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Table S1. ^{13}C NMR and IR data for Compounds **1 - 9**

Compound (X)	^{13}C NMR δ (ppm)	IR (cm^{-1}), KBr pellet
1 (*p*-OCH_3)	161.5, 156.0, 143.4, 125.5, 114.1, 55.6	1619(s), 1597(m), 1500(s), 1461(w), 1439(w), 1345(w), 1292(w), 1242(m), 1229(m), 1181(w), 1107(w), 1035(m), 966(w), 833(w), 769(w), 700(w), 595(w), 539(w).
2 (*p*-CH_3)	162.0, 147.3, 132.5, 129.2, 124.5, 20.8	1624(s), 1592(s), 1544(w), 1504(s), 1342(m), 1304(w), 1231(m), 1183(w), 1110(w), 965(w), 819(w), 768(w), 700(w), 531(w), 461(w).
3 (-H)	162.6, 149.6, 128.7, 124.8, 123.5	1621(s), 1571(s), 1540(w), 1487(s), 1451(w), 1388(w), 1343(m), 1230(m), 1178(w), 1152(w), 1078(w), 1026(w), 968(w), 847(w), 755(w), 698(m), 527(w).
4 (*m*-OCH_3)	162.7, 160.3, 151.2, 129.5, 117.2, 110.5, 110.1, 55.4	1624(w), 1593(s), 1573(s), 1535(w), 1484(m), 1446(w), 1344(w), 1319(w), 1286(w), 1266(w), 1199(w), 1151(m), 1085(w), 1042(w), 986(w), 973(w), 940(w), 862(w), 780(w), 760(w), 699(w).
5 (*p*-Cl)	162.5, 147.3, 129.8, 129.2, 125.4	1616(s), 1576(s), 1542(w), 1486(s), 1403(w), 1383(w), 1344(m), 1295(w), 1233(m), 1176(w), 1094(m), 1011(w), 972(w), 827(w), 702(w).
6 (*m*-Cl)	162.6, 149.6, 134.9, 130.1, 124.6, 124.5, 122.4	1619(m), 1571(s), 1536(w), 1475(m), 1345(m), 1226(w), 1164(w), 1098(w), 1076(w), 1000(w), 970(w), 897(w), 781(w), 744(w), 691(w).
7 (*m*-CF_3)	163.0, 148.5, 132.1, 130.0, 126.9, 125.1, 121.4, 120.9	1629(m), 1601(m), 1578(s), 1542(m), 1488(m), 1445(m), 1327(s), 1286(w), 1278(w), 1222(w), 1165(m), 1127(s), 1099(m), 1068(m), 1001(w), 978(w), 901(w), 888(w), 801(w), 760(w), 701(m), 665(m).
8 (*p*-CF_3)	163.5, 151.0, 127.1, 126.8, 126.6, 124.0	1632(w), 1613(m), 1583(s), 1541(w), 1508(m), 1411(w), 1328(s), 1240(m), 1187(m), 1170(m), 1115(s), 1068(s), 1015(w), 974(w), 836(w), 705(w), 683(w), 603(w), 539(w), 514(w), 476(w).
9 (3,5-Cl_2)	162.6, 149.1, 136.0, 125.3, 122.5	1621(m), 1561(s), 1529(m), 1427(m), 1344(m), 1260(w), 1219(w), 1112(m), 1096(w), 1010(w), 997(w), 939(m), 848(m), 808(m), 725(w), 704(w), 681(w), 670(w).

