Table 8. Non-bonded Contacts out to 6.06 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
Cl(1)	F(9)	4.90(2)	56501	Cl(1)	C(20)	4.91(2)	75603
Cl(1)	C(11)	4.91(1)	56501	Cl(1)	F(7)	4.95(1)	75603
Cl(1)	F(11)	5.03(2)	1	Cl(1)	Cl(1)	5.12(3)	75604
Cl(1)	C(19)	5.18(2)	75603	Cl(1)	C(21)	5.18(1)	56501
Cl(1)	C(24)	5.24(2)	1	Cl(1)	F(12)	5.26(1)	76604
Cl(1)	C(13)	5.36(1)	76604	Cl(1)	C(8)	5.42(1)	66501
Cl(1)	F(9)	5.47(1)	75603	Cl(1)	C(9)	5.47(1)	66604
Cl(1)	C(4)	5.490(10)	66501	Cl(1)	O(6)	5.53(1)	56501
Cl(1)	O(1)	5.567(9)	56501	Cl(1)	C(17)	5.61(1)	75603
Cl(1)	C(20)	5.70(2)	56501	Cl(1)	F(10)	5.74(2)	75604
Cl(1)	C(18)	5.76(2)	75603	Cl(1)	O(5)	5.82(1)	56501
Cl(1)	F(2)	5.82(2)	76603	Cl(1)	O(5)	5.85(1)	75603
Cl(1)	N(1)	5.865(10)	56501	Cl(1)	F(8)	5.87(1)	56501
Cl(1)	C(12)	5.88(1)	56501	Cl(1)	F(1)	5.89(1)	75603
Cl(1)	N(2)	5.949(9)	66501	Cl(1)	F(10)	5.97(1)	56501
Cl(1)	F(1)	6.01(2)	76603	Cl(1)	C(21)	6.05(1)	75603
Cl(2)	F(4)	3.810(9)	75603	Cl(2)	F(1)	3.924(9)	75603
Cl(2)	F(11)	4.01(1)	1	Cl(2)	C(9)	4.032(9)	66501
Cl(2)	C(4)	4.078(8)	66501	Cl(2)	C(8)	4.081(10)	65501
Cl(2)	C(13)	4.23(1)	76604	Cl(2)	C(17)	4.242(10)	75603
Cl(2)	C(5)	4.421(9)	66501	Cl(2)	F(6)	4.431(9)	75603
Cl(2)	F(10)	4.44(1)	1	Cl(2)	C(10)	4.51(1)	66501
Cl(2)	C(19)	4.55(1)	75603	Cl(2)	C(24)	4.78(1)	1
Cl(2)	C(15)	4.84(1)	75603	Cl(2)	C(7)	4.875(8)	66501

Table 8. Non-bonded Contacts out to 6.06 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
Cl(2)	C(18)	4.886(10)	75603	Cl(2)	F(10)	4.94(1)	75604
Cl(2)	F(8)	5.00(1)	75603	Cl(2)	C(16)	5.004(10)	75603
Cl(2)	F(5)	5.235(9)	66501	Cl(2)	C(3)	5.279(8)	66501
Cl(2)	F(3)	5.36(1)	75603	Cl(2)	F(7)	5.50(1)	75603
Cl(2)	C(7)	5.499(9)	65501	Cl(2)	F(12)	5.51(1)	1
Cl(2)	N(2)	5.581(7)	66501	Cl(2)	C(11)	5.605(9)	76604
Cl(2)	C(20)	5.62(2)	75603	Cl(2)	F(2)	5.762(9)	75603
Cl(2)	F(5)	5.776(8)	75603	Cl(2)	F(12)	5.79(1)	75604
Cl(2)	C(10)	5.85(1)	65501	Cl(2)	C(6)	5.859(8)	66501
Cl(2)	F(3)	5.86(1)	65501	Cl(2)	O(5)	5.869(7)	75603
Cl(2)	C(14)	5.91(1)	56501	Cl(2)	C(23)	5.910(9)	1
Cl(2)	O(2)	5.919(7)	65501	Cl(2)	N(1)	5.930(7)	76604
Cl(2)	C(24)	6.01(1)	75604	Cl(2)	O(4)	6.032(8)	75603
F(1)	C(10)	3.51(1)	65603	F(1)	C(8)	3.75(1)	65603
F(1)	F(11)	3.76(1)	75603	F(1)	C(7)	4.25(1)	65603
F(1)	F(6)	4.442(10)	56501	F(1)	F(3)	4.59(2)	65603
F(1)	C(25)	4.61(4)	75603	F(1)	F(9)	4.67(2)	75603
F(1)	C(22)	4.69(2)	75603	F(1)	C(24)	4.84(2)	75603
F(1)	F(5)	4.961(10)	56501	F(1)	C(9)	5.16(1)	65603
F(1)	C(19)	5.19(1)	56501	F(1)	C(12)	5.26(1)	56501
F(1)	F(4)	5.28(1)	56501	F(1)	F(7)	5.29(2)	75603
F(1)	C(23)	5.34(2)	75603	F(1)	C(17)	5.40(2)	65603
F(1)	N(2)	5.44(1)	65603	F(1)	F(10)	5.45(2)	75603
F(1)	C(20)	5.50(2)	75603	F(1)	C(21)	5.57(2)	75603

Table 8. Non-bonded Contacts out to 6.06 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
F(1)	F(12)	5.58(1)	75603	F(1)	C(16)	5.63(2)	65603
F(1)	O(2)	5.72(1)	65603	F(1)	F(4)	5.77(1)	65603
F(1)	F(1)	5.84(3)	65603	F(1)	C(15)	5.84(2)	65603
F(1)	C(18)	5.96(2)	65603	F(2)	F(6)	3.056(9)	56501
F(2)	C(12)	3.37(1)	56501	F(2)	F(9)	3.49(2)	75603
F(2)	F(5)	3.55(1)	56501	F(2)	C(19)	3.86(1)	56501
F(2)	C(10)	4.13(1)	65603	F(2)	F(7)	4.31(2)	75603
F(2)	F(4)	4.38(1)	56501	F(2)	C(20)	4.54(2)	75603
F(2)	C(22)	4.61(2)	75603	F(2)	F(11)	4.76(1)	75603
F(2)	C(11)	4.87(1)	56501	F(2)	C(21)	5.08(2)	75603
F(2)	C(18)	5.12(1)	56501	F(2)	C(5)	5.18(1)	56501
F(2)	C(8)	5.22(1)	65603	F(2)	F(8)	5.26(1)	75603
F(2)	C(7)	5.271(10)	65603	F(2)	C(14)	5.27(1)	56501
F(2)	O(4)	5.287(8)	56501	F(2)	F(4)	5.32(1)	65603
F(2)	F(3)	5.49(2)	65603	F(2)	N(1)	5.590(9)	56501
F(2)	C(6)	5.60(1)	56501	F(2)	C(24)	5.65(2)	75603
F(2)	C(23)	5.67(2)	75603	F(2)	C(25)	5.70(3)	76603
F(2)	C(4)	5.74(1)	56501	F(2)	C(17)	5.79(1)	65603
F(2)	C(13)	5.79(1)	56501	F(2)	C(1)	5.824(10)	56501
F(2)	C(9)	5.97(1)	65603	F(2)	F(8)	6.02(1)	56501
F(3)	C(10)	3.67(1)	65603	F(3)	F(5)	3.76(1)	56501
F(3)	F(3)	3.76(2)	65603	F(3)	F(6)	4.00(1)	56501
F(3)	C(17)	4.25(1)	65603	F(3)	C(19)	4.36(1)	56501
F(3)	F(4)	4.41(1)	65603	F(3)	F(4)	4.54(1)	56501

