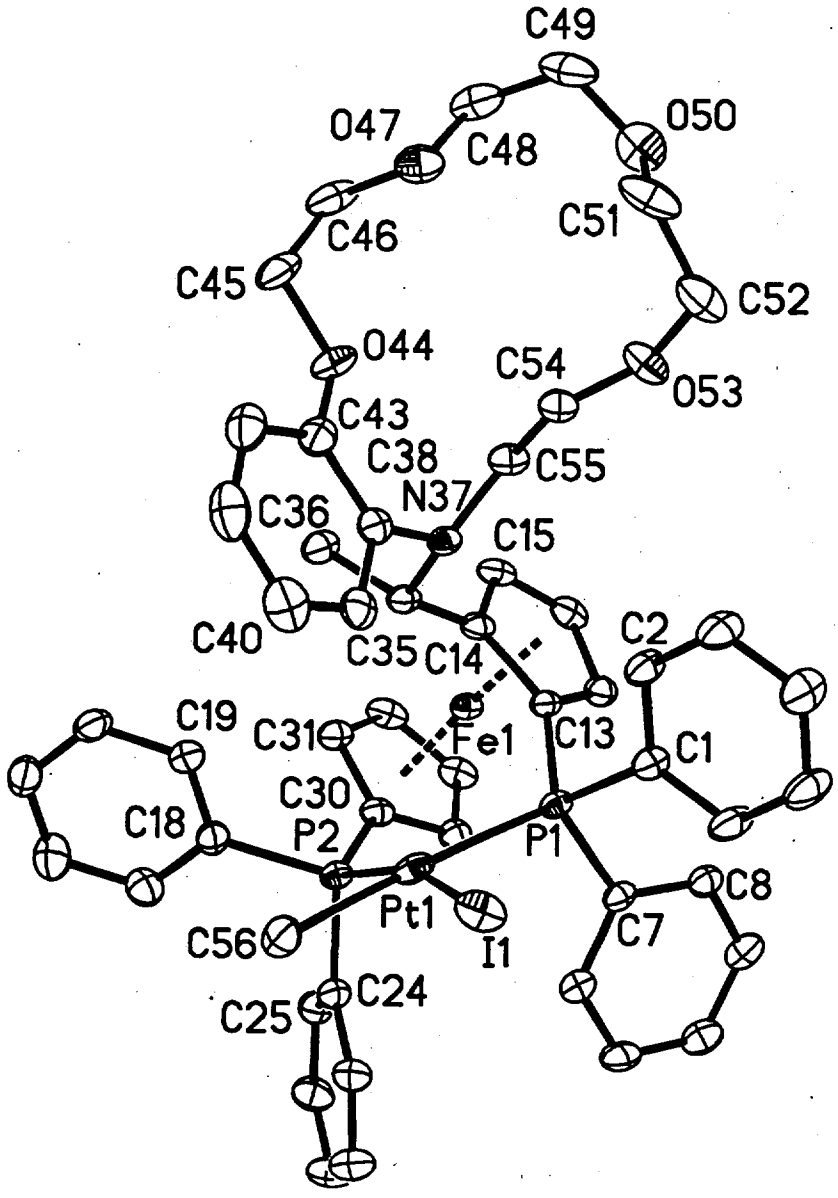

Figure 1. Complete structure and numbering scheme for PtMeI(**1**).

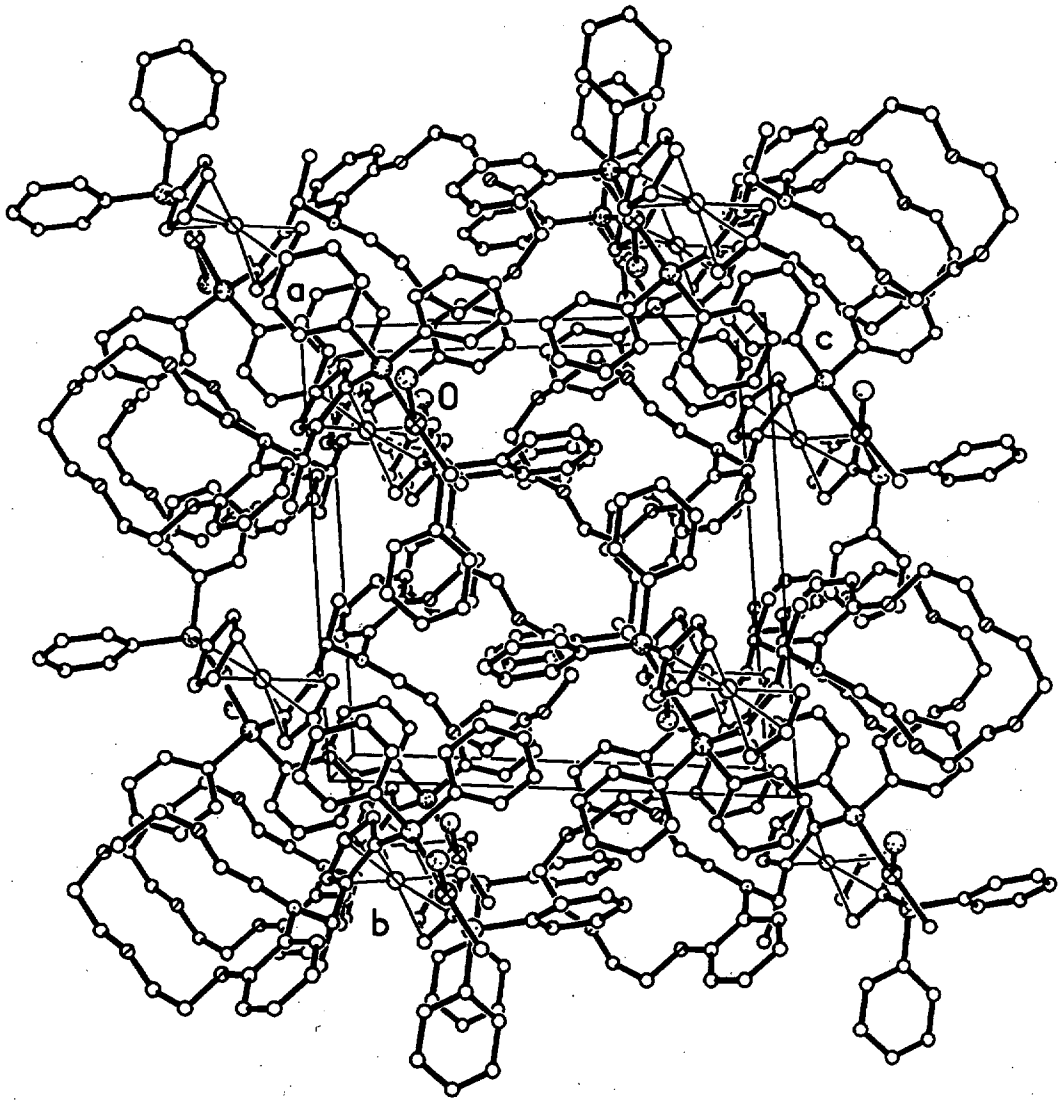

Figure 2. Unit cell diagram for PtMeI(**1**).

Table 1. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for PtMeI(**1**).

	x	y	z	U(eq)
Pt(1)	0.158675(13)	0.222907(13)	0.250128(12)	0.02236(6)
I(1)	0.34949(5)	0.13548(5)	0.24390(4)	0.0298(2)
C(56')	0.3114(6)	0.1345(7)	0.2206(8)	0.0299(2)
I(1')	0.25136(6)	0.34466(5)	0.32056(5)	0.0298(2)
P(1)	0.10393(8)	0.09805(7)	0.18245(7)	0.0176(2)
P(2)	-0.01233(8)	0.31305(7)	0.29807(7)	0.0183(2)
Fe(1)	-0.10453(4)	0.22580(4)	0.13032(4)	0.01785(12)
C(1)	0.2161(3)	0.0100(3)	0.1142(3)	0.0205(8)
C(2)	0.2881(3)	0.0340(3)	0.0160(3)	0.0260(9)
C(3)	0.3740(4)	-0.0317(3)	-0.0381(3)	0.0322(10)
C(4)	0.3884(4)	-0.1221(4)	0.0054(4)	0.0340(11)
C(5)	0.3186(4)	-0.1462(4)	0.1028(3)	0.0389(12)
C(6)	0.2335(4)	-0.0807(3)	0.1570(3)	0.0328(11)
C(7)	-0.0033(3)	0.0175(3)	0.2796(3)	0.0183(8)
C(8)	-0.0522(4)	-0.0661(3)	0.2626(3)	0.0242(9)
C(9)	-0.1363(4)	-0.1220(3)	0.3407(3)	0.0288(10)
C(10)	-0.1699(4)	-0.0959(3)	0.4362(3)	0.0288(9)
C(11)	-0.1189(3)	-0.0166(3)	0.4546(3)	0.0259(9)
C(12)	-0.0364(3)	0.0405(3)	0.3766(3)	0.0224(8)
C(13)	0.0369(3)	0.1351(3)	0.0966(3)	0.0178(7)
C(14)	0.0647(3)	0.2214(3)	0.0256(3)	0.0193(8)
C(15)	-0.0170(3)	0.2205(3)	-0.0202(3)	0.0226(8)
C(16)	-0.0931(3)	0.1387(3)	0.0202(3)	0.0243(9)
C(17)	-0.0606(3)	0.0853(3)	0.0908(3)	0.0214(8)
C(18)	0.0108(3)	0.4467(3)	0.2747(3)	0.0213(8)
C(19)	0.0972(4)	0.4831(3)	0.1852(3)	0.0267(9)
C(20)	0.1168(4)	0.5836(3)	0.1637(3)	0.0290(9)
C(21)	0.0531(4)	0.6496(3)	0.2323(4)	0.0306(10)
C(22)	-0.0318(4)	0.6145(3)	0.3220(4)	0.0348(11)
C(23)	-0.0529(4)	0.5134(3)	0.3428(3)	0.0298(9)
C(24)	-0.1008(3)	0.2946(3)	0.4298(3)	0.0205(8)
C(25)	-0.2193(4)	0.3212(3)	0.4708(3)	0.0244(8)
C(26)	-0.2854(4)	0.3078(4)	0.5712(3)	0.0309(10)
C(27)	-0.2358(4)	0.2647(4)	0.6326(3)	0.0370(11)
C(28)	-0.1189(4)	0.2357(4)	0.5929(3)	0.0324(10)
C(29)	-0.0507(4)	0.2518(3)	0.4927(3)	0.0252(9)
C(30)	-0.1247(3)	0.2963(3)	0.2520(3)	0.0198(8)
C(31)	-0.1521(3)	0.3634(3)	0.1844(3)	0.0230(8)
C(32)	-0.2463(3)	0.3225(3)	0.1693(3)	0.0264(9)
C(33)	-0.2787(3)	0.2310(3)	0.2267(3)	0.0257(9)
C(34)	-0.2043(3)	0.2137(3)	0.2775(3)	0.0219(8)

C(35)	0.1616(3)	0.2959(3)	-0.0030(3)	0.0194(8)
C(36)	0.1276(4)	0.3966(3)	-0.0395(3)	0.0258(9)
N(37)	0.2743(3)	0.2585(2)	-0.0766(2)	0.0190(7)
C(38)	0.3724(3)	0.3203(3)	-0.0927(3)	0.0205(8)
C(39)	0.4176(4)	0.3122(3)	-0.0210(3)	0.0252(9)
C(40)	0.5116(4)	0.3697(4)	-0.0282(4)	0.0359(11)
C(41)	0.5624(4)	0.4361(4)	-0.1094(4)	0.0367(11)
C(42)	0.5190(4)	0.4465(3)	-0.1809(4)	0.0327(10)
C(43)	0.4233(3)	0.3903(3)	-0.1724(3)	0.0262(9)
O(44)	0.3726(3)	0.3985(2)	-0.2393(2)	0.0317(7)
C(45)	0.4190(4)	0.4686(3)	-0.3221(3)	0.0342(11)
C(46)	0.3757(4)	0.4396(4)	-0.3962(3)	0.0366(12)
O(47)	0.4407(3)	0.3549(2)	-0.4404(2)	0.0323(7)
C(48)	0.3995(4)	0.3168(4)	-0.5066(4)	0.0384(12)
C(49)	0.4691(4)	0.2275(4)	-0.5502(4)	0.0436(13)
O(50)	0.4383(3)	0.1426(3)	-0.4828(3)	0.0390(8)
C(51)	0.5173(4)	0.1189(5)	-0.4372(4)	0.0421(13)
C(52)	0.4556(5)	0.0520(4)	-0.3461(4)	0.0427(12)
O(53)	0.3558(3)	0.0952(2)	-0.2738(2)	0.0347(7)
C(54)	0.3841(4)	0.1692(3)	-0.2255(3)	0.0253(9)
C(55)	0.2672(3)	0.2138(3)	-0.1603(3)	0.0233(8)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2. Bond lengths (Å) and angles (•) for PtMeI(**1**).

