
Ru(1)	20(1)	17(1)	20(1)	0(1)	6(1)	0(1)
P(1)	22(1)	21(1)	21(1)	0(1)	4(1)	2(1)
P(2)	28(1)	19(1)	21(1)	-1(1)	6(1)	1(1)
P(3)	22(1)	21(1)	22(1)	1(1)	4(1)	0(1)
P(4)	24(1)	19(1)	22(1)	-1(1)	7(1)	1(1)
C(1)	23(2)	19(2)	26(2)	3(1)	7(1)	3(1)
C(2)	23(2)	19(2)	28(2)	2(1)	8(1)	-2(1)
C(3)	23(2)	28(2)	26(2)	6(2)	10(1)	3(2)
C(4)	23(2)	20(2)	30(2)	0(1)	12(1)	0(1)
C(5)	27(2)	19(2)	23(2)	2(1)	6(1)	2(1)
C(6)	37(2)	27(2)	28(2)	2(2)	12(2)	1(2)
C(7)	61(3)	40(3)	31(2)	-10(2)	21(2)	-3(2)
C(8)	53(3)	42(3)	24(2)	-3(2)	4(2)	1(2)
C(9)	35(2)	35(3)	36(2)	-6(2)	-2(2)	-5(2)
C(10)	28(2)	27(2)	34(2)	-3(2)	9(2)	1(2)
C(11)	27(2)	20(2)	24(2)	2(1)	3(1)	2(2)
C(12)	33(2)	27(2)	34(2)	1(2)	11(2)	5(2)
C(13)	27(2)	38(3)	47(2)	1(2)	3(2)	8(2)
C(14)	32(2)	33(3)	39(2)	9(2)	-6(2)	5(2)
C(15)	41(2)	39(3)	27(2)	5(2)	2(2)	-7(2)
C(16)	36(2)	26(2)	31(2)	6(2)	12(2)	-1(2)
C(17)	22(2)	22(2)	24(2)	-1(1)	2(1)	1(1)
C(18)	40(2)	27(2)	31(2)	-2(2)	15(2)	0(2)
C(19)	46(2)	31(3)	40(2)	-6(2)	20(2)	5(2)
C(20)	46(2)	14(2)	50(2)	-3(2)	13(2)	7(2)
C(21)	46(2)	25(2)	51(2)	5(2)	22(2)	-1(2)
C(22)	41(2)	29(2)	44(2)	6(2)	22(2)	7(2)
C(23)	28(2)	16(2)	28(2)	1(1)	1(1)	3(1)
C(24)	49(2)	31(3)	33(2)	-5(2)	11(2)	-6(2)
C(25)	74(3)	46(3)	34(2)	-18(2)	11(2)	-9(3)
C(26)	55(3)	49(4)	60(3)	-23(3)	-4(3)	-8(2)
C(27)	45(3)	32(3)	81(4)	-9(2)	14(2)	-13(2)
C(28)	38(2)	31(3)	49(2)	-2(2)	14(2)	-1(2)
C(29)	21(2)	24(2)	27(2)	2(1)	3(1)	4(1)
C(30)	32(2)	30(2)	31(2)	-1(2)	0(2)	-2(2)
C(31)	44(2)	32(3)	46(2)	-5(2)	4(2)	-5(2)
C(32)	34(2)	54(3)	30(2)	-12(2)	0(2)	2(2)
C(33)	36(2)	42(3)	29(2)	-1(2)	7(2)	9(2)
C(34)	37(2)	33(3)	25(2)	1(2)	8(2)	3(2)
C(35)	26(2)	22(2)	27(2)	2(1)	5(1)	4(2)
C(36)	29(2)	34(3)	35(2)	2(2)	7(2)	6(2)
C(37)	28(2)	40(3)	46(2)	4(2)	0(2)	11(2)
C(38)	56(3)	39(3)	35(2)	5(2)	-6(2)	16(2)
C(39)	56(3)	33(3)	37(2)	11(2)	13(2)	2(2)
C(40)	37(2)	26(2)	33(2)	5(2)	10(2)	2(2)
C(41)	32(2)	22(2)	29(2)	3(2)	13(2)	4(2)
C(42)	38(2)	29(2)	44(2)	2(2)	16(2)	6(2)
C(43)	58(3)	33(3)	70(3)	5(2)	32(2)	16(2)
C(44)	89(4)	19(3)	74(3)	-1(2)	43(3)	8(3)
C(45)	52(3)	27(3)	51(2)	-2(2)	21(2)	-5(2)
C(46)	39(2)	22(2)	38(2)	3(2)	17(2)	1(2)