Table 8. Non-bonded Contacts out to 6.06 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
F(3)	C(12)	4.61(1)	56501	F(3)	C(8)	4.71(2)	65603
F(3)	C(16)	4.71(1)	65603	F(3)	C(7)	4.82(1)	65603
F(3)	C(15)	4.84(2)	65603	F(3)	C(18)	4.96(1)	65603
F(3)	C(19)	5.17(1)	65603	F(3)	F(9)	5.22(1)	75603
F(3)	C(5)	5.23(2)	56501	F(3)	F(11)	5.42(1)	75603
F(3)	F(5)	5.52(1)	65603	F(3)	O(3)	5.67(1)	65603
F(3)	C(4)	5.69(2)	56501	F(3)	N(2)	5.73(1)	65603
F(3)	C(18)	5.80(1)	56501	F(3)	O(4)	5.88(1)	65603
F(3)	C(9)	5.90(1)	65603	F(3)	F(7)	5.97(2)	75603
F(3)	C(22)	6.00(1)	75603	F(3)	C(6)	6.01(2)	56501
F(4)	F(4)	3.17(1)	64603	F(4)	F(5)	3.180(8)	64603
F(4)	C(10)	3.58(1)	64603	F(4)	C(19)	3.76(1)	64603
F(4)	C(25)	3.96(2)	75603	F(4)	C(4)	4.600(8)	64603
F(4)	F(6)	4.658(10)	64603	F(4)	C(18)	4.755(9)	64603
F(4)	C(7)	4.923(9)	64603	F(4)	C(15)	5.10(1)	54501
F(4)	C(5)	5.205(8)	64603	F(4)	C(9)	5.230(10)	64603
F(4)	C(17)	5.250(10)	64603	F(4)	O(4)	5.462(7)	64603
F(4)	C(3)	5.466(7)	64603	F(4)	N(2)	5.585(7)	64603
F(4)	C(15)	5.63(1)	65603	F(4)	F(9)	5.72(1)	74603
F(4)	C(8)	6.00(1)	64603	F(5)	C(19)	4.31(1)	64603
F(5)	C(15)	4.36(1)	54501	F(5)	F(5)	4.38(1)	64603
F(5)	C(10)	4.666(10)	64603	F(5)	F(6)	5.115(9)	64603
F(5)	C(17)	5.222(9)	64603	F(5)	C(18)	5.226(9)	64603
F(5)	O(3)	5.282(7)	54501	F(5)	C(16)	5.301(10)	54501

Table 8. Non-bonded Contacts out to 6.06 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
F(5)	F(9)	5.34(1)	74603	F(5)	C(25)	5.46(2)	75603
F(6)	C(25)	3.60(2)	75603	F(6)	F(9)	3.67(1)	74603
F(6)	C(15)	4.00(1)	54501	F(6)	C(10)	4.119(10)	64603
F(6)	C(20)	5.02(2)	74603	F(6)	F(8)	5.14(1)	74603
F(6)	C(16)	5.306(10)	54501	F(6)	F(7)	5.33(1)	74603
F(6)	O(3)	5.347(8)	54501	F(6)	C(22)	5.43(1)	74603
F(6)	C(7)	5.430(9)	64603	F(6)	C(19)	5.49(1)	64603
F(6)	C(21)	5.63(1)	74603	F(6)	C(9)	5.633(10)	64603
F(6)	F(11)	5.98(1)	74603	F(7)	C(22)	3.39(1)	75603
F(7)	F(7)	3.42(2)	75603	F(7)	C(21)	3.59(1)	75603
F(7)	C(23)	3.76(1)	75603	F(7)	C(20)	3.94(2)	75603
F(7)	C(14)	4.01(1)	74603	F(7)	C(12)	4.06(1)	74603
F(7)	O(5)	4.15(1)	75603	F(7)	C(25)	4.24(3)	75603
F(7)	O(6)	4.253(9)	75603	F(7)	C(24)	4.31(2)	75603
F(7)	F(10)	4.33(1)	75603	F(7)	F(11)	4.45(1)	75603
F(7)	F(9)	4.58(2)	75603	F(7)	O(3)	4.60(1)	75603
F(7)	C(11)	4.60(1)	74603	F(7)	C(15)	4.72(2)	75603
F(7)	F(8)	5.02(1)	74603	F(7)	F(8)	5.05(1)	75603
F(7)	C(13)	5.06(1)	74603	F(7)	C(16)	5.09(2)	75603
F(7)	F(9)	5.41(2)	74603	F(7)	F(12)	5.57(1)	75603
F(7)	C(20)	5.84(2)	74603	F(7)	O(7)	6.02(1)	75603
F(7)	N(1)	6.02(1)	74603	F(8)	C(25)	3.37(2)	75603
F(8)	F(8)	3.46(2)	74603	F(8)	C(14)	3.48(1)	74603
F(8)	F(9)	3.51(2)	74603	F(8)	C(20)	4.12(2)	74603