Pt(1)-C(56)	2.109(4)	C(18)-C(23)	1.388(6)
Pt(1)-C(56')	2.115(4)	C(18)-C(19)	1.396(6)
Pt(1)-P(2)	2.2891(10)	C(19)-C(20)	1.385(6)
Pt(1)-P(1)	2.3002(11)	C(20)-C(21)	1.385(7)
Pt(1)-I(1')	2.5663(6)	C(21)-C(22)	1.384(7)
Pt(1)-I(1)	2.5835(5)	C(22)-C(23)	1.394(6)
P(1)-C(1)	1.826(4)	C(24)-C(25)	1.391(5)
P(1)-C(13)	1.825(4)	C(24)-C(29)	1.404(5)
P(1)-C(7),	1.832(4)	C(25)-C(26)	1.387(6)
P(2)-C(30)	1.819(4)	C(26)-C(27)	1.384(6)
P(2)-C(24)	1.823(4)	C(27)-C(28)	1.383(6)
P(2)-C(18)	1.831(4)	C(28)-C(29)	1.390(6)
Fe(1)-C(13)	2.020(4)	C(30)-C(31)	1.441(5)
Fe(1)-C(17)	2.033(4)	C(30)-C(34)	1.445(6)
Fe(1)-C(34)	2.034(4)	C(31)-C(32)	1.419(6)
Fe(1)-C(30)	2.045(4)	C(32)-C(33)	1.424(6)
Fe(1)-C(14)	2.049(4)	C(33)-C(34)	1.420(5)
Fe(1)-C(33)	2.057(4)	C(35)-N(37)	1.488(5)
Fe(1)-C(16)	2.061(4)	C(35)-C(36)	1.540(5)
Fe(1)-C(31)	2.067(4)	N(37)-C(38)	1.433(5)
Fe(1)-C(15)	2.068(4)	N(37)-C(55)	1.470(5)
Fe(1)-C(32)	2.071(4)	C(38)-C(39)	1.394(6)
C(1)-C(6)	1.392(5)	C(38)-C(43)	1.403(6)
C(1)-C(2)	1.390(5)	C(39)-C(40)	1.392(6)
C(2)-C(3)	1.391(6)	C(40)-C(41)	1.387(7)
C(3)-C(4)	1.382(6)	C(41)-C(42)	1.377(7)
C(4)-C(5)	1.377(6)	C(42)-C(43)	1.394(6)
C(5)-C(6)	1.385(6)	C(43)-O(44)	1.378(5)
C(7)-C(8)	1.396(6)	O(44)-C(45)	1.427(5)
C(7)-C(12)	1.396(6)	C(45)-C(46)	1.497(7)
C(8)-C(9)	1.397(6)	C(46)-O(47)	1.426(6)
C(9)-C(10)	1.388(7)	O(47)-C(48)	1.424(6)
C(10)-C(11)	1.371(6)	C(48)-C(49)	1.495(8)
C(11)-C(12)	1.396(5)	C(49)-O(50)	1.422(6)
C(13)-C(17)	1.444(5)	O(50)-C(51)	1.421(6)
C(13)-C(14)	1.466(5)	C(51)-C(52)	1.505(8)
C(14)-C(15)	1.439(5)	C(52)-O(53)	1.417(6)
C(14)-C(35)	1.502(5)	O(53)-C(54)	1.417(5)
C(15)-C(16)	1.413(6)	C(54)-C(55)	1.518(6)
C(16)-C(17)	1.416(5)		

C(56)-Pt(1)-P(2)	82.5(3)	C(56')-Pt(1)-P(1)	82.9(3)
C(56')-Pt(1)-P(2)	174.3(3)	P(2)-Pt(1)-P(1)	98.49(3)
C(56)-Pt(1)-P(1)	176.6(3)	C(56')-Pt(1)-I(1')	87.4(3)

P(2)-Pt(1)-I(1')	91.16(3)	C(17)-Fe(1)-C(15)	68.0(2)
P(1)-Pt(1)-I(1')	170.29(3)	C(34)-Fe(1)-C(15)	171.5(2)
C(56)-Pt(1)-I(1)	84.0(3)	C(30)-Fe(1)-C(15)	147.0(2)
P(2)-Pt(1)-I(1)	163.39(3)	C(14)-Fe(1)-C(15)	40.91(14)
P(1)-Pt(1)-I(1)	94.47(3)	C(33)-Fe(1)-C(15)	134.7(2)
C(1)-P(1)-C(13)	102.0(2)	C(16)-Fe(1)-C(15)	40.0(2)
C(1)-P(1)-C(7)	102.1(2)	C(31)-Fe(1)-C(15)	117.4(2)
C(13)-P(1)-C(7)	105.9(2)	C(13)-Fe(1)-C(32)	177.0(2)
C(1)-P(1)-Pt(1)	118.52(13)	C(17)-Fe(1)-C(32)	140.9(2)
C(13)-P(1)-Pt(1)	116.70(13)	C(34)-Fe(1)-C(32)	68.4(2)
C(7)-P(1)-Pt(1)	109.99(13)	C(30)-Fe(1)-C(32)	68.4(2)
C(30)-P(2)-C(24)	100.0(2)	C(14)-Fe(1)-C(32)	137.7(2)
C(30)-P(2)-C(18)	101.2(2)	C(33)-Fe(1)-C(32)	40.4(2)
C(24)-P(2)-C(18)	104.7(2)	C(16)-Fe(1)-C(32)	113.4(2)
C(30)-P(2)-Pt(1)	122.81(13)	C(31)-Fe(1)-C(32)	40.1(2)
C(24)-P(2)-Pt(1)	112.03(12)	C(15)-Fe(1)-C(32)	112.4(2)
C(18)-P(2)-Pt(1)	113.78(13)	C(6)-C(1)-C(2)	118.3(4)
C(13)-Fe(1)-C(17)	41.8(2)	C(6)-C(1)-P(1)	122.4(3)
C(13)-Fe(1)-C(34)	110.2(2)	C(2)-C(1)-P(1)	119.3(3)
C(17)-Fe(1)-C(34)	105.8(2)	C(3)-C(2)-C(1)	120.6(4)
C(13)-Fe(1)-C(30)	108.8(2)	C(4)-C(3)-C(2)	120.1(4)
C(17)-Fe(1)-C(30)	133.6(2)	C(5)-C(4)-C(3)	119.8(4)
C(34)-Fe(1)-C(30)	41.5(2)	C(4)-C(5)-C(6)	120.2(4)
C(13)-Fe(1)-C(14)	42.22(14)	C(5)-C(6)-C(1)	121.0(4)
C(17)-Fe(1)-C(14)	69.9(2)	C(8)-C(7)-C(12)	118.2(4)
C(34)-Fe(1)-C(14)	143.8(2)	C(8)-C(7)-P(1)	124.0(3)
C(30)-Fe(1)-C(14)	115.0(2)	C(12)-C(7)-P(1)	117.7(3)
C(13)-Fe(1)-C(33)	140.1(2)	C(7)-C(8)-C(9)	120.5(4)
C(17)-Fe(1)-C(33)	109.6(2)	C(10)-C(9)-C(8)	120.0(4)
C(34)-Fe(1)-C(33)	40.6(2)	C(11)-C(10)-C(9)	120.2(4)
C(30)-Fe(1)-C(33)	68.8(2)	C(10)-C(11)-C(12)	119.9(4)
C(14)-Fe(1)-C(33)	175.6(2)	C(11)-C(12)-C(7)	121.1(4)
C(13)-Fe(1)-C(16)	69.5(2)	C(17)-C(13)-C(14)	107.0(3)
C(17)-Fe(1)-C(16)	40.5(2)	C(17)-C(13)-P(1)	124.9(3)
C(34)-Fe(1)-C(16)	131.6(2)	C(14)-C(13)-P(1)	128.0(3)
C(30)-Fe(1)-C(16)	172.5(2)	C(17)-C(13)-Fe(1)	69.6(2)
C(14)-Fe(1)-C(16)	69.0(2)	C(14)-C(13)-Fe(1)	70.0(2)
C(33)-Fe(1)-C(16)	107.6(2)	P(1)-C(13)-Fe(1)	123.0(2)
C(13)-Fe(1)-C(31)	137.1(2)	C(15)-C(14)-C(13)	106.4(3)
C(17)-Fe(1)-C(31)	174.4(2)	C(15)-C(14)-C(35)	123.6(3)
C(34)-Fe(1)-C(31)	69.0(2)	C(13)-C(14)-C(35)	129.9(3)
C(30)-Fe(1)-C(31)	41.0(2)	C(15)-C(14)-Fe(1)	70.3(2)
C(14)-Fe(1)-C(31)	112.9(2)	C(13)-C(14)-Fe(1)	67.8(2)
C(33)-Fe(1)-C(31)	68.1(2)	C(35)-C(14)-Fe(1)	129.4(3)
C(16)-Fe(1)-C(31)	144.7(2)	C(16)-C(15)-C(14)	109.5(3)
C(13)-Fe(1)-C(15)	69.4(2)	C(16)-C(15)-Fe(1)	69.7(2)

C(14)-C(15)-Fe(1)	68.8(2)	C(55)-N(37)-C(35)	116.1(3)
C(15)-C(16)-C(17)	108.4(3)	C(39)-C(38)-C(43)	117.8(4)
C(15)-C(16)-Fe(1)	70.3(2)	C(39)-C(38)-N(37)	116.8(3)
C(17)-C(16)-Fe(1)	68.7(2)	C(43)-C(38)-N(37)	125.3(4)
C(16)-C(17)-C(13)	108.8(3)	C(40)-C(39)-C(38)	121.7(4)
C(16)-C(17)-Fe(1)	70.8(2)	C(41)-C(40)-C(39)	119.2(4)
C(13)-C(17)-Fe(1)	68.6(2)	C(42)-C(41)-C(40)	120.4(4)
C(23)-C(18)-C(19)	118.4(4)	C(41)-C(42)-C(43)	120.2(4)
C(23)-C(18)-P(2)	122.8(3)	O(44)-C(43)-C(42)	123.6(4)
C(19)-C(18)-P(2)	118.8(3)	O(44)-C(43)-C(38)	115.8(4)
C(20)-C(19)-C(18)	120.8(4)	C(42)-C(43)-C(38)	120.6(4)
C(19)-C(20)-C(21)	120.3(4)	C(43)-O(44)-C(45)	119.1(3)
C(20)-C(21)-C(22)	119.6(4)	O(44)-C(45)-C(46)	107.0(4)
C(21)-C(22)-C(23)	120.1(5)	O(47)-C(46)-C(45)	108.2(3)
C(18)-C(23)-C(22)	120.8(4)	C(48)-O(47)-C(46)	112.4(4)
C(25)-C(24)-C(29)	118.1(4)	O(47)-C(48)-C(49)	110.6(4)
C(25)-C(24)-P(2)	121.4(3)	O(50)-C(49)-C(48)	112.4(4)
C(29)-C(24)-P(2)	120.4(3)	C(49)-O(50)-C(51)	115.0(4)
C(26)-C(25)-C(24)	120.9(4)	O(50)-C(51)-C(52)	108.8(4)
C(27)-C(26)-C(25)	120.6(4)	O(53)-C(52)-C(51)	114.2(4)
C(28)-C(27)-C(26)	119.2(4)	C(52)-O(53)-C(54)	113.8(4)
C(27)-C(28)-C(29)	120.6(4)	O(53)-C(54)-C(55)	105.7(3)
C(28)-C(29)-C(24)	120.5(4)	N(37)-C(55)-C(54)	111.9(3
C(31)-C(30)-C(34)	107.2(3)		
C(31)-C(30)-P(2)	126.4(3)		
C(34)-C(30)-P(2)	126.3(3)		
C(31)-C(30)-Fe(1)	70.3(2)		
C(34)-C(30)-Fe(1)	68.9(2)		
P(2)-C(30)-Fe(1)	126.6(2)		
C(32)-C(31)-C(30)	108.0(4)		
C(32)-C(31)-Fe(1)	70.1(2)		
C(30)-C(31)-Fe(1)	68.7(2)		
C(31)-C(32)-C(33)	108.5(3)		
C(31)-C(32)-Fe(1)	69.8(2)		
C(33)-C(32)-Fe(1)	69.3(2)		
C(34)-C(33)-C(32)	108.4(4)		
C(34)-C(33)-Fe(1)	68.8(2)		
C(32)-C(33)-Fe(1)	70.3(2)		
C(33)-C(34)-C(30)	107.9(3)		
C(33)-C(34)-Fe(1)	70.5(2)		
C(30)-C(34)-Fe(1)	69.7(2)		
N(37)-C(35)-C(14)	111.4(3)		
N(37)-C(35)-C(36)	111.3(3)		
C(14)-C(35)-C(36)	112.0(3)		
C(38)-N(37)-C(55)	119.4(3)		
C(38)-N(37)-C(35)	112.5(3)		