C(47)	31(2)	18(2)	24(2)	1(1)	9(1)	-3(1)
C(48)	37(2)	22(2)	31(2)	-2(2)	13(2)	-1(2)
C(49)	46(2)	27(2)	26(2)	-4(2)	11(2)	4(2)
C(50)	54(3)	25(2)	27(2)	-3(2)	3(2)	-6(2)
C(51)	30(2)	29(2)	34(2)	2(2)	3(2)	-2(2)
C(52)	31(2)	27(2)	24(2)	0(2)	9(2)	-1(2)
C(53)	28(2)	21(2)	31(2)	2(2)	13(2)	2(1)

C(54)	34(2)	26(2)	31(2)	1(2)	16(2)	-1(2)
C(55)	42(2)	25(2)	43(2)	-4(2)	21(2)	-3(2)
C(56)	54(3)	26(3)	48(2)	12(2)	25(2)	4(2)
C(57)	66(3)	37(3)	31(2)	6(2)	22(2)	3(2)
C(58)	53(2)	25(2)	32(2)	-2(2)	20(2)	-3(2)
C(59)	23(2)	34(2)	24(2)	1(2)	9(1)	0(2)
C(60)	25(2)	31(2)	42(2)	-4(2)	12(2)	0(2)
C(61)	28(2)	50(3)	46(2)	-15(2)	15(2)	-13(2)
C(62)	25(2)	55(3)	28(2)	-3(2)	4(2)	6(2)
C(63)	35(2)	42(3)	37(2)	8(2)	10(2)	9(2)
C(64)	26(2)	35(3)	36(2)	3(2)	9(2)	0(2)
C(65)	30(2)	25(2)	27(2)	-4(2)	12(2)	-3(2)
C(66)	28(2)	33(2)	38(2)	-7(2)	11(2)	0(2)
C(67)	42(2)	40(3)	53(3)	-17(2)	24(2)	1(2)
C(68)	51(3)	43(3)	35(2)	-10(2)	20(2)	-6(2)
C(69)	42(2)	44(3)	26(2)	2(2)	5(2)	-4(2)
C(70)	36(2)	28(2)	32(2)	2(2)	13(2)	5(2)
C(71)	30(2)	22(2)	32(2)	2(2)	13(2)	1(2)
C(72)	33(2)	43(3)	37(2)	4(2)	16(2)	3(2)
C(73)	56(3)	34(3)	45(2)	12(2)	20(2)	11(2)
C(74)	56(3)	28(3)	35(2)	4(2)	16(2)	-9(2)
C(75)	55(3)	38(3)	57(3)	2(2)	38(2)	-5(2)
C(76)	44(2)	27(2)	66(3)	11(2)	35(2)	4(2)
C(77)	25(2)	31(2)	29(2)	4(2)	11(2)	-1(2)
C(78)	32(2)	34(3)	55(3)	-4(2)	5(2)	-2(2)
C(79)	50(3)	41(3)	52(3)	-6(2)	2(2)	-5(2)
C(80)	36(2)	58(3)	32(2)	7(2)	2(2)	-9(2)
C(81)	38(2)	63(4)	45(3)	7(2)	8(2)	16(2)
C(82)	32(2)	41(3)	35(2)	2(2)	7(2)	3(2)
C(83)	27(2)	28(2)	32(2)	-2(2)	13(2)	-1(2)
C(84)	35(2)	35(3)	34(2)	0(2)	13(2)	-1(2)
C(85)	47(2)	58(3)	31(2)	-12(2)	18(2)	-10(2)
C(86)	47(3)	46(3)	59(3)	-21(2)	32(2)	-5(2)
C(87)	38(2)	27(3)	59(3)	-3(2)	23(2)	2(2)
C(88)	36(2)	32(2)	36(2)	0(2)	16(2)	-1(2)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table 10. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**

atom	x	y	z	U(eq)
H(89)	3561	-1938	3597	170(40)
H(6)	9300	-1152	7481	50(10)
H(7)	10373	-973	9341	50(10)
H(8)	12276	-961	10046	70(10)
H(9)	13151	-1124	8987	60(10)
H(10)	12113	-1302	7131	40(10)