Table 8. Non-bonded Contacts out to 6.06 $\AA$ (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
F(8)	C(21)	4.47(1)	74603	F(8)	C(12)	4.51(1)	74603
F(8)	C(11)	4.628(10)	74603	F(8)	O(5)	4.82(1)	74603
F(8)	C(22)	4.97(1)	74603	F(8)	C(22)	5.14(1)	75603
F(8)	F(10)	5.19(1)	75603	F(8)	C(23)	5.35(1)	75603
F(8)	C(13)	5.36(1)	74603	F(8)	F(11)	5.44(1)	75603
F(8)	C(24)	5.48(2)	75603	F(8)	C(21)	5.50(1)	75603
F(8)	C(20)	5.74(2)	75603	F(8)	N(1)	5.822(9)	74603
F(8)	O(6)	5.84(1)	75603	F(8)	C(25)	5.84(2)	54501
F(8)	O(1)	5.868(8)	74603	F(8)	C(23)	5.89(1)	74603
F(8)	C(15)	5.91(2)	75603	F(9)	C(12)	3.62(1)	74603
F(9)	C(14)	3.62(1)	74603	F(9)	C(15)	4.17(2)	75603
F(9)	C(11)	4.307(10)	74603	F(9)	F(9)	4.41(2)	74603
F(9)	C(20)	4.50(2)	74603	F(9)	O(5)	4.78(1)	74603
F(9)	O(3)	4.79(1)	75603	F(9)	C(25)	4.87(3)	54501
F(9)	C(21)	4.88(1)	74603	F(9)	C(19)	4.93(1)	74603
F(9)	C(25)	5.03(2)	75603	F(9)	C(21)	5.04(2)	75603
F(9)	C(16)	5.06(1)	75603	F(9)	C(22)	5.10(2)	75603
F(9)	C(20)	5.25(2)	75603	F(9)	O(5)	5.28(1)	75603
F(9)	C(13)	5.28(1)	74603	F(9)	C(23)	5.35(1)	75603
F(9)	O(4)	5.40(1)	74603	F(9)	N(1)	5.417(9)	74603
F(9)	C(18)	5.47(1)	74603	F(9)	O(6)	5.54(1)	75603
F(9)	O(1)	5.718(9)	74603	F(9)	F(10)	5.72(1)	75603
F(9)	C(22)	5.73(2)	74603	F(9)	C(24)	5.93(2)	75603
F(10)	C(13)	3.69(1)	56501	F(10)	F(12)	3.94(1)	75604

Table 8. Non-bonded Contacts out to 6.06 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
F(10)	F(10)	4.04(2)	75604	F(10)	C(25)	4.23(3)	1
F(10)	F(11)	4.34(1)	75604	F(10)	C(24)	4.46(1)	75604
F(10)	C(11)	4.64(1)	56501	F(10)	C(14)	4.67(1)	56501
F(10)	C(12)	4.98(1)	56501	F(10)	C(20)	5.18(2)	75603
F(10)	C(8)	5.29(1)	65501	F(10)	C(25)	5.90(2)	75604
F(10)	C(9)	5.92(1)	65501	F(10)	C(23)	5.92(1)	75604
F(10)	N(1)	6.049(10)	56501	F(11)	F(12)	3.77(1)	75604
F(11)	C(8)	3.770(10)	65501	F(11)	C(25)	4.35(4)	1
F(11)	C(9)	4.37(1)	65501	F(11)	C(15)	4.48(2)	75603
F(11)	C(7)	4.50(1)	65501	F(11)	C(24)	4.68(1)	75604
F(11)	C(10)	4.75(1)	65501	F(11)	F(11)	4.97(2)	75604
F(11)	C(20)	5.27(2)	75603	F(11)	C(16)	5.55(1)	75603
F(11)	C(25)	5.56(4)	54501	F(11)	C(13)	5.58(1)	56501
F(11)	C(17)	5.80(1)	75603	F(11)	C(23)	5.88(1)	75604
F(11)	O(6)	5.933(8)	75604	F(11)	N(2)	5.975(9)	65501
F(12)	F(12)	2.89(1)	75604	F(12)	C(24)	3.84(1)	75604
F(12)	C(9)	4.59(1)	65501	F(12)	C(8)	4.77(1)	65501
F(12)	C(23)	5.14(1)	75604	F(12)	C(7)	5.27(1)	65501
F(12)	C(13)	5.32(1)	56501	F(12)	C(25)	5.49(4)	54501
F(12)	O(6)	5.565(8)	75604	F(12)	C(25)	5.79(3)	1
F(12)	C(10)	5.80(1)	65501	F(12)	C(22)	6.03(1)	75604
O(2)	C(5)	4.982(7)	56501	O(2)	C(6)	5.210(7)	56501
O(2)	C(13)	5.300(10)	66604	O(2)	C(6)	5.445(7)	66604
O(2)	C(12)	6.023(9)	56501	O(3)	C(12)	3.593(9)	56501

Table 8. Non-bonded Contacts out to 6.06 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(3)	C(11)	4.958(8)	56501	O(3)	C(13)	5.193(10)	56501
O(3)	C(5)	5.206(8)	56501	O(3)	C(6)	5.301(7)	56501
O(3)	C(20)	5.35(1)	75603	O(3)	C(14)	5.763(10)	56501
O(3)	C(22)	5.877(10)	75603	O(3)	C(25)	5.93(3)	75603
O(3)	N(1)	5.941(7)	56501	O(3)	C(19)	5.99(1)	56501
O(3)	C(1)	6.029(7)	56501	O(4)	C(25)	5.49(2)	75603
O(5)	C(25)	4.80(2)	75603	O(5)	C(20)	5.10(1)	75603
O(5)	C(22)	5.43(1)	75603	O(5)	C(12)	5.485(9)	56501
O(5)	C(21)	5.53(1)	75603	O(5)	C(20)	5.59(2)	74603
O(5)	C(14)	6.045(9)	74603	O(6)	C(13)	4.267(9)	56501
O(6)	C(12)	4.499(9)	56501	O(6)	C(11)	4.952(9)	56501
O(6)	C(20)	5.31(1)	75603	O(6)	C(14)	5.49(1)	56501
O(7)	C(12)	3.997(9)	56501	O(7)	C(13)	4.160(10)	56501
O(7)	C(6)	4.292(7)	56501	O(7)	C(11)	4.706(9)	56501
O(7)	C(5)	4.731(8)	56501	O(7)	C(6)	4.889(7)	66604
O(7)	C(5)	5.100(7)	66604	O(7)	C(1)	5.383(7)	56501
O(7)	N(1)	5.538(6)	56501	O(7)	C(14)	5.927(10)	56501
O(7)	C(4)	6.027(8)	56501	C(4)	C(25)	5.36(2)	44501
C(4)	C(19)	5.84(1)	64603	C(4)	C(8)	5.94(1)	54501
C(5)	C(8)	5.26(1)	54501	C(5)	C(16)	5.78(1)	54501
C(5)	C(15)	5.79(1)	54501	C(5)	C(25)	6.00(2)	44501
C(7)	C(15)	5.11(1)	65603	C(7)	C(25)	5.11(3)	44501
C(7)	C(24)	5.51(1)	45501	C(7)	C(19)	5.76(1)	64603
C(8)	C(15)	4.79(1)	65603	C(8)	C(24)	4.84(1)	45501