Table 3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for PtMeI(**1**).

	U11	U22	U33	U23	U13	U12
Pt(1)	17(1)	29(1)	22(1)	10(1)	-10(1)	-5(1)
I(1)	20(1)	46(1)	26(1)	-9(1)	-12(1)	14(1)
C(56)	32(1)	28(1)	38(1)	4(1)	-24(1)	-9(1)
C(56')	20(1)	46(1)	26(1)	-9(1)	-12(1)	14(1)
I(1')	32(1)	28(1)	38(1)	4(1)	-24(1)	-9(1)
P(1)	16(1)	20(1)	15(1)	2(1)	-5(1)	3(1)
P(2)	17(1)	21(1)	17(1)	1(1)	-7(1)	1(1)
Fe(1)	15(1)	23(1)	15(1)	-1(1)	-6(1)	3(1)
C(1)	16(2)	23(2)	20(2)	2(2)	-5(2)	3(2)
C(2)	23(2)	25(2)	23(2)	5(2)	-4(2)	5(2)
C(3)	24(2)	35(2)	23(2)	5(2)	3(2)	6(2)
C(4)	25(2)	34(3)	33(3)	2(2)	-4(2)	14(2)
C(5)	38(3)	35(3)	29(3)	10(2)	-3(2)	18(2)
C(6)	34(2)	33(2)	22(2)	7(2)	-4(2)	13(2)
C(7)	16(2)	18(2)	18(2)	2(2)	-4(2)	4(1)
C(8)	28(2)	23(2)	24(2)	2(2)	-13(2)	1(2)
C(9)	28(2)	28(2)	34(2)	8(2)	-17(2)	-7(2)
C(10)	20(2)	35(2)	27(2)	7(2)	-6(2)	-5(2)
C(11)	23(2)	32(2)	16(2)	3(2)	-3(2)	1(2)
C(12)	21(2)	24(2)	21(2)	3(2)	-8(2)	0(2)
C(13)	19(2)	20(2)	14(2)	0(2)	-6(2)	2(1)
C(14)	19(2)	23(2)	13(2)	-2(2)	-4(2)	6(2)
C(15)	21(2)	32(2)	15(2)	-4(2)	-8(2)	9(2)
C(16)	23(2)	32(2)	20(2)	-7(2)	-11(2)	6(2)
C(17)	23(2)	23(2)	18(2)	-2(2)	-7(2)	3(2)
C(18)	23(2)	21(2)	23(2)	0(2)	-13(2)	2(2)
C(19)	35(2)	24(2)	22(2)	1(2)	-12(2)	0(2)
C(20)	35(2)	28(2)	26(2)	6(2)	-15(2)	-4(2)
C(21)	39(2)	22(2)	39(3)	1(2)	-24(2)	-3(2)
C(22)	32(2)	28(2)	42(3)	-5(2)	-12(2)	1(2)
C(23)	27(2)	32(2)	29(2)	-5(2)	-9(2)	-2(2)
C(24)	21(2)	22(2)	18(2)	0(2)	-8(2)	1(2)
C(25)	25(2)	26(2)	21(2)	-2(2)	-9(2)	2(2)
C(26)	25(2)	41(3)	22(2)	-5(2)	-4(2)	1(2)
C(27)	35(2)	55(3)	17(2)	2(2)	-6(2)	-5(2)
C(28)	33(2)	43(3)	22(2)	4(2)	-13(2)	-2(2)
C(29)	26(2)	31(2)	20(2)	0(2)	-11(2)	0(2)
C(30)	17(2)	24(2)	16(2)	-2(2)	-5(2)	4(2)

C(31)	22(2)	26(2)	19(2)	-1(2)	-7(2)	8(2)
C(32)	22(2)	38(2)	21(2)	-8(2)	-11(2)	13(2)
C(33)	16(2)	39(2)	21(2)	-5(2)	-7(2)	1(2)
C(34)	20(2)	24(2)	19(2)	-1(2)	-5(2)	2(2)
C(35)	20(2)	22(2)	14(2)	0(2)	-5(2)	3(2)
C(36)	24(2)	25(2)	22(2)	2(2)	-4(2)	7(2)
N(37)	17(1)	22(2)	14(2)	1(1)	-3(1)	0(1)
C(38)	18(2)	20(2)	20(2)	-4(2)	-5(2)	6(2)
C(39)	26(2)	22(2)	27(2)	-6(2)	-10(2)	7(2)
C(40)	33(2)	35(3)	49(3)	-10(2)	-24(2)	8(2)
C(41)	25(2)	31(2)	53(3)	-12(2)	-14(2)	0(2)
C(42)	25(2)	28(2)	36(3)	-2(2)	-3(2)	-3(2)
C(43)	21(2)	25(2)	24(2)	-2(2)	-1(2)	2(2)
O(44)	31(2)	35(2)	22(2)	13(1)	-6(1)	-8(1)
C(45)	32(2)	27(2)	25(2)	10(2)	5(2)	3(2)
C(46)	29(2)	42(3)	26(2)	15(2)	-2(2)	8(2)
O(47)	26(2)	44(2)	27(2)	2(1)	-11(1)	0(1)
C(48)	33(2)	53(3)	29(3)	14(2)	-14(2)	-13(2)
C(49)	34(2)	72(4)	20(2)	-5(2)	-4(2)	-15(3)
O(50)	32(2)	45(2)	43(2)	-7(2)	-17(2)	0(2)
C(51)	25(2)	74(4)	27(3)	-22(3)	-8(2)	12(2)
C(52)	44(3)	52(3)	35(3)	-21(2)	-16(2)	17(2)
O(53)	34(2)	42(2)	27(2)	-16(2)	-9(1)	5(1)
C(54)	23(2)	30(2)	20(2)	-1(2)	-6(2)	0(2)
C(55)	20(2)	30(2)	16(2)	1(2)	-5(2)	0(2)

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$.

Table 4. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for PtMeI(**1**).

	x	y	z	U(eq)
H(56A)	0.147(3)	0.383(2)	0.339(4)	0.045
H(56B)	0.283(3)	0.361(3)	0.273(2)	0.045
H(56C)	0.217(6)	0.3008(10)	0.377(3)	0.045
H(56D)	0.341(4)	0.115(5)	0.153(2)	0.045
H(56E)	0.292(2)	0.076(3)	0.266(4)	0.045
H(56F)	0.372(2)	0.172(2)	0.228(5)	0.045
H(2)	0.2784(3)	0.0958(3)	-0.0145(3)	0.031
H(3)	0.4230(4)	-0.0145(3)	-0.1050(3)	0.039
H(4)	0.4462(4)	-0.1674(4)	-0.0319(4)	0.041
H(5)	0.3288(4)	-0.2081(4)	0.1330(3)	0.047
H(6)	0.1863(4)	-0.0978(3)	0.2243(3)	0.039
H(8)	-0.0281(4)	-0.0851(3)	0.1975(3)	0.029
H(9)	-0.1706(4)	-0.1779(3)	0.3283(3)	0.035
H(10)	-0.2283(4)	-0.1332(3)	0.4891(3)	0.035
H(11)	-0.1396(3)	-0.0005(3)	0.5203(3)	0.031
H(12)	-0.0022(3)	0.0960(3)	0.3898(3)	0.027
H(15)	-0.0221(3)	0.2719(3)	-0.0702(3)	0.027
H(16)	-0.1597(3)	0.1221(3)	0.0029(3)	0.029
H(17)	-0.0996(3)	0.0241(3)	0.1310(3)	0.026
H(19)	0.1432(4)	0.4384(3)	0.1384(3)	0.032
H(20)	0.1741(4)	0.6074(3)	0.1016(3)	0.035
H(21)	0.0675(4)	0.7185(3)	0.2179(4)	0.037
H(22)	-0.0758(4)	0.6594(3)	0.3694(4)	0.042
H(23)	-0.1115(4)	0.4899(3)	0.4043(3)	0.036
H(25)	-0.2554(4)	0.3490(3)	0.4294(3)	0.029
H(26)	-0.3656(4)	0.3283(4)	0.5980(3)	0.037
H(27)	-0.2815(4)	0.2553(4)	0.7013(3)	0.044
H(28)	-0.0848(4)	0.2044(4)	0.6343(3)	0.039
H(29)	0.0302(4)	0.2338(3)	0.4667(3)	0.030
H(31)	-0.1109(3)	0.4269(3)	0.1528(3)	0.028
H(32)	-0.2825(3)	0.3523(3)	0.1246(3)	0.032
H(33)	-0.3422(3)	0.1860(3)	0.2298(3)	0.031
H(34)	-0.2073(3)	0.1552(3)	0.3237(3)	0.026
H(35)	0.1745(3)	0.3063(3)	0.0573(3)	0.023
H(36A)	0.1884(13)	0.4452(6)	-0.049(2)	0.039
H(36B)	0.0519(13)	0.4184(11)	0.0094(10)	0.039
H(36C)	0.121(3)	0.3902(6)	-0.1018(11)	0.039

H(39)	0.3834(4)	0.2662(3)	0.0343(3)	0.030
H(40)	0.5406(4)	0.3635(4)	0.0218(4)	0.043
H(41)	0.6276(4)	0.4748(4)	-0.1156(4)	0.044
H(42)	0.5545(4)	0.4921(3)	-0.2363(4)	0.039
H(45A)	0.5062(4)	0.4678(3)	-0.3500(3)	0.041
H(45B)	0.3913(4)	0.5359(3)	-0.3025(3)	0.041
H(46A)	0.2906(4)	0.4241(4)	-0.3637(3)	0.044
H(46B)	0.3874(4)	0.4946(4)	-0.4469(3)	0.044
H(48A)	0.4066(4)	0.3681(4)	-0.5597(4)	0.046
H(48B)	0.3152(4)	0.2991(4)	-0.4713(4)	0.046
H(49A)	0.4556(4)	0.2139(4)	-0.6088(4)	0.052
H(49B)	0.5540(4)	0.2412(4)	-0.5718(4)	0.052
H(51A)	0.5427(4)	0.1800(5)	-0.4196(4)	0.051
H(51B)	0.5882(4)	0.0855(5)	-0.4830(4)	0.051
H(52A)	0.4305(5)	-0.0084(4)	-0.3651(4)	0.051
H(52B)	0.5124(5)	0.0318(4)	-0.3170(4)	0.051
H(54A)	0.4351(4)	0.2201(3)	-0.2738(3)	0.030
H(54B)	0.4258(4)	0.1401(3)	-0.1855(3)	0.030
H(55A)	0.2430(3)	0.2649(3)	-0.1997(3)	0.028
H(55B)	0.2062(3)	0.1617(3)	-0.1356(3)	0.028