Table S2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 9. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni(1)	9222(1)	1290(1)	2542(1)	29(1)
N(1)	9202(3)	2094(2)	2385(2)	35(1)
N(2)	9836(3)	1419(2)	3469(2)	32(1)
N(3)	9381(3)	486(2)	2691(2)	33(1)
N(4)	8750(3)	1160(2)	1608(2)	34(1)
Cl(11)	5857(1)	2655(1)	2071(1)	117(1)
Cl(12)	7517(1)	3316(1)	369(1)	86(1)
Cl(21)	6884(2)	1706(1)	3997(2)	141(1)
Cl(22)	9958(2)	2907(1)	5244(1)	107(1)
Cl(31)	6398(1)	-7(1)	3109(1)	117(1)
Cl(32)	9712(2)	-759(1)	4715(1)	81(1)
Cl(41)	5395(1)	998(1)	1504(1)	99(1)
Cl(42)	6620(2)	-150(2)	-179(1)	151(1)
C(1)	10000	2368(4)	2500	40(2)
C(2)	10724(4)	1291(2)	3737(2)	32(1)
C(3)	10000	217(4)	2500	35(2)
C(11)	8389(4)	2401(2)	2025(3)	39(1)
C(12)	7624(5)	2392(3)	2217(3)	56(2)
C(13)	6821(4)	2676(3)	1832(4)	67(2)
C(14)	6780(5)	2978(3)	1272(4)	67(2)
C(15)	7542(4)	2972(3)	1083(3)	55(2)
C(16)	8344(4)	2699(3)	1454(3)	44(2)
C(21)	9392(4)	1698(2)	3861(2)	37(1)
C(22)	8475(4)	1570(3)	3760(3)	56(2)
C(23)	8038(5)	1864(4)	4135(4)	80(2)
C(24)	8476(6)	2263(4)	4592(4)	82(3)
C(25)	9392(5)	2380(3)	4688(3)	63(2)
C(26)	9855(4)	2102(3)	4326(3)	50(2)
C(31)	8957(4)	182(2)	3080(3)	38(1)
C(32)	7993(4)	223(3)	2915(3)	49(2)
C(33)	7594(4)	-54(3)	3315(3)	61(2)
C(34)	8097(5)	-367(3)	3867(3)	60(2)
C(35)	9036(5)	-391(3)	4011(3)	49(2)
C(36)	9497(4)	-124(3)	3634(3)	45(2)
C(41)	7860(4)	929(3)	1278(2)	40(2)
C(42)	7135(4)	1064(3)	1498(3)	45(2)
C(43)	6280(4)	822(3)	1199(3)	57(2)
C(44)	6091(5)	466(4)	679(3)	76(3)
C(45)	6813(5)	326(4)	466(3)	76(2)
C(46)	7700(5)	545(3)	760(3)	60(2)
C(102)	5853(15)	-1275(9)	1710(10)	265(9)
C(105)	8285(14)	-1099(8)	1618(9)	265(9)
C(104)	7289(17)	-1290(10)	1473(11)	284(11)
C(103)	6802(17)	-1069(10)	1706(11)	302(12)
C(106)	8584(12)	-1364(8)	1149(8)	257(9)
C(100)	5147(14)	-1052(8)	1327(9)	280(10)

Table S3. Bond lengths [Å] and angles [°] for 9.