Table 8. Non-bonded Contacts out to 6.06 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(8)	C(13)	4.90(1)	66604	C(8)	C(25)	5.67(3)	45501
C(8)	C(17)	5.95(1)	65603	C(8)	C(16)	5.96(1)	65603
C(8)	C(25)	6.04(3)	44501	C(8)	C(23)	6.05(1)	45501
C(9)	C(25)	4.31(3)	44501	C(9)	C(24)	5.15(1)	45501
C(9)	C(15)	5.96(1)	65603	C(10)	C(15)	4.14(1)	65603
C(10)	C(19)	4.35(1)	64603	C(10)	C(25)	4.63(3)	44501
C(10)	C(16)	5.55(1)	65603	C(10)	C(18)	5.77(1)	64603
C(10)	C(24)	5.83(2)	45501	C(10)	C(17)	6.02(1)	65603
C(11)	C(20)	4.91(1)	74603	C(11)	C(23)	5.44(1)	54501
C(11)	C(25)	5.46(2)	54501	C(11)	C(24)	5.56(2)	54501
C(11)	C(15)	5.72(1)	54501	C(11)	C(16)	5.90(1)	54501
C(12)	C(15)	4.20(1)	54501	C(12)	C(16)	4.44(1)	54501
C(12)	C(20)	4.44(1)	74603	C(12)	C(23)	5.09(1)	54501
C(12)	C(24)	5.62(2)	54501	C(12)	C(22)	5.69(1)	54501
C(12)	C(21)	5.74(1)	74603	C(12)	C(21)	5.80(1)	54501
C(12)	C(17)	5.80(1)	54501	C(13)	C(24)	4.73(2)	54501
C(13)	C(23)	4.83(1)	54501	C(13)	C(25)	5.44(2)	54501
C(13)	C(20)	5.60(1)	74603	C(13)	C(25)	5.62(2)	74604
C(13)	C(22)	5.89(1)	54501	C(14)	C(20)	4.06(1)	74603
C(14)	C(25)	4.26(2)	54501	C(14)	C(21)	5.48(1)	74603
C(14)	C(24)	5.59(2)	54501	C(14)	C(23)	5.65(1)	54501
C(15)	C(19)	4.74(1)	56501	C(15)	C(22)	4.77(2)	75603
C(15)	C(20)	5.05(2)	75603	C(15)	C(25)	5.24(4)	75603
C(15)	C(21)	5.41(2)	75603	C(15)	C(24)	5.45(2)	75603

Table 8. Non-bonded Contacts out to 6.06 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(15)	C(17)	5.60(2)	65603	C(15)	C(23)	5.67(2)	75603
C(15)	C(16)	5.98(2)	65603	C(15)	C(15)	6.06(3)	65603
C(16)	C(25)	5.07(3)	75603	C(16)	C(22)	5.70(1)	75603
C(16)	C(20)	5.70(2)	75603	C(16)	C(19)	5.94(1)	56501
C(17)	C(25)	4.31(3)	75603	C(17)	C(19)	5.86(1)	64603
C(18)	C(25)	4.58(2)	75603	C(18)	C(19)	5.62(1)	64603
C(19)	C(25)	4.22(2)	75603	C(19)	C(19)	4.64(2)	64603
C(20)	C(25)	4.19(2)	75603	C(20)	C(22)	4.40(2)	75603
C(20)	C(21)	4.54(2)	75603	C(20)	C(20)	4.66(3)	75603
C(20)	C(23)	4.82(2)	75603	C(20)	C(20)	4.97(3)	74603
C(20)	C(24)	5.25(2)	75603	C(20)	C(21)	5.42(2)	74603
C(20)	C(25)	5.85(3)	54501	C(20)	C(22)	6.05(2)	74603
C(21)	C(21)	4.90(2)	75603	C(21)	C(22)	4.99(1)	75603
C(21)	C(25)	5.15(2)	75603	C(21)	C(25)	5.66(3)	54501
C(21)	C(23)	5.73(1)	75603	C(22)	C(25)	5.29(4)	54501
C(22)	C(22)	5.43(2)	75603	C(22)	C(25)	5.80(4)	1
C(23)	C(25)	5.59(3)	1	C(23)	C(25)	5.78(4)	54501
C(23)	C(24)	6.04(1)	75604	C(24)	C(24)	4.68(2)	75604
C(24)	C(25)	4.78(4)	1	C(24)	C(25)	5.90(4)	54501

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ±4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

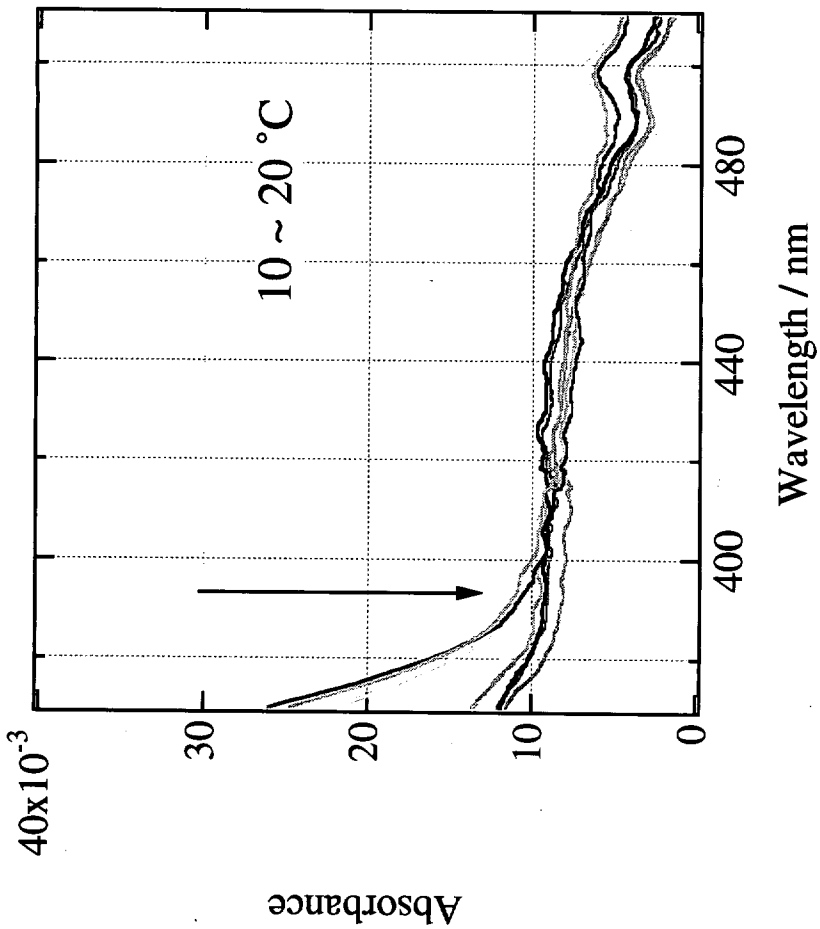
The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