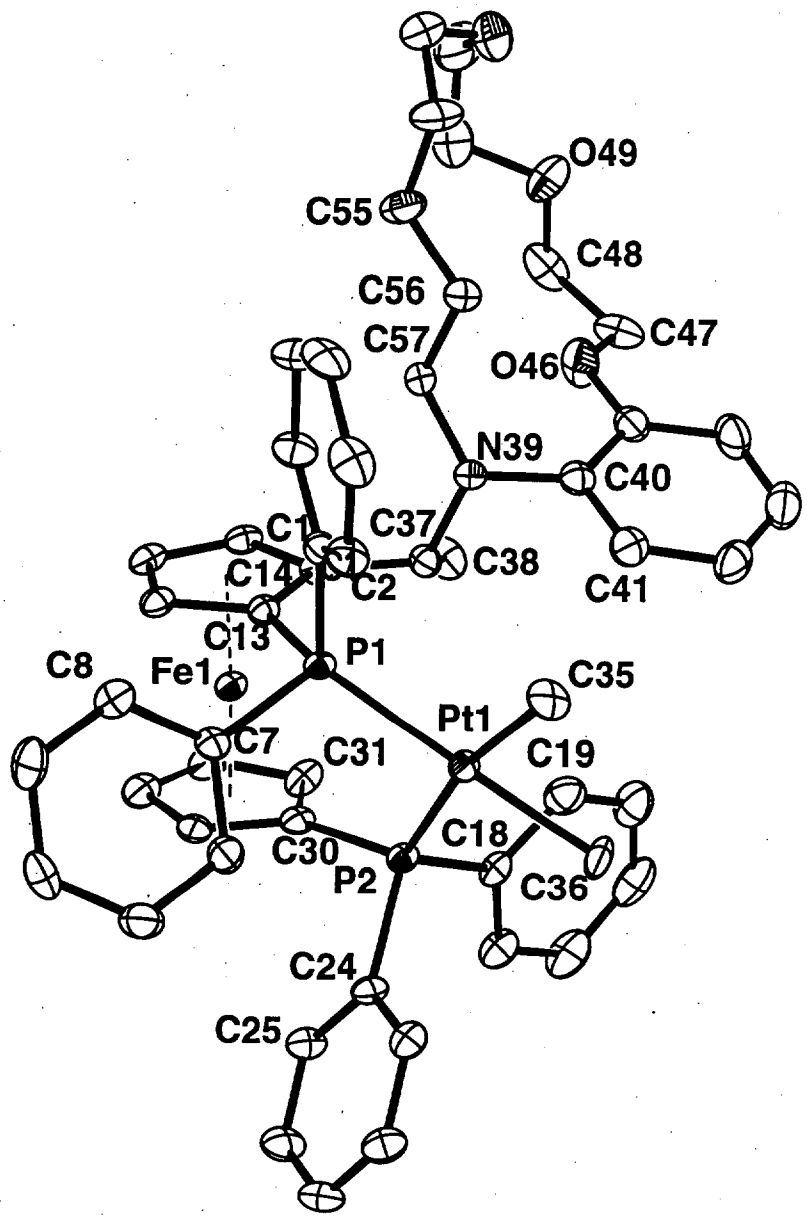

Figure 3. Structure and numbering scheme for $PtMe_2$(**1**).

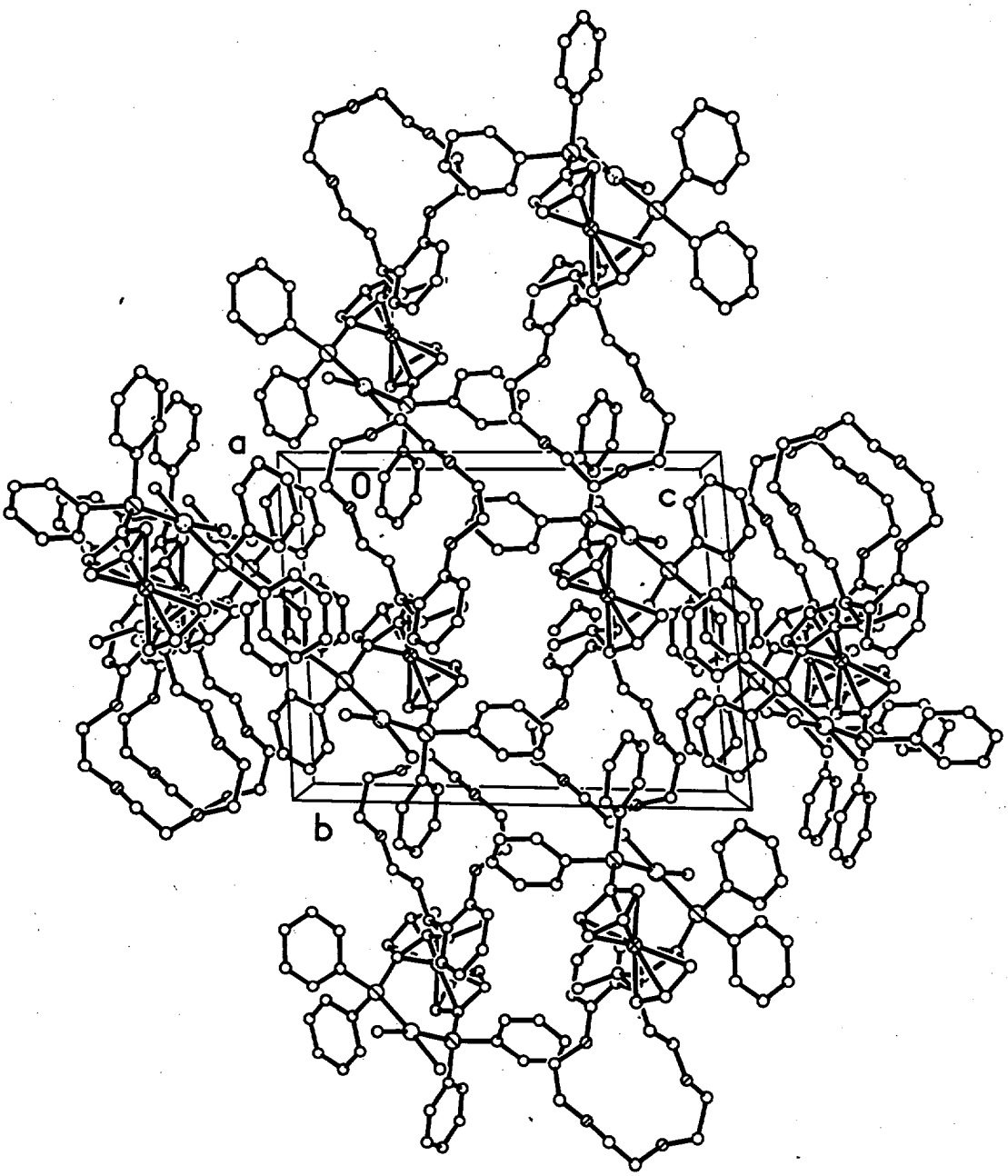

Figure 4. Unit cell diagram for $PtMe_2$(**1**).

Table 5. Crystal data and structure refinement for $PtMe_2$(**1**).

Empirical formula	C52 H57 Fe N O4 P2 Pt	
Formula weight	1072.87	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.3177(13) Å	α= 82.564(2)°
	b = 12.6345(13) Å	β= 79.477(2)°
	c = 15.6691(17) Å	γ= 71.587(2)°
Volume	2268.1(4) Å^3	
Z	2	
Density (calculated)	1.571 Mg/m^3	
Wavelength	0.71073 Å	
Temperature	133(2) K	
F(000)	1084	
Absorption coefficient	3.518 mm^{-1}	
Absorption correction	Empirical	
Max. and min. transmission	0.928 and 0.539	
Theta range for data collection	1.76 to 28.34°.	
Reflections collected	30607	
Independent reflections	10615 [R(int) = 0.0544]	
Data / restraints / parameters	10615 / 0 / 553	
wR(F^2 all data)	wR = 0.1014	
R(F obsd data)	R = 0.0388	
Goodness-of-fit on F^2	1.034	
Observed data [I > 2σ(I)]	9415	
Largest and mean shift / s.u.	0.001and 0.000	
Largest diff. peak and hole	2.509 and -2.058 e/Å^3	

Table 6. Atomic coordinates and equivalent isotropic displacement parameters for $PtMe_2$(**1**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pt(1)	0.652926(13)	0.777775(13)	0.195534(10)	0.01532(6)
Fe(1)	0.40202(5)	0.59216(5)	0.26432(4)	0.01629(13)
P(1)	0.60455(9)	0.66784(9)	0.11165(7)	0.0143(2)
P(2)	0.48390(9)	0.82138(9)	0.29243(7)	0.0158(2)
C(1)	0.7126(4)	0.5847(4)	0.0291(3)	0.0187(9)
C(2)	0.7744(4)	0.6363(4)	-0.0378(3)	0.0241(10)
C(3)	0.8584(4)	0.5728(5)	-0.0981(3)	0.0289(11)
C(4)	0.8808(4)	0.4579(5)	-0.0945(3)	0.0300(11)
C(5)	0.8184(4)	0.4050(4)	-0.0292(3)	0.0299(11)
C(6)	0.7345(4)	0.4698(4)	0.0322(3)	0.0236(10)
C(7)	0.4975(4)	0.7551(4)	0.0444(3)	0.0170(8)
C(8)	0.4639(4)	0.7131(4)	-0.0220(3)	0.0221(9)
C(9)	0.3801(4)	0.7817(4)	-0.0694(3)	0.0279(11)
C(10)	0.3300(4)	0.8933(5)	-0.0539(3)	0.0283(11)
C(11)	0.3650(4)	0.9373(4)	0.0093(3)	0.0278(10)
C(12)	0.4487(4)	0.8686(4)	0.0581(3)	0.0213(9)
C(13)	0.5388(4)	0.5633(4)	0.1679(3)	0.0160(8)
C(14)	0.5694(4)	0.4918(4)	0.2467(3)	0.0176(8)
C(15)	0.4920(4)	0.4246(4)	0.2672(3)	0.0197(9)
C(16)	0.4160(4)	0.4516(4)	0.2043(3)	0.0217(9)
C(17)	0.4448(4)	0.5361(4)	0.1429(3)	0.0186(8)
C(18)	0.5115(4)	0.8139(4)	0.4049(3)	0.0206(9)
C(19)	0.6136(5)	0.7386(4)	0.4284(3)	0.0302(11)
C(20)	0.6390(5)	0.7327(5)	0.5123(3)	0.0367(13)
C(21)	0.5632(6)	0.8014(5)	0.5728(3)	0.0369(13)
C(22)	0.4615(5)	0.8757(5)	0.5508(3)	0.0367(13)
C(23)	0.4356(5)	0.8819(4)	0.4673(3)	0.0271(10)
C(24)	0.3909(4)	0.9652(4)	0.2746(3)	0.0194(9)
C(25)	0.2723(4)	0.9975(4)	0.3071(3)	0.0225(9)
C(26)	0.2047(4)	1.1071(4)	0.2938(3)	0.0288(11)