H(12)	11993	-1940	5848	14(8)
H(13)	13467	-2125	7440	40(10)
H(14)	13477	-2138	9279	50(10)
H(15)	12010	-1956	9565	40(10)
H(16)	10519	-1770	7965	30(10)
H(18)	10235	-2081	3212	30(10)
H(19)	10531	-2512	3025	40(10)
H(20)	10132	-2816	4164	50(10)
H(21)	9545	-2679	5565	40(10)
H(22)	9322	-2243	5814	60(10)
H(24)	8383	-1830	1297	50(10)
H(25)	7325	-2129	-126	80(20)
H(26)	5993	-2368	144	100(20)
H(27)	5719	-2314	1830	60(10)
H(28)	6846	-2031	3306	20(10)
H(30)	5985	-1549	1553	30(10)
H(31)	4932	-1743	-265	50(10)
H(32)	4457	-1514	-1997	50(10)
H(33)	5035	-1093	-1934	20(10)
H(34)	6097	-897	-114	40(10)
H(36)	4563	-776	1315	40(10)
H(37)	3336	-557	-386	60(10)
H(38)	4007	-264	-1307.0001	70(10)
H(39)	5904	-168	-482	40(10)
H(40)	7149	-385	1223	20(10)
H(42)	5701	-370	3225	30(10)
H(43)	5465	55	3589	40(10)
H(44)	6993	334	4276	70(10)
H(45)	8749	179	4659	30(10)
H(46)	8989	-247.0000	4330	16(8)
H(48)	8237	-521	6351	30(10)
H(49)	9502	-301	8004	50(10)
H(50)	11378	-314	8484	70(10)
H(51)	12043	-561	7393	50(10)
H(52)	10793	-781.0001	5736	30(10)
H(54)	9986	-540	3660	50(10)
H(55)	9834	-139	2786	60(10)
H(56)	9228	-104	745	40(10)
H(57)	8802	-476	-391	40(10)
H(58)	8946	-868	457	30(10)
H(60)	11777	-776.9999	4137	30(10)
H(61)	13672	-816	5425	40(10)
H(62)	14454	-1211	6098	30(10)
H(63)	13338	-1577	5567	80(20)
H(64)	11443	-1543	4358	50(10)
H(66)	10967	-1537	2150	40(10)
H(67)	10685	-1805	572	50(10)
H(68)	9003	-1796	-1136	60(10)
H(69)	7585	-1522	-1227	50(10)
H(70)	7867	-1256	369	50(10)
H(72)	8209	-1848	5790	30(10)
H(73)	8137	-2208	6843	50(10)
H(74)	6800	-2236	7562	30(10)
H(75)	5528	-1908	7202	40(10)
H(76)	5568	-1552	6114	70(10)
H(78)	5410	-1729.0001	2992	80(20)
H(79)	3646	-1803	1474	110(20)

H(80)	2263	-1491	1012	40(10)
H(81)	2655	-1122	2119	60(10)
H(82)	4446	-1037	3556	40(10)
H(84)	7361	-1191	7421	30(10)
H(85)	7156	-864	8537	40(10)
H(86)	6264	-484	7647	40(10)
H(87)	5654	-430	5632	40(10)
H(88)	5879	-754.9999	4491	13(8)

Figure S2. Ortep view of complex **5** structure (Phenyl atoms of triphenyltin groups, solvent and hydrogen atoms have been omitted for clarity).