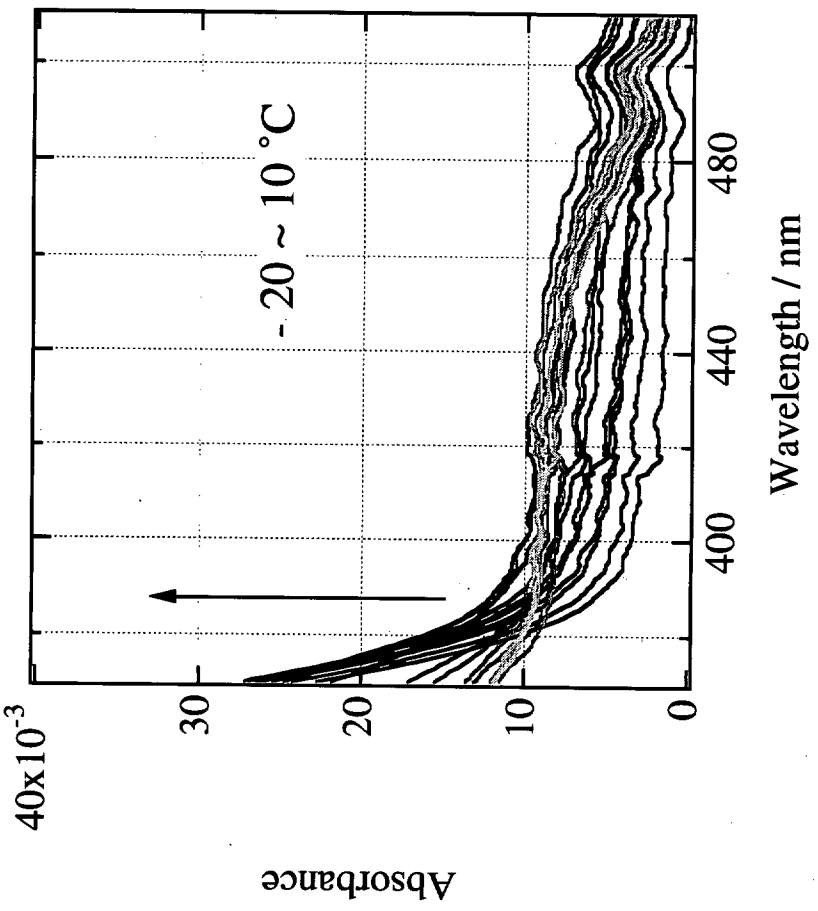
For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

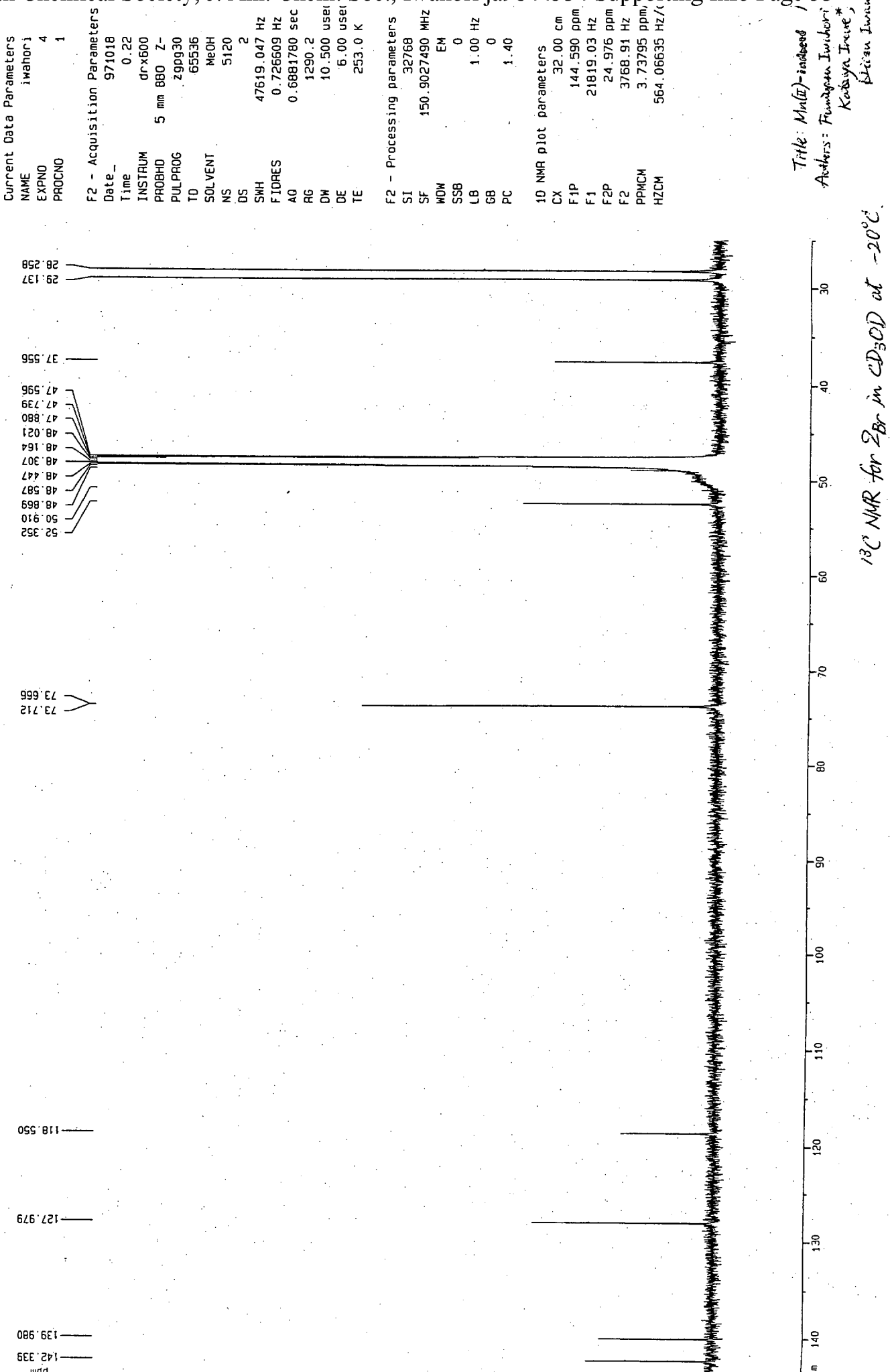
Symmetry Operators:

(1)	X,	Y,	Z	(2)	1/2+X,	-Y,	1/2+Z
(3)	-X,	-Y,	-Z	(4)	1/2-X,	Y,	1/2-Z





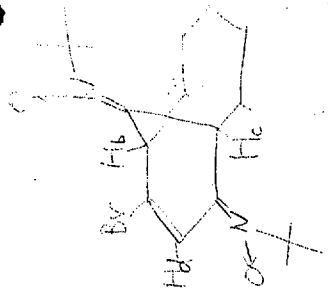
Temperature dependence of UV spectrum for $\mathbf{2_{Br}}$•[$Mn(hfac)_2$•$H_2O]_2$•CH_2Cl_2.
Title; Mn(II)-Induced Formation and ..
Authors; F. Iwahori, K. Inoue and H. Iwamura