C(27)	0.2532(4)	1.1859(4)	0.2476(3)	0.0274(10)
C(28)	0.3702(4)	1.1548(4)	0.2126(3)	0.0266(10)
C(29)	0.4391(4)	1.0450(4)	0.2259(3)	0.0220(9)
C(30)	0.3771(4)	0.7449(4)	0.3082(3)	0.0184(8)
C(31)	0.3598(4)	0.6669(4)	0.3808(3)	0.0226(9)
C(32)	0.2702(4)	0.6253(4)	0.3673(3)	0.0288(11)
C(33)	0.2304(4)	0.6762(4)	0.2882(3)	0.0278(11)
C(34)	0.2961(4)	0.7510(4)	0.2509(3)	0.0216(9)
C(35)	0.8147(4)	0.7621(4)	0.1180(3)	0.0240(10)
C(36)	0.7068(4)	0.8817(4)	0.2626(3)	0.0248(10)
C(37)	0.6610(4)	0.4888(4)	0.3002(3)	0.0192(9)
C(38)	0.6332(4)	0.4437(5)	0.3944(3)	0.0294(11)
N(39)	0.7784(3)	0.4257(3)	0.2581(2)	0.0188(7)
C(40)	0.8660(4)	0.4389(4)	0.3017(3)	0.0211(9)
C(41)	0.8901(4)	0.5400(4)	0.2854(3)	0.0259(10)
C(42)	0.9672(4)	0.5656(5)	0.3280(4)	0.0320(12)
C(43)	1.0238(5)	0.4870(5)	0.3875(4)	0.0367(13)
C(44)	1.0031(5)	0.3839(5)	0.4053(4)	0.0349(12)
C(45)	0.9235(4)	0.3604(4)	0.3640(3)	0.0259(10)
O(46)	0.8956(3)	0.2627(3)	0.3809(3)	0.0375(9)
C(47)	0.9202(5)	0.1935(4)	0.4585(3)	0.0338(12)
C(48)	0.8814(5)	0.0942(5)	0.4525(4)	0.0388(13)
O(49)	0.9626(4)	0.0263(3)	0.3911(3)	0.0407(10)
C(50)	0.9030(6)	-0.0241(6)	0.3439(5)	0.0512(17)
C(51)	0.9916(6)	-0.0982(6)	0.2858(5)	0.058(2)
O(52)	1.0621(3)	-0.0497(4)	0.2184(3)	0.0441(10)
C(53)	1.0306(6)	-0.0229(5)	0.1359(5)	0.0506(17)
C(54)	1.0106(5)	0.0999(5)	0.1079(4)	0.0440(15)
O(55)	0.9043(3)	0.1616(3)	0.1550(3)	0.0431(10)
C(56)	0.9056(4)	0.2652(4)	0.1801(3)	0.0269(10)
C(57)	0.7896(4)	0.3143(4)	0.2342(3)	0.0233(9)

Table 7. Bond lengths [Å] and angles [°] for $PtMe_2$(**1**).

Pt(1)-C(35)	2.101(4)	C(14)-C(37)	1.511(6)
Pt(1)-C(36)	2.105(4)	C(15)-C(16)	1.419(7)
Pt(1)-P(2)	2.2980(11)	C(16)-C(17)	1.428(6)
Pt(1)-P(1)	2.3007(11)	C(18)-C(23)	1.395(6)
Fe(1)-C(13)	2.019(4)	C(18)-C(19)	1.395(7)
Fe(1)-C(34)	2.028(5)	C(19)-C(20)	1.394(7)
Fe(1)-C(33)	2.033(5)	C(20)-C(21)	1.379(8)
Fe(1)-C(17)	2.035(4)	C(21)-C(22)	1.379(9)
Fe(1)-C(14)	2.041(4)	C(22)-C(23)	1.389(7)
Fe(1)-C(30)	2.046(4)	C(24)-C(29)	1.402(6)
Fe(1)-C(32)	2.050(4)	C(24)-C(25)	1.403(6)
Fe(1)-C(15)	2.055(4)	C(25)-C(26)	1.384(7)
Fe(1)-C(16)	2.061(4)	C(26)-C(27)	1.379(7)
Fe(1)-C(31)	2.070(4)	C(27)-C(28)	1.393(7)
P(1)-C(13)	1.815(4)	C(28)-C(29)	1.391(7)
P(1)-C(7)	1.831(4)	C(30)-C(31)	1.437(6)
P(1)-C(1)	1.840(4)	C(30)-C(34)	1.440(6)
P(2)-C(30)	1.829(5)	C(31)-C(32)	1.421(7)
P(2)-C(24)	1.834(5)	C(32)-C(33)	1.416(8)
P(2)-C(18)	1.840(5)	C(33)-C(34)	1.434(7)
C(1)-C(6)	1.386(7)	C(37)-N(39)	1.490(5)
C(1)-C(2)	1.396(6)	C(37)-C(38)	1.531(6)
C(2)-C(3)	1.387(6)	N(39)-C(40)	1.439(6)
C(3)-C(4)	1.385(8)	N(39)-C(57)	1.461(6)
C(4)-C(5)	1.394(7)	C(40)-C(41)	1.382(7)
C(5)-C(6)	1.405(6)	C(40)-C(45)	1.413(7)
C(7)-C(12)	1.396(6)	C(41)-C(42)	1.391(7)
C(7)-C(8)	1.405(6)	C(42)-C(43)	1.379(8)
C(8)-C(9)	1.384(7)	C(43)-C(44)	1.389(8)
C(9)-C(10)	1.383(7)	C(44)-C(45)	1.390(7)
C(10)-C(11)	1.389(7)	C(45)-O(46)	1.365(6)
C(11)-C(12)	1.396(7)	O(46)-C(47)	1.423(6)
C(13)-C(17)	1.436(6)	C(47)-C(48)	1.496(8)
C(13)-C(14)	1.466(6)	C(48)-O(49)	1.407(7)
C(14)-C(15)	1.435(6)	O(49)-C(50)	1.453(7)

C(50)-C(51)	1.452(9)	C(54)-O(55)	1.420(7)
C(51)-O(52)	1.442(8)	O(55)-C(56)	1.421(6)
O(52)-C(53)	1.386(8)	C(56)-C(57)	1.510(6)
C(53)-C(54)	1.510(9)		

C(35)-Pt(1)-C(36)	82.58(19)	C(32)-Fe(1)-C(15)	110.96(19)
C(35)-Pt(1)-P(2)	168.82(14)	C(13)-Fe(1)-C(16)	69.62(17)
C(36)-Pt(1)-P(2)	86.36(14)	C(34)-Fe(1)-C(16)	130.75(19)
C(35)-Pt(1)-P(1)	92.92(14)	C(33)-Fe(1)-C(16)	106.63(19)
C(36)-Pt(1)-P(1)	175.00(14)	C(17)-Fe(1)-C(16)	40.80(17)
P(2)-Pt(1)-P(1)	98.07(4)	C(14)-Fe(1)-C(16)	69.17(18)
C(13)-Fe(1)-C(34)	111.21(18)	C(30)-Fe(1)-C(16)	171.42(19)
C(13)-Fe(1)-C(33)	142.0(2)	C(32)-Fe(1)-C(16)	113.69(19)
C(34)-Fe(1)-C(33)	41.37(19)	C(15)-Fe(1)-C(16)	40.33(18)
C(13)-Fe(1)-C(17)	41.47(16)	C(13)-Fe(1)-C(31)	135.53(17)
C(34)-Fe(1)-C(17)	105.80(19)	C(34)-Fe(1)-C(31)	69.02(19)
C(33)-Fe(1)-C(17)	110.58(19)	C(33)-Fe(1)-C(31)	68.6(2)
C(13)-Fe(1)-C(14)	42.32(16)	C(17)-Fe(1)-C(31)	173.37(18)
C(34)-Fe(1)-C(14)	145.19(18)	C(14)-Fe(1)-C(31)	111.81(19)
C(33)-Fe(1)-C(14)	173.43(19)	C(30)-Fe(1)-C(31)	40.88(17)
C(17)-Fe(1)-C(14)	69.84(17)	C(32)-Fe(1)-C(31)	40.37(18)
C(13)-Fe(1)-C(30)	108.52(17)	C(15)-Fe(1)-C(31)	117.18(19)
C(34)-Fe(1)-C(30)	41.39(18)	C(16)-Fe(1)-C(31)	145.78(18)
C(33)-Fe(1)-C(30)	69.37(18)	C(13)-P(1)-C(7)	103.9(2)
C(17)-Fe(1)-C(30)	132.49(18)	C(13)-P(1)-C(1)	100.5(2)
C(14)-Fe(1)-C(30)	115.48(17)	C(7)-P(1)-C(1)	100.89(19)
C(13)-Fe(1)-C(32)	175.85(19)	C(13)-P(1)-Pt(1)	117.52(14)
C(34)-Fe(1)-C(32)	68.8(2)	C(7)-P(1)-Pt(1)	110.03(14)
C(33)-Fe(1)-C(32)	40.6(2)	C(1)-P(1)-Pt(1)	121.49(14)
C(17)-Fe(1)-C(32)	142.68(19)	C(30)-P(2)-C(24)	100.6(2)
C(14)-Fe(1)-C(32)	135.6(2)	C(30)-P(2)-C(18)	100.5(2)
C(30)-Fe(1)-C(32)	68.60(18)	C(24)-P(2)-C(18)	103.6(2)
C(13)-Fe(1)-C(15)	69.72(17)	C(30)-P(2)-Pt(1)	124.12(14)
C(34)-Fe(1)-C(15)	170.79(18)	C(24)-P(2)-Pt(1)	113.70(14)
C(33)-Fe(1)-C(15)	132.60(19)	C(18)-P(2)-Pt(1)	111.76(15)
C(17)-Fe(1)-C(15)	68.50(18)	C(6)-C(1)-C(2)	118.7(4)
C(14)-Fe(1)-C(15)	41.03(17)	C(6)-C(1)-P(1)	120.8(3)
C(30)-Fe(1)-C(15)	147.69(18)	C(2)-C(1)-P(1)	120.5(4)

C(3)-C(2)-C(1)	120.2(5)	C(21)-C(20)-C(19)	120.2(6)
C(4)-C(3)-C(2)	121.0(5)	C(22)-C(21)-C(20)	120.1(5)
C(3)-C(4)-C(5)	119.7(4)	C(21)-C(22)-C(23)	120.0(5)
C(4)-C(5)-C(6)	119.0(5)	C(22)-C(23)-C(18)	120.8(5)
C(1)-C(6)-C(5)	121.4(4)	C(29)-C(24)-C(25)	118.8(4)
C(12)-C(7)-C(8)	118.3(4)	C(29)-C(24)-P(2)	119.2(3)
C(12)-C(7)-P(1)	119.0(3)	C(25)-C(24)-P(2)	121.9(3)
C(8)-C(7)-P(1)	122.6(3)	C(26)-C(25)-C(24)	120.6(4)
C(9)-C(8)-C(7)	120.5(4)	C(27)-C(26)-C(25)	120.3(4)
C(10)-C(9)-C(8)	120.8(4)	C(26)-C(27)-C(28)	120.0(5)
C(9)-C(10)-C(11)	119.5(4)	C(29)-C(28)-C(27)	120.2(5)
C(10)-C(11)-C(12)	120.1(5)	C(28)-C(29)-C(24)	120.0(4)
C(11)-C(12)-C(7)	120.7(4)	C(31)-C(30)-C(34)	107.6(4)
C(17)-C(13)-C(14)	107.1(4)	C(31)-C(30)-P(2)	125.7(3)
C(17)-C(13)-P(1)	125.6(3)	C(34)-C(30)-P(2)	126.7(3)
C(14)-C(13)-P(1)	127.3(3)	C(31)-C(30)-Fe(1)	70.4(2)
C(17)-C(13)-Fe(1)	69.9(2)	C(34)-C(30)-Fe(1)	68.6(3)
C(14)-C(13)-Fe(1)	69.6(2)	P(2)-C(30)-Fe(1)	126.1(2)
P(1)-C(13)-Fe(1)	125.2(2)	C(32)-C(31)-C(30)	107.7(4)
C(15)-C(14)-C(13)	106.8(4)	C(32)-C(31)-Fe(1)	69.1(3)
C(15)-C(14)-C(37)	124.8(4)	C(30)-C(31)-Fe(1)	68.7(2)
C(13)-C(14)-C(37)	128.4(4)	C(33)-C(32)-C(31)	109.1(4)
C(15)-C(14)-Fe(1)	70.0(2)	C(33)-C(32)-Fe(1)	69.1(3)
C(13)-C(14)-Fe(1)	68.0(2)	C(31)-C(32)-Fe(1)	70.6(2)
C(37)-C(14)-Fe(1)	125.4(3)	C(32)-C(33)-C(34)	107.9(4)
C(16)-C(15)-C(14)	109.3(4)	C(32)-C(33)-Fe(1)	70.4(3)
C(16)-C(15)-Fe(1)	70.1(3)	C(34)-C(33)-Fe(1)	69.1(3)
C(14)-C(15)-Fe(1)	69.0(2)	C(33)-C(34)-C(30)	107.7(4)
C(15)-C(16)-C(17)	107.9(4)	C(33)-C(34)-Fe(1)	69.5(3)
C(15)-C(16)-Fe(1)	69.6(2)	C(30)-C(34)-Fe(1)	70.0(3)
C(17)-C(16)-Fe(1)	68.6(2)	N(39)-C(37)-C(14)	111.1(3)
C(16)-C(17)-C(13)	108.9(4)	N(39)-C(37)-C(38)	112.2(4)
C(16)-C(17)-Fe(1)	70.6(2)	C(14)-C(37)-C(38)	111.7(4)
C(13)-C(17)-Fe(1)	68.7(2)	C(40)-N(39)-C(57)	118.5(4)
C(23)-C(18)-C(19)	118.5(4)	C(40)-N(39)-C(37)	110.4(3)
C(23)-C(18)-P(2)	122.8(4)	C(57)-N(39)-C(37)	115.4(4)
C(19)-C(18)-P(2)	118.7(4)	C(41)-C(40)-C(45)	117.4(4)
C(20)-C(19)-C(18)	120.4(5)	C(41)-C(40)-N(39)	117.0(4)