Ni(1)-N(3)	1.914(4)	Ni(1)-N(4)	1.916(4)
Ni(1)-N(1)	1.918(4)	Ni(1)-N(2)	1.919(4)
Ni(1)-Ni(1)#1	2.4618(13)	N(1)-C(1)	1.330(6)
N(1)-C(11)	1.419(6)	N(2)-C(2)	1.320(6)
N(2)-C(21)	1.419(6)	N(3)-C(3)	1.321(5)
N(3)-C(31)	1.422(6)	N(4)-C(2)#1	1.311(6)
N(4)-C(41)	1.414(6)	Cl(11)-C(13)	1.732(7)
Cl(12)-C(15)	1.729(7)	Cl(21)-C(23)	1.734(7)
Cl(22)-C(25)	1.734(7)	Cl(31)-C(33)	1.739(7)
Cl(32)-C(35)	1.744(6)	Cl(41)-C(43)	1.754(7)
Cl(42)-C(45)	1.731(7)	C(1)-N(1)#1	1.330(6)
C(2)-N(4)#1	1.311(6)	C(3)-N(3)#1	1.321(5)
C(11)-C(12)	1.377(8)	C(11)-C(16)	1.397(8)
C(12)-C(13)	1.395(9)	C(13)-C(14)	1.383(10)
C(14)-C(15)	1.367(9)	C(15)-C(16)	1.375(8)
C(21)-C(22)	1.382(8)	C(21)-C(26)	1.384(8)
C(22)-C(23)	1.400(9)	C(23)-C(24)	1.358(11)
C(24)-C(25)	1.380(10)	C(25)-C(26)	1.388(8)
C(31)-C(36)	1.396(8)	C(31)-C(32)	1.402(8)
C(32)-C(33)	1.383(8)	C(33)-C(34)	1.386(9)
C(34)-C(35)	1.369(9)	C(35)-C(36)	1.399(8)
C(41)-C(42)	1.390(8)	C(41)-C(46)	1.392(8)
C(42)-C(43)	1.372(8)	C(43)-C(44)	1.349(10)
C(44)-C(45)	1.379(10)	C(45)-C(46)	1.388(9)
C(102)-C(100)	1.23(2)	C(102)-C(103)	1.54(2)
C(105)-C(106)	1.39(2)	C(105)-C(104)	1.52(2)
C(104)-C(103)	1.16(3)		

N(3)-Ni(1)-N(4)	90.0(2)	N(3)-Ni(1)-N(1)	173.4(2)
N(4)-Ni(1)-N(1)	89.7(2)	N(3)-Ni(1)-N(2)	89.6(2)
N(4)-Ni(1)-N(2)	173.3(2)	N(1)-Ni(1)-N(2)	89.9(2)
N(3)-Ni(1)-Ni(1)#1	86.61(12)	N(4)-Ni(1)-Ni(1)#1	86.97(13)
N(1)-Ni(1)-Ni(1)#1	86.76(13)	N(2)-Ni(1)-Ni(1)#1	86.31(12)
C(1)-N(1)-C(11)	116.0(5)	C(1)-N(1)-Ni(1)	119.1(4)
C(11)-N(1)-Ni(1)	123.6(4)	C(2)-N(2)-C(21)	118.8(4)

C(2)-N(2)-Ni(1)	118.8(3)	C(21)-N(2)-Ni(1)	122.1(3)
C(3)-N(3)-C(31)	118.1(5)	C(3)-N(3)-Ni(1)	118.9(4)
C(31)-N(3)-Ni(1)	122.4(3)	C(2)#1-N(4)-C(41)	119.0(4)