Title: Mn(II)-indeed [illegible]
Authors: Fumiyasu Iwahori, Kazuya Ikeue*, and Ritsuo Imamura

^{13}C NMR for 2Br in CD_3OD at -20°C

h2



Br 体

'H cosy NMR for 2Br

Title: NMR(II)-induced formation and

Authors: Fumiyasu Iwahori,

Katsuya Inoue, and

Current Data Parameters
NAME inoue2
EXPNO 2
PROCNO 1

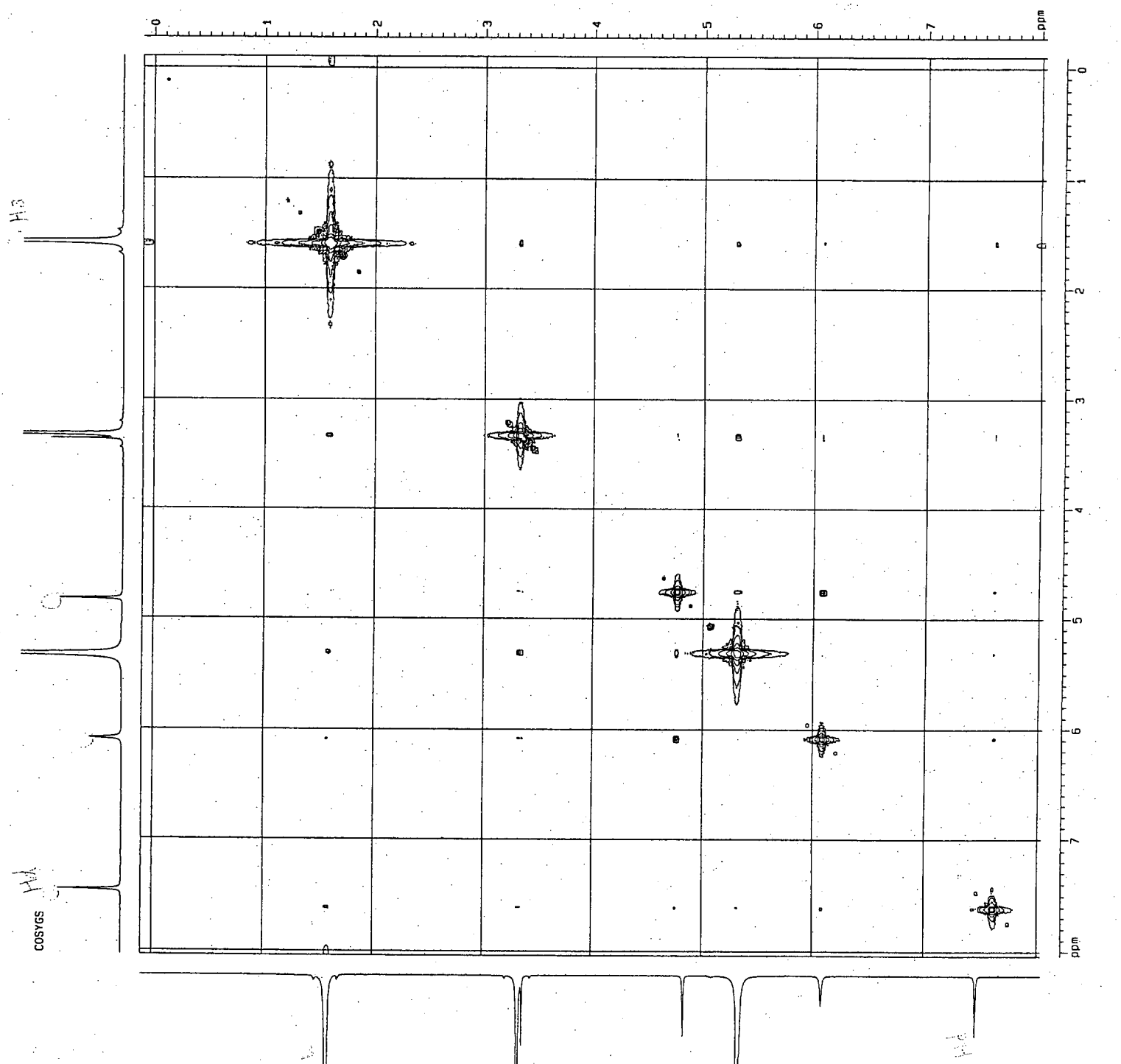
F2 - Acquisition Parameters
Date_ 971029
Time 16.06
INSTRUM drx600
PROBHD 5 mm BBO Z-
PULPROG cosygs
TD 2048
SOLVENT MeOH
NS 16
DS 2
SWH 4882.812 Hz
FIDRES 2.384186 Hz
AQ 0.2097652 sec
RG 362
DW 102.400 usec
DE 6.00 usec
TE 300.0 K