C(45)-C(40)-N(39)	125.4(4)	O(49)-C(48)-C(47)	108.1(4)
C(40)-C(41)-C(42)	122.4(5)	C(48)-O(49)-C(50)	109.3(5)
C(43)-C(42)-C(41)	119.2(5)	C(51)-C(50)-O(49)	106.7(5)
C(42)-C(43)-C(44)	120.3(5)	O(52)-C(51)-C(50)	118.2(6)
C(43)-C(44)-C(45)	119.9(5)	C(53)-O(52)-C(51)	119.2(5)
O(46)-C(45)-C(44)	123.0(5)	O(52)-C(53)-C(54)	111.9(5)
O(46)-C(45)-C(40)	116.3(4)	O(55)-C(54)-C(53)	108.5(6)
C(44)-C(45)-C(40)	120.8(5)	C(54)-O(55)-C(56)	114.1(4)
C(45)-O(46)-C(47)	120.6(4)	O(55)-C(56)-C(57)	106.5(4)
O(46)-C(47)-C(48)	105.0(5)	N(39)-C(57)-C(56)	111.0(4)

Table 8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $PtMe_2$(**1**). 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}
Pt(1)	13(1)	16(1)	16(1)	-3(1)	1(1)	-6(1)
Fe(1)	14(1)	17(1)	17(1)	-5(1)	4(1)	-6(1)
P(1)	13(1)	15(1)	14(1)	-4(1)	2(1)	-4(1)
P(2)	16(1)	16(1)	15(1)	-4(1)	3(1)	-5(1)
C(1)	15(2)	21(2)	19(2)	-4(2)	-2(2)	-3(2)
C(2)	21(2)	26(3)	24(2)	-2(2)	2(2)	-7(2)
C(3)	20(2)	41(3)	21(2)	0(2)	5(2)	-9(2)
C(4)	18(2)	41(3)	21(2)	-10(2)	5(2)	3(2)
C(5)	31(3)	22(3)	29(3)	-8(2)	2(2)	2(2)
C(6)	23(2)	24(2)	18(2)	-2(2)	4(2)	-3(2)
C(7)	15(2)	21(2)	13(2)	-4(2)	2(2)	-3(2)
C(8)	29(2)	21(2)	17(2)	0(2)	-2(2)	-10(2)
C(9)	35(3)	36(3)	19(2)	3(2)	-9(2)	-19(2)
C(10)	21(2)	35(3)	28(2)	6(2)	-11(2)	-7(2)
C(11)	31(3)	18(2)	31(3)	-3(2)	-6(2)	-1(2)
C(12)	21(2)	23(2)	19(2)	-4(2)	-3(2)	-5(2)
C(13)	15(2)	16(2)	16(2)	-3(2)	1(2)	-5(2)
C(14)	17(2)	20(2)	15(2)	-1(2)	3(2)	-7(2)
C(15)	22(2)	15(2)	21(2)	-3(2)	4(2)	-7(2)
C(16)	24(2)	19(2)	23(2)	-7(2)	3(2)	-9(2)
C(17)	19(2)	18(2)	19(2)	-7(2)	2(2)	-6(2)
C(18)	25(2)	20(2)	21(2)	-3(2)	-2(2)	-11(2)
C(19)	39(3)	25(3)	28(3)	0(2)	-8(2)	-10(2)
C(20)	51(4)	36(3)	29(3)	3(2)	-19(2)	-17(3)
C(21)	62(4)	40(3)	22(2)	1(2)	-8(2)	-34(3)
C(22)	49(3)	47(3)	21(2)	-12(2)	5(2)	-26(3)
C(23)	34(3)	30(3)	19(2)	-6(2)	2(2)	-14(2)
C(24)	21(2)	15(2)	21(2)	-5(2)	2(2)	-4(2)
C(25)	22(2)	19(2)	23(2)	-2(2)	4(2)	-6(2)
C(26)	21(2)	26(3)	34(3)	-6(2)	6(2)	-3(2)
C(27)	30(3)	18(2)	28(2)	-1(2)	-3(2)	0(2)
C(28)	33(3)	21(3)	24(2)	-2(2)	1(2)	-9(2)

C(29)	25(2)	25(2)	18(2)	-4(2)	1(2)	-10(2)
C(30)	14(2)	18(2)	21(2)	-7(2)	6(2)	-4(2)
C(31)	25(2)	27(3)	17(2)	-9(2)	9(2)	-14(2)
C(32)	26(2)	32(3)	30(2)	-15(2)	16(2)	-18(2)
C(33)	15(2)	30(3)	38(3)	-16(2)	8(2)	-8(2)
C(34)	13(2)	21(2)	27(2)	-11(2)	1(2)	0(2)
C(35)	12(2)	27(3)	29(2)	-2(2)	9(2)	-8(2)
C(36)	26(2)	30(3)	26(2)	-10(2)	-6(2)	-15(2)
C(37)	19(2)	21(2)	17(2)	-2(2)	-3(2)	-5(2)
C(38)	27(3)	39(3)	18(2)	2(2)	-1(2)	-7(2)
N(39)	18(2)	16(2)	22(2)	-4(1)	-3(1)	-3(1)
C(40)	18(2)	24(2)	20(2)	-4(2)	0(2)	-5(2)
C(41)	23(2)	28(3)	27(2)	-3(2)	2(2)	-9(2)
C(42)	27(3)	36(3)	38(3)	-12(2)	4(2)	-17(2)
C(43)	29(3)	50(4)	37(3)	-14(3)	-5(2)	-16(3)
C(44)	29(3)	42(3)	34(3)	-3(2)	-15(2)	-6(2)
C(45)	22(2)	25(3)	29(2)	-1(2)	-5(2)	-5(2)
O(46)	44(2)	30(2)	44(2)	16(2)	-27(2)	-16(2)
C(47)	35(3)	27(3)	26(3)	2(2)	2(2)	4(2)
C(48)	26(3)	40(3)	45(3)	15(3)	-4(2)	-9(2)
O(49)	54(3)	38(2)	41(2)	-6(2)	-8(2)	-26(2)
C(50)	39(3)	56(4)	64(4)	-10(3)	-13(3)	-17(3)
C(51)	42(4)	60(5)	82(5)	-30(4)	13(3)	-32(3)
O(52)	29(2)	52(3)	55(3)	-8(2)	-6(2)	-17(2)
C(53)	45(4)	41(4)	68(4)	-29(3)	-19(3)	1(3)
C(54)	43(3)	34(3)	48(4)	-23(3)	-2(3)	2(3)
O(55)	32(2)	30(2)	68(3)	-26(2)	-1(2)	-6(2)
C(56)	23(2)	23(3)	33(3)	-10(2)	-7(2)	0(2)
C(57)	20(2)	21(2)	31(2)	-6(2)	-8(2)	-4(2)

Table 9. Hydrogen coordinates and isotropic displacement parameters for $PtMe_2$(**1**).

	x	y	z	U(eq)
H(2)	0.7588	0.7153	-0.0420	0.029
H(3)	0.9013	0.6086	-0.1425	0.035
H(4)	0.9384	0.4153	-0.1364	0.036
H(5)	0.8325	0.3263	-0.0264	0.036
H(6)	0.6918	0.4342	0.0769	0.028
H(8)	0.4989	0.6371	-0.0345	0.027
H(9)	0.3567	0.7517	-0.1131	0.033
H(10)	0.2719	0.9396	-0.0863	0.034
H(11)	0.3321	1.0143	0.0195	0.033
H(12)	0.4726	0.8993	0.1010	0.026
H(15)	0.4899	0.3697	0.3191	0.024
H(16)	0.3521	0.4188	0.2040	0.026
H(17)	0.4046	0.5720	0.0918	0.022
H(19)	0.6661	0.6911	0.3870	0.036
H(20)	0.7087	0.6811	0.5279	0.044
H(21)	0.5812	0.7977	0.6298	0.044
H(22)	0.4091	0.9225	0.5927	0.044
H(23)	0.3652	0.9330	0.4526	0.032
H(25)	0.2380	0.9437	0.3386	0.027
H(26)	0.1246	1.1282	0.3165	0.035
H(27)	0.2069	1.2614	0.2397	0.033
H(28)	0.4030	1.2087	0.1796	0.032
H(29)	0.5188	1.0240	0.2019	0.026
H(31)	0.4045	0.6440	0.4309	0.027
H(32)	0.2412	0.5679	0.4066	0.035
H(33)	0.1676	0.6625	0.2630	0.033
H(34)	0.2870	0.7990	0.1951	0.026
H(35A)	0.8689	0.7707	0.1533	0.036
H(35B)	0.8061	0.8201	0.0696	0.036
H(35C)	0.8444	0.6881	0.0950	0.036
H(36A)	0.6409	0.9234	0.3027	0.037
H(36B)	0.7365	0.9344	0.2207	0.037

H(36C)	0.7680	0.8358	0.2956	0.037
H(37)	0.6607	0.5677	0.3017	0.023
H(38A)	0.6911	0.4482	0.4281	0.044
H(38B)	0.6346	0.3655	0.3956	0.044
H(38C)	0.5562	0.4884	0.4200	0.044
H(41)	0.8526	0.5939	0.2436	0.031
H(42)	0.9808	0.6364	0.3163	0.038
H(43)	1.0772	0.5035	0.4165	0.044
H(44)	1.0432	0.3296	0.4456	0.042
H(47A)	0.8772	0.2335	0.5106	0.041
H(47B)	1.0040	0.1704	0.4619	0.041
H(48A)	0.8763	0.0516	0.5100	0.047
H(48B)	0.8040	0.1188	0.4340	0.047
H(50A)	0.8579	-0.0668	0.3848	0.061
H(50B)	0.8493	0.0343	0.3101	0.061
H(51A)	1.0440	-0.1544	0.3219	0.070
H(51B)	0.9532	-0.1391	0.2574	0.070
H(53A)	0.9589	-0.0424	0.1356	0.061
H(53B)	1.0923	-0.0678	0.0937	0.061
H(54A)	1.0749	0.1242	0.1199	0.053
H(54B)	1.0074	0.1131	0.0446	0.053
H(56A)	0.9175	0.3161	0.1280	0.032
H(56B)	0.9689	0.2532	0.2145	0.032
H(57A)	0.7271	0.3191	0.2008	0.028
H(57B)	0.7810	0.2646	0.2877	0.028