C(2)#1-N(4)-Ni(1)	118.4(3)	C(41)-N(4)-Ni(1)	122.6(3)
N(1)-C(1)-N(1)#1	122.3(8)	N(4)#1-C(2)-N(2)	123.6(4)
N(3)-C(3)-N(3)#1	122.8(7)	C(12)-C(11)-C(16)	119.1(6)
C(12)-C(11)-N(1)	120.6(5)	C(16)-C(11)-N(1)	120.2(5)
C(11)-C(12)-C(13)	119.0(6)	C(14)-C(13)-C(12)	121.9(7)
C(14)-C(13)-Cl(11)	119.3(5)	C(12)-C(13)-Cl(11)	118.8(6)
C(15)-C(14)-C(13)	118.1(6)	C(14)-C(15)-C(16)	121.3(6)
C(14)-C(15)-Cl(12)	120.3(5)	C(16)-C(15)-Cl(12)	118.4(5)
C(15)-C(16)-C(11)	120.5(6)	C(22)-C(21)-C(26)	120.2(5)
C(22)-C(21)-N(2)	118.7(5)	C(26)-C(21)-N(2)	121.0(5)
C(21)-C(22)-C(23)	117.9(7)	C(24)-C(23)-C(22)	122.9(7)
C(24)-C(23)-Cl(21)	119.5(6)	C(22)-C(23)-Cl(21)	117.6(6)
C(23)-C(24)-C(25)	118.1(7)	C(24)-C(25)-C(26)	121.1(7)
C(24)-C(25)-Cl(22)	119.2(5)	C(26)-C(25)-Cl(22)	119.6(6)
C(21)-C(26)-C(25)	119.7(6)	C(36)-C(31)-C(32)	121.0(5)
C(36)-C(31)-N(3)	120.4(5)	C(32)-C(31)-N(3)	118.5(5)
C(33)-C(32)-C(31)	117.9(6)	C(32)-C(33)-C(34)	123.4(6)
C(32)-C(33)-Cl(31)	118.0(5)	C(34)-C(33)-Cl(31)	118.6(5)
C(35)-C(34)-C(33)	116.6(6)	C(34)-C(35)-C(36)	123.7(6)
C(34)-C(35)-Cl(32)	118.8(5)	C(36)-C(35)-Cl(32)	117.4(5)
C(31)-C(36)-C(35)	117.3(6)	C(42)-C(41)-C(46)	118.9(6)
C(42)-C(41)-N(4)	119.4(5)	C(46)-C(41)-N(4)	121.6(5)
C(43)-C(42)-C(41)	119.7(6)	C(44)-C(43)-C(42)	122.9(6)
C(44)-C(43)-Cl(41)	119.2(5)	C(42)-C(43)-Cl(41)	117.9(6)
C(43)-C(44)-C(45)	117.3(6)	C(44)-C(45)-C(46)	122.5(7)
C(44)-C(45)-Cl(42)	119.2(6)	C(46)-C(45)-Cl(42)	118.3(6)
C(45)-C(46)-C(41)	118.6(6)	C(100)-C(102)-C(103)	119(2)
C(106)-C(105)-C(104)	106(2)	C(103)-C(104)-C(105)	122(3)
C(104)-C(103)-C(102)	128(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+1/2