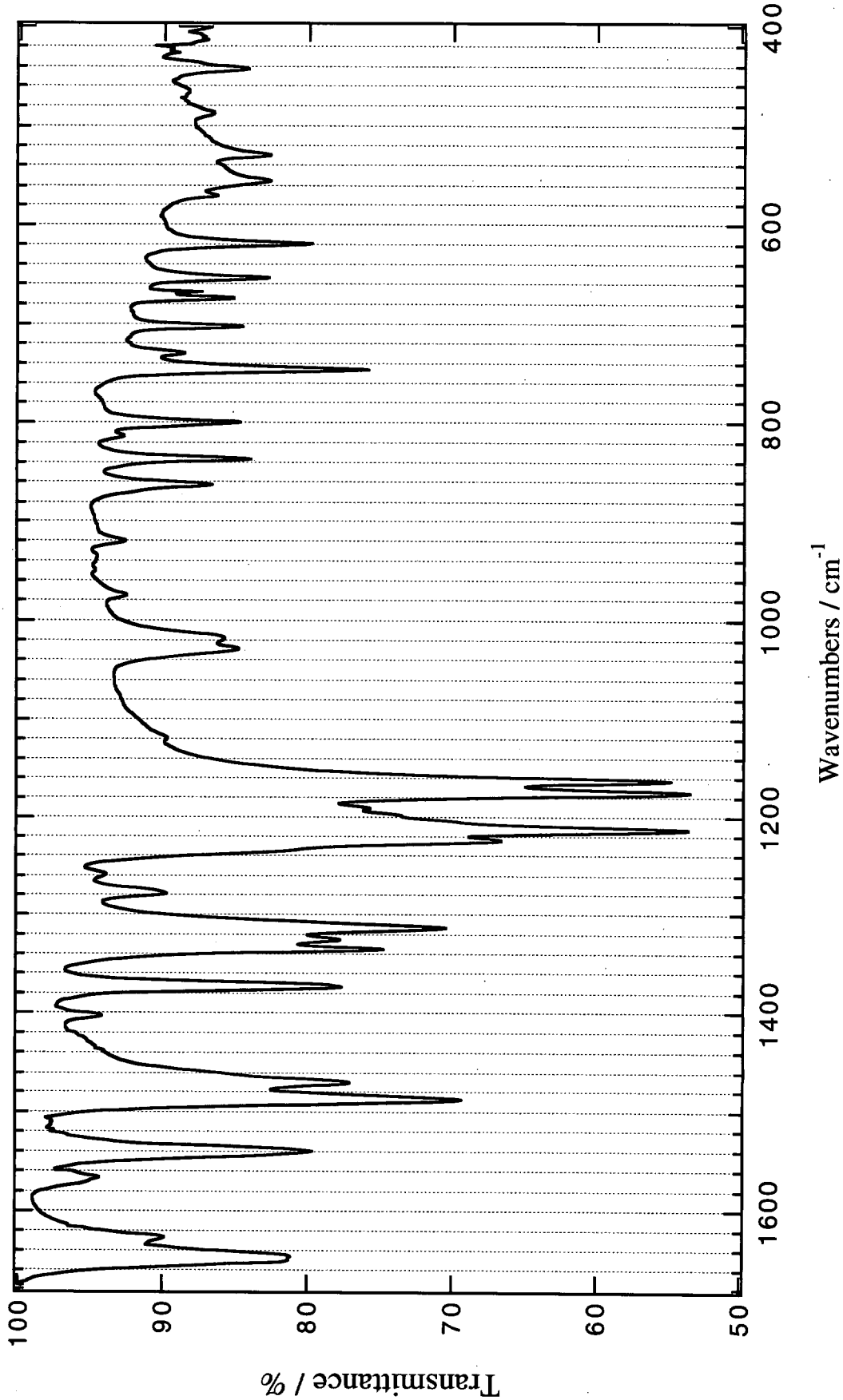
F1 - Acquisition parameters
NDO 1
TD 128
SFO1 600.1327 MHz
FIDRES 38.146969 Hz
SW 8.136 ppm

F2 - Processing parameters
SI 1024
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1303034 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 23.00 cm
CX1 23.00 cm
F2PLO 8.039 ppm
F2LO 4824.64 Hz
F2HI -0.097 ppm
F2HI -58.18 Hz
F1PLO 8.037 ppm
F1LO 4822.97 Hz
F1HI -0.100 ppm
F1HI -59.84 Hz
F2PPMCM 0.35375 ppm/cm
F2HZCM 212.29620 Hz/cm
F1PPMCM 0.35375 ppm/cm
F1HZCM 212.29619 Hz/cm