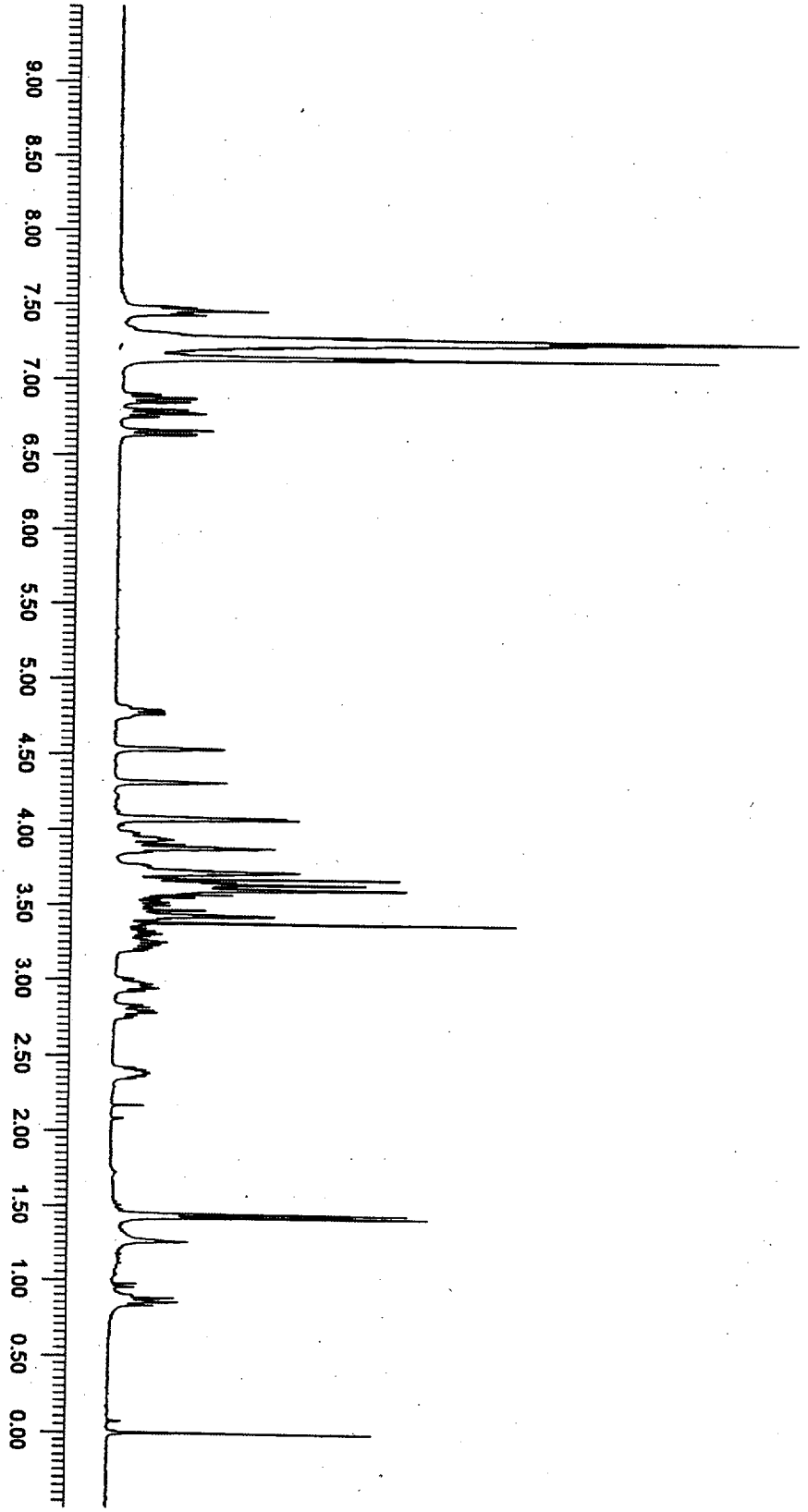

Figure.5 300 MHz ^{1}H -NMR Spectrum of BPPF-crown (**1**) in $CDCl_3$

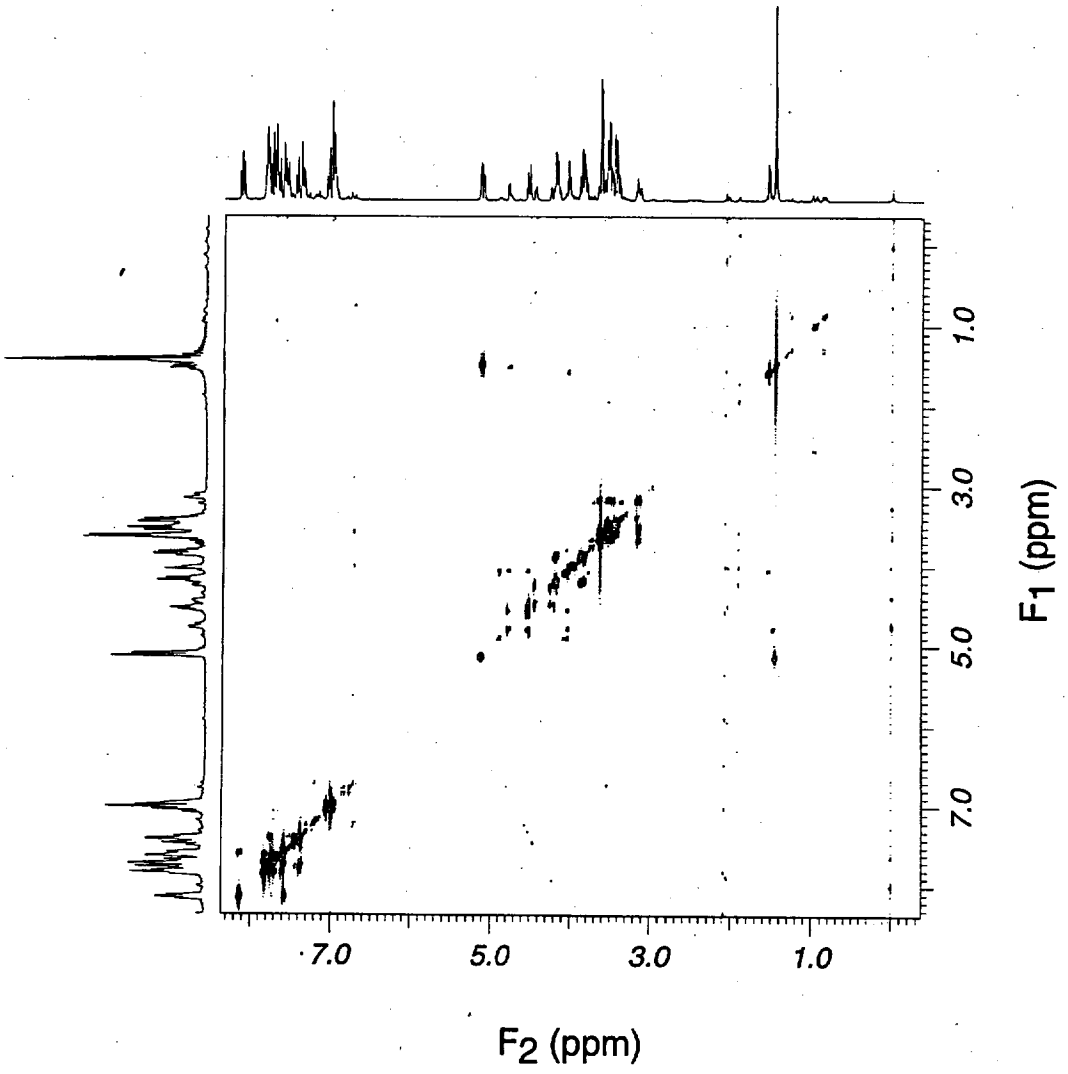

Figure 6. 500 MHz ^{1}H-DQF-COSY spectrum of [RhNBD(*rac*-**1**)]OTf (**9**) in acetone-d_6

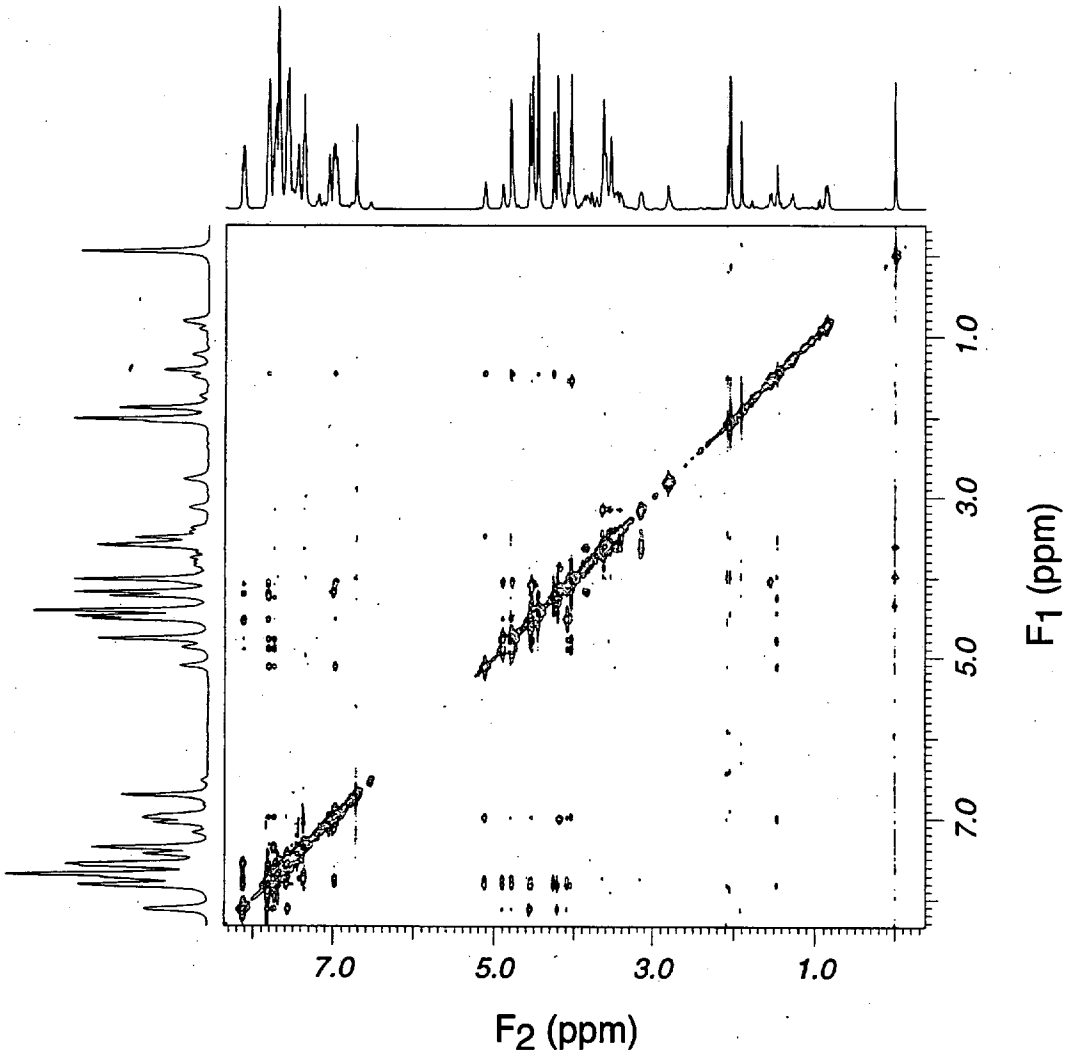

Figure 7. 500 MHz ^{1}H-NOESY spectrum of [RhNBD(*rac*-**1**)]OTf (**9**) in acetone-d_6