Table S4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 9.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ni(1)	24(1)	37(1)	25(1)	1(1)	8(1)	1(1)
N(1)	30(2)	39(3)	33(3)	1(2)	6(2)	3(2)
N(2)	25(2)	42(3)	27(2)	2(2)	9(2)	8(2)
N(3)	34(3)	36(3)	31(3)	6(2)	15(2)	2(2)
N(4)	27(2)	44(3)	27(2)	4(2)	5(2)	-5(2)
Cl(11)	57(1)	161(3)	146(2)	12(2)	52(1)	32(2)
Cl(12)	85(1)	93(2)	65(1)	32(1)	8(1)	28(1)
Cl(21)	74(2)	198(3)	187(3)	-60(2)	89(2)	-18(2)
Cl(22)	116(2)	110(2)	87(2)	-55(1)	26(1)	15(2)
Cl(31)	52(1)	194(3)	117(2)	46(2)	44(1)	-6(2)
Cl(32)	95(2)	84(2)	59(1)	36(1)	22(1)	-2(1)
Cl(41)	42(1)	128(2)	132(2)	16(2)	37(1)	-1(1)
Cl(42)	146(2)	226(3)	94(2)	-95(2)	57(2)	-127(2)
C(1)	34(5)	50(6)	35(4)	0	9(4)	0
C(2)	35(3)	34(3)	23(2)	0(3)	4(2)	6(3)
C(3)	41(5)	32(5)	34(4)	0	18(4)	0
C(11)	31(3)	40(4)	41(3)	-2(3)	6(3)	2(3)
C(12)	42(4)	55(5)	69(5)	-4(4)	16(4)	0(3)
C(13)	40(4)	76(5)	84(5)	-7(5)	21(4)	11(4)
C(14)	46(4)	65(5)	75(5)	1(4)	-1(4)	23(4)
C(15)	48(4)	49(4)	55(4)	12(3)	1(3)	13(3)
C(16)	43(4)	38(4)	44(3)	6(3)	7(3)	12(3)
C(21)	41(3)	45(4)	27(3)	5(3)	13(3)	13(3)
C(22)	46(4)	70(5)	59(4)	-5(4)	28(3)	3(4)
C(23)	52(5)	116(7)	84(5)	-15(5)	41(4)	4(5)
C(24)	76(6)	111(7)	72(5)	-18(5)	43(5)	10(5)
C(25)	70(5)	74(5)	44(4)	-14(4)	19(3)	18(4)
C(26)	50(4)	60(4)	37(3)	-1(3)	13(3)	15(3)
C(31)	45(4)	37(3)	35(3)	0(3)	20(3)	-4(3)
C(32)	46(4)	56(4)	53(4)	6(3)	25(3)	-4(3)
C(33)	46(4)	72(5)	73(5)	10(4)	29(4)	-12(4)
C(34)	66(5)	60(5)	65(5)	9(4)	37(4)	-12(4)
C(35)	70(5)	44(4)	39(3)	10(3)	25(3)	-6(3)
C(36)	57(4)	38(4)	43(3)	3(3)	20(3)	-7(3)
C(41)	34(3)	51(4)	27(3)	9(3)	2(3)	-4(3)
C(42)	31(3)	52(4)	47(4)	12(3)	7(3)	-5(3)