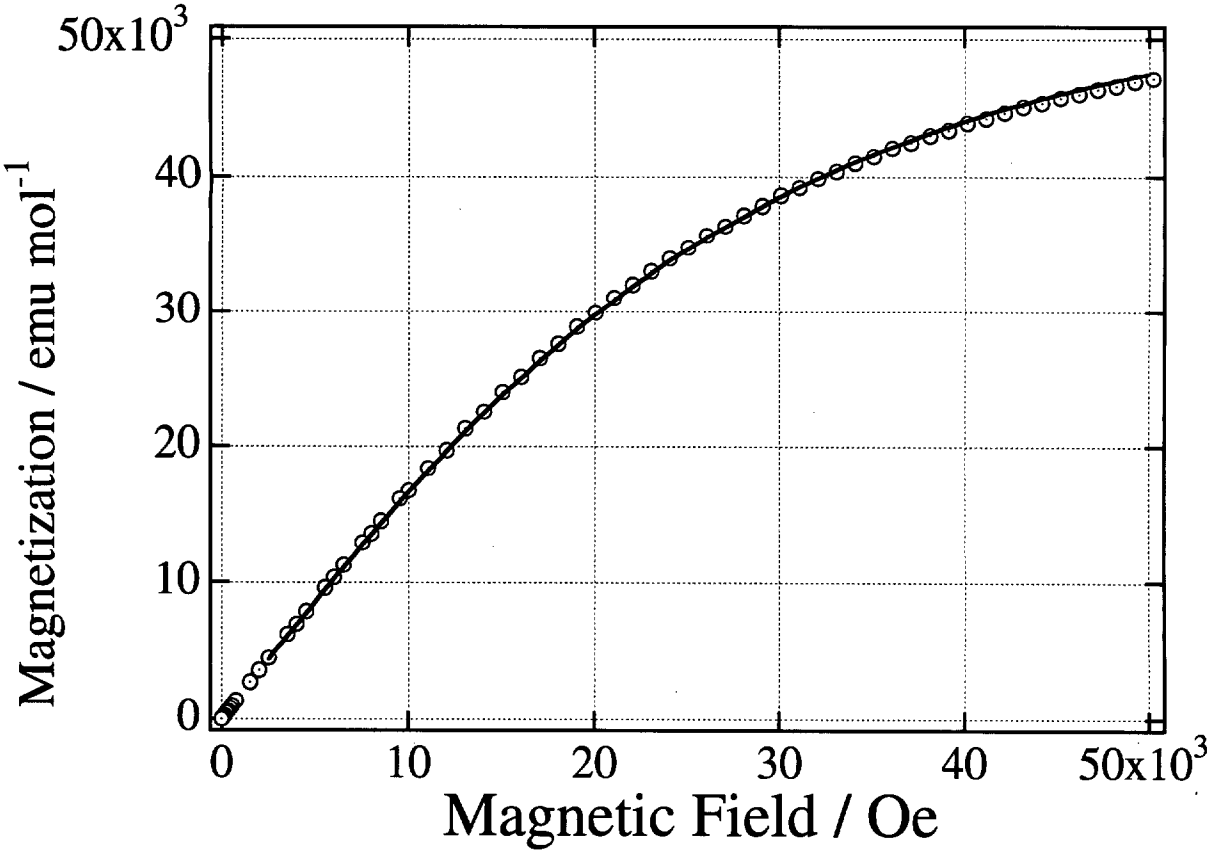


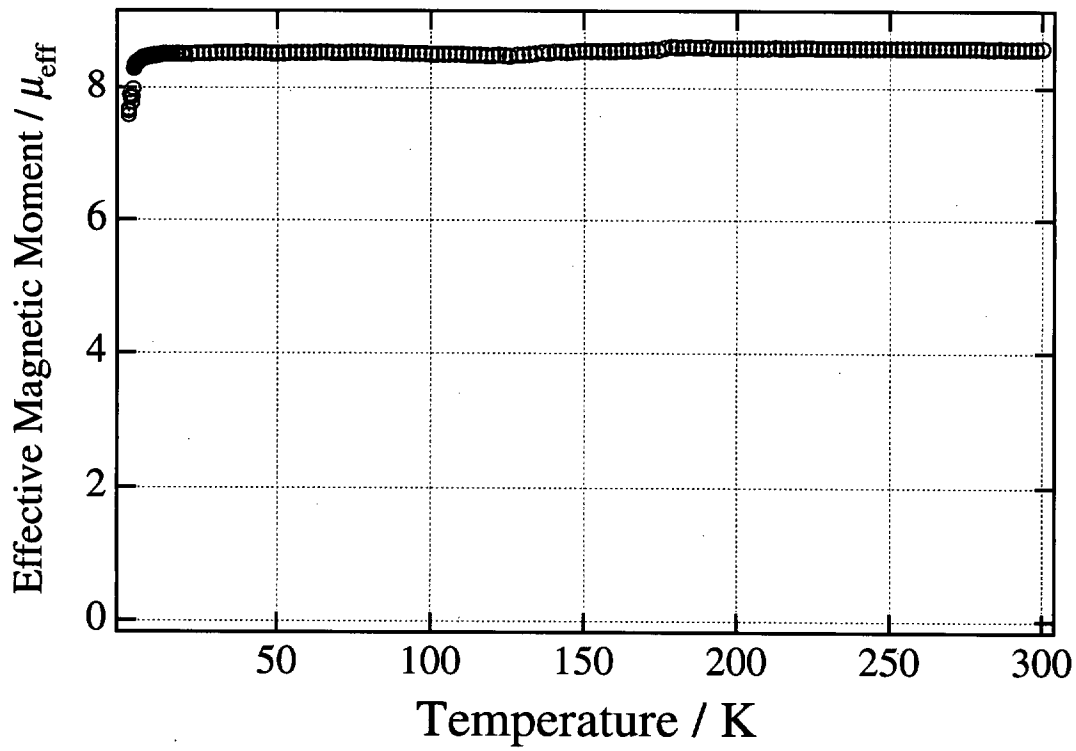


IR spectrum for $\mathbf{2}_{\mathbf{Br}}$.

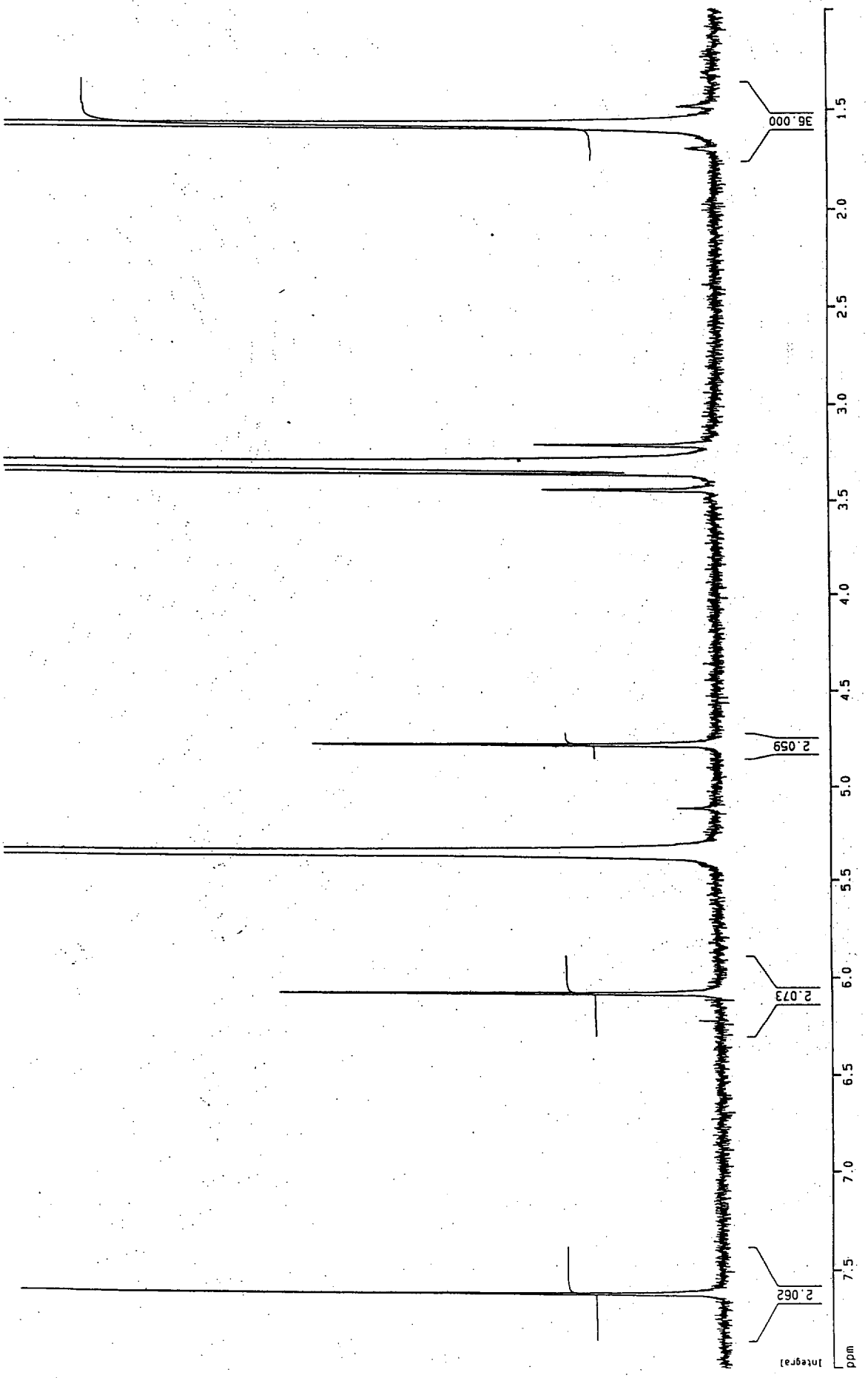
Title; Mn(II)-Induced Formation and Structural Elucidation of [3+3] Benzene-Dimer Derivative from *m*-Phenylenebis(*N-tert*-butylaminoxyl)

Authors; Fumiyasu Iwahori, Katsuya Inoue and Hiizu Iwamura





Field dependence of magnetization (top)
and temperature dependence of effective magnetic moment
in the field of 0.5 T (bottom) for 2_{Br}•[Mn(hfac)$_2$•H$_2$O]•CH$_2$Cl$_2$
Mn(II)-Induced ...
F. Iwahori, K. Inoue and H. Iwamura



Title: Mn(II)-induced formation and ...
Authors: Fumiyasu Iwahori, Katsuya Inoue and Hiroshi Iwamura