C(43)	32(4)	73(5)	62(4)	19(4)	10(3)	-7(3)
C(44)	44(4)	117(7)	54(4)	-4(5)	1(4)	-45(5)
C(45)	71(5)	107(7)	44(4)	-17(4)	14(4)	-47(5)
C(46)	56(4)	85(6)	39(4)	-13(4)	17(3)	-28(4)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 9.

	x	y	z	U(eq)
H(2)	11017(44)	1289(29)	4238(33)	90
H(34)	7781(46)	-553(30)	4157(32)	90
H(42)	7271(48)	1325(30)	1861(33)	90
H(3)	10000	-234(43)	2500	90
H(16)	8779(47)	2697(30)	1255(32)	90
H(26)	10549(47)	2223(29)	4417(31)	90
H(12)	7570(52)	2227(32)	2558(35)	90
H(46)	8168(48)	434(32)	633(34)	90
H(14)	6190(47)	3131(29)	967(33)	90
H(22)	8109(49)	1292(30)	3408(34)	90
H(44)	5508(49)	295(30)	484(33)	90
H(10M)	5812(15)	-1681(9)	1620(10)	319
H(10N)	5845(15)	-1226(9)	2154(10)	319
H(10B)	8316(14)	-688(8)	1583(9)	317
H(10C)	8670(14)	-1213(8)	2060(9)	317
H(10A)	6983(17)	-1269(10)	998(11)	340
H(10D)	7312(17)	-1690(10)	1591(11)	340
H(10E)	6691(17)	-692(10)	1511(11)	363
H(10L)	7176(17)	-1013(10)	2167(11)	363
H(10F)	9213(12)	-1256(8)	1220(8)	386
H(10G)	8196(12)	-1249(8)	715(8)	386
H(10H)	8549(12)	-1770(8)	1190(8)	386
H(10I)	4612(14)	-1221(8)	1384(9)	420
H(10J)	5123(14)	-1109(8)	881(9)	420
H(10K)	5157(14)	-651(8)	1417(9)	420
H(24)	8366(129)	2441(96)	4894(100)	420
H(1)	10000	2837(123)	2500	420
H(32)	7661(143)	478(83)	2624(100)	420
H(36)	10032(137)	-79(85)	3850(96)	420

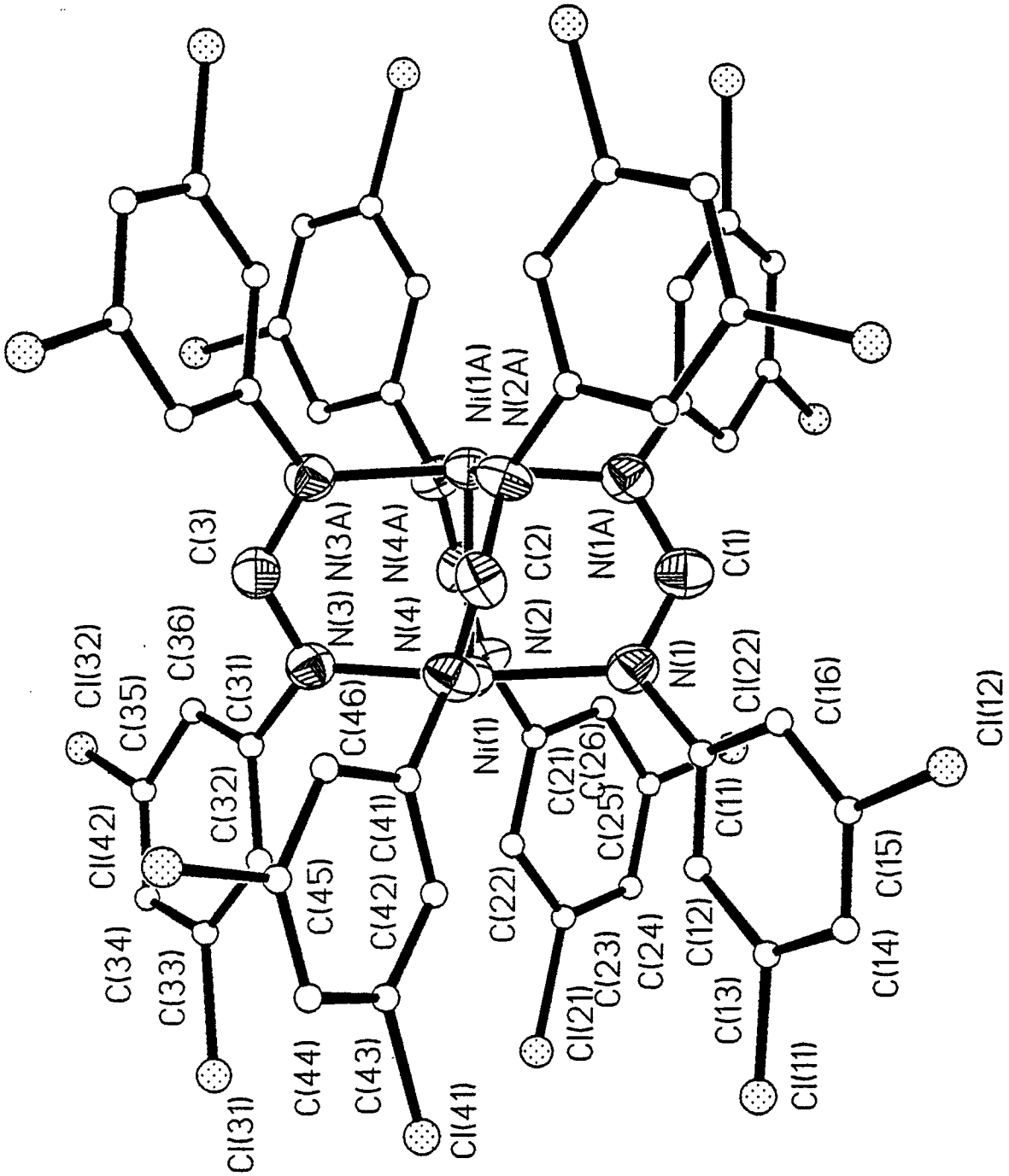
Ni(1A)
N(2A)
C(3)
N(3A)
N(4A)
C(2)
N(1A)
C(1)
N(3)
N(4)
N(2)
N(1)
Cl(32)
C(35)
C(36)
C(31)
C(46)
Ni(1)
C(21)
C(26)
C(22)
C(16)
Cl(12)
Cl(42)
C(32)
C(45)
C(41)
C(25)
C(11)
C(34)
C(33)
C(42)
C(22)
C(24)
C(12)
C(15)
C(44)
C(43)
C(23)
C(13)
C(14)
Cl(31)
Cl(41)
Cl(21)
Cl(11)

Figure S1