2DCPA Input Data of 500 MHz ^{1}H-NOESY of [RhNBD(*rac*-1)]OTf in acetone-d_6

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31\number of well-defined NOESY groups of [Rh(NBD)(rac-1)]OTf(9)
# 1st number indicates whether methyl or not 1 = not methyl, 3 = methyl
# 2nd number is the number of protons in the group.
# 3rd number to the last number are the atom number from the conformer file
3       3
        68      69      70      67\#1 Me
1       2
        128     129\#2 CH2 NBD
1       1
        109\#3 CH - N, (used 2DCPA for the assignment)
1       2
        87      88\#4 CH2-CH2-OAP (AP=Amino Phenol)
1       2
        122     123\#5 CH NBD
1       1
        125\#6 vinyl, (used 2DCPA for the assignment)
1       2
        84      85\#7 CH2-OAP
1       1
        64\#8 Cp proton on the left, bottom one (looking from NBD-Rh-Fe and crown-ether is on the top of Rh)
1       1
        58\#9 Cp proton on the left, (used 2DCPA for the assignment)
1       2
        60      62\#10 Cp proton on the left, (used 2DCPA for the assignment)
1       1
        126\#11 vinyl, (used 2DCPA for the assignment)
1       2
        31      33\#12 Cp proton on the right, (used 2DCPA for the assignment)
1       2
        127     29\#13 vinyl and Cp proton on the right, (used 2DCPA for the assignment)
1       1
        124\#14 vinyl, (used 2DCPA for the assignment).
1       1
        66\#15 CH
1       1
        76\#16 AP
1       2
        74      80\#17 AP
1       1
        102\#18 crown ether, (used 2DCPA for the assignment)
1       2
        38      42\#19 meta A
1       1
        40\#20 para A
1       2
        19      23\#21 meta D
1       2
        8       12\#22 meta C
```

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1       4
        51      10      49      53\#23 para B,C and meta B (B and C could be switched)
1       1
        21\#24 para D
1       2
        36      44\#25 ortho A
1       4
        47      55      6       14\#26 ortho B,C
1       2
        17      25\#27 ortho D
1       6
        108     91      92      101     98      99\#28
1       3
        106     94      95\#29 no.107 is close to Me
1       1
        105\#30
1       1
        78\#31 AP
#1st number is isotropic rotational correlation time (in ns)
#2nd number is methyl spin correlation time (in ps)
#3rd number is external relaxation rate ( in sec.)
#4th number is a bit flag that determines which relaxation parameter(s) is/are optimized
# by comparison with experimental data. This flag is integer sum of three binary numbers
# 1=optimize tau(1), 2=optimize tau(2), 4=optimize r_ex;
#5th number is optimization gradient cutoff
0.2549  0       0       0       1E-8\
6\#number of mixing times
0       0.3     0.45    0.6     0.9     1.2\mixing time (in sec.)
# 496 total data points, 31 diagonal peaks, 49 good peaks, 3 noisy peaks ,117 unresolved peaks and 296 absent peaks
# RMS of data is 7.415E+04 and RMSD is 1.363E+05
# RMS+3RMSD=4.831E+05
# if 3 of 5 of each data set is less than RMS+3RMSD, it is a noisy peak

#1st two numbers are the group (group matrix elements)
#the input file only requires upper triangular part of the matrix
#next six number are the volumes at each mixing time (arbitrary units)
#next number is the exchange rate which was calculated from the ratio method. Only well-defined pairs of group number 6 and 11 were chosen for the calculation.
#next number is weighting factor which can be of several types
# 995 for good peaks, 997 for absent peaks and noisy peaks, 0 for diagonal peaks and unresolved peaks
1       1       1.311E+09       6.810E+08       5.070E+08       3.770E+08       1.980E+08       1.020E+08       0       0       0\Diagonal
1       2       0.000E+00       -1.919E+04      -5.875E+03      -9.796E+04      -2.971E+03      -9.712E+03      0       997     0\absent peak
1       3       0.000E+00       -0.356E+06      -0.103E+06      -0.228E+05      -0.223E+06      -0.380E+05      0       997     0\noisy peak
1       4       0.000E+00       -4.557E+04      -4.141E+04      -6.968E+04      -4.806E+04      -9.557E+04      0       997     0\absent peak
1       5       0.000E+00       -1.880E+04      -4.288E+04      -3.705E+04      -5.098E+04      -4.314E+04      0       997     0\absent peak
1       6       0.000E+00       -4.336E+04      -8.603E+04      -8.610E+04      -3.518E+04      -9.319E+04      0       997     0\absent peak
1       7       0.000E+00       -5.377E+04      -7.129E+04      -3.895E+03      -7.891E+04      -3.376E+04      0       997     0\absent peak
1       8       0.000E+00       -4.356E+04      -3.705E+04      -1.186E+04      -7.769E+04      -3.833E+04      0       997     0\absent peak
1       9       0.000E+00       -5.600E+06      -7.260E+06      -8.320E+06      -7.990E+06      -6.875E+06      0       995     0\good peak
1       10      0.000E+00       -1.245E+06      -1.625E+06      -1.790E+06      -1.920E+06      -1.690E+06      0       995     0\good peak
1       11      0.000E+00       -4.822E+04      -4.252E+04      -5.378E+04      -4.675E+04      -9.385E+04      0       997     0\absent peak
1       12      0.000E+00       -7.550E+04      -9.641E+04      -5.170E+03      -7.921E+04      -9.415E+04      0       997     0\absent peak
1       13      0.000E+00       -7.525E+06      -8.555E+06      -1.027E+07      -9.865E+06      -8.810E+06      0       995     0\good peak
1       14      0.000E+00       -9.783E+04      -2.936E+04      -3.072E+04      -6.916E+04      -9.431E+04      0       997     0\absent peak
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1	15	0.000E+00	-6.175E+06	-7.355E+06	-8.155E+06	-7.365E+06	-6.010E+06	0	995	2\tau2opt
1	16	0.000E+00	-2.322E+04	-1.529E+04	-6.482E+04	-4.619E+04	-8.215E+04	0	997	0\absent peak
1	17	0.000E+00	-3.850E+06	-3.900E+06	-4.065E+06	-4.030E+06	-3.595E+06	0	995	0\good peak
1	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
1	19	0.000E+00	-6.114E+04	-1.705E+03	-3.026E+04	-4.797E+03	-3.206E+04	0	997	0\absent peak
1	20	0.000E+00	-7.442E+04	-1.008E+04	-5.976E+04	-9.466E+04	-4.952E+04	0	997	0\absent peak
1	21	0.000E+00	-5.240E+04	-8.660E+04	-5.378E+04	-9.171E+04	-9.019E+04	0	997	0\absent peak
1	22	0.000E+00	-6.503E+04	-3.903E+04	-9.419E+04	-3.228E+04	-9.656E+04	0	997	0\absent peak
1	23	0.000E+00	-3.870E+04	-6.718E+04	-6.441E+04	-8.920E+04	-6.327E+04	0	997	0\absent peak
1	24	0.000E+00	-5.574E+03	-3.205E+04	-4.342E+04	-1.237E+04	-5.538E+04	0	997	0\absent peak
1	25	0.000E+00	-2.738E+04	-3.778E+04	-1.810E+04	-1.369E+04	-7.034E+04	0	997	0\absent peak
1	26	0.000E+00	-2.375E+06	-2.945E+06	-2.600E+06	-2.835E+06	-2.315E+06	0	995	0\good peak
1	27	0.000E+00	-1.980E+04	-5.940E+04	-5.076E+04	-3.719E+04	-2.917E+04	0	997	0\absent peak
1	28	0.000E+00	-0.359E+06	-0.589E+06	-0.847E+06	-0.421E+06	-0.106E+06	0	0	0\unresolved
1	29	0.000E+00	-0.152E+07	-0.122E+07	-0.199E+07	-0.103E+07	-0.193E+05	0	0	0\unresolved
1	30	0.000E+00	-0.103E+07	-0.110E+07	-0.174E+07	-0.110E+07	-0.151E+06	0	0	0\unresolved
1	31	0.000E+00	-5.577E+04	-6.130E+04	-9.398E+04	-9.559E+04	-7.301E+04	0	997	0\absent peak
2	2	8.459E+08	4.760E+08	3.250E+08	2.540E+08	1.380E+08	7.480E+07	0	0	0\Diagonal
2	3	0.000E+00	-2.738E+04	-3.778E+04	-1.810E+04	-1.369E+04	-7.034E+04	0	997	0\absent peak
2	4	0.000E+00	-2.404E+04	-7.227E+04	-8.630E+03	-2.782E+04	-6.383E+04	0	997	0\absent peak
2	5	0.000E+00	-1.170E+07	-1.415E+07	-1.635E+07	-1.620E+07	-1.495E+07	0	995	1\tau1opt
2	6	0.000E+00	-0.149E+07	-0.100E+07	-0.143E+07	-0.147E+07	-0.145E+07	0	995	0\good peak
2	7	0.000E+00	-6.502E+04	-3.686E+04	-7.614E+04	-1.654E+04	-4.704E+04	0	997	0\absent peak
2	8	0.000E+00	-5.502E+04	-1.562E+04	-7.985E+04	-2.188E+04	-1.265E+04	0	997	0\absent peak
2	9	0.000E+00	-7.242E+04	-8.361E+04	-8.291E+04	-7.972E+04	-4.878E+04	0	997	0\absent peak
2	10	0.000E+00	-6.349E+04	-7.594E+04	-3.923E+04	-5.621E+04	-1.656E+04	0	997	0\absent peak
2	11	0.000E+00	-0.417E+06	-0.911E+06	-0.803E+06	-0.606E+06	-0.577E+06	0	995	0\good peak
2	12	0.000E+00	-9.306E+04	-4.816E+04	-1.857E+04	-9.189E+04	-3.991E+04	0	997	0\absent peak
2	13	0.000E+00	-0.235E+06	-0.517E+06	-0.565E+06	-0.483E+06	-0.361E+06	0	997	0\noisy peak
2	14	0.000E+00	-0.592E+06	-0.739E+06	-0.704E+06	-0.752E+06	-0.618E+06	0	995	0\good peak
2	15	0.000E+00	-2.108E+04	-2.759E+03	-7.643E+04	-6.519E+04	-8.699E+04	0	997	0\absent peak
2	16	0.000E+00	-3.233E+04	-1.354E+04	-7.347E+04	-8.408E+04	-5.206E+04	0	997	0\absent peak
2	17	0.000E+00	-2.425E+04	-8.868E+04	-8.157E+04	-7.609E+04	-1.389E+04	0	997	0\absent peak
2	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
2	19	0.000E+00	-6.506E+04	-7.641E+04	-9.137E+04	-2.736E+04	-4.272E+04	0	997	0\absent peak
2	20	0.000E+00	-5.669E+04	-2.212E+04	-9.398E+04	-5.985E+04	-4.554E+04	0	997	0\absent peak
2	21	0.000E+00	-1.654E+02	-4.257E+04	-8.922E+03	-6.035E+04	-8.587E+04	0	997	0\absent peak
2	22	0.000E+00	-5.596E+04	-4.234E+04	-1.506E+04	-9.618E+04	-1.330E+04	0	997	0\absent peak
2	23	0.000E+00	-9.593E+04	-3.840E+04	-4.703E+04	-3.491E+04	-8.146E+04	0	997	0\absent peak
2	24	0.000E+00	-9.673E+04	-3.609E+04	-6.869E+04	-5.371E+03	-3.335E+04	0	997	0\absent peak
2	25	0.000E+00	-9.271E+04	-9.731E+03	-4.921E+04	-9.904E+04	-8.922E+04	0	997	0\absent peak
2	26	0.000E+00	-6.867E+04	-7.656E+04	-6.831E+04	-3.334E+03	-8.287E+04	0	997	0\absent peak
2	27	0.000E+00	-1.143E+04	-5.470E+04	-9.437E+04	-1.377E+04	-8.833E+04	0	997	0\absent peak
2	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
2	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
2	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
2	31	0.000E+00	-9.429E+04	-3.938E+04	-8.238E+04	-5.299E+04	-9.204E+04	0	997	0\absent peak
3	3	4.370E+08	2.910E+08	2.450E+08	2.010E+08	1.320E+08	9.100E+07	0	0	0\Diagonal
3	4	0.000E+00	-5.688E+04	-6.074E+04	-2.273E+04	-6.911E+04	-5.813E+04	0	997	0\absent peak
3	5	0.000E+00	-2.115E+04	-2.379E+04	-5.342E+04	-9.693E+04	-5.145E+04	0	997	0\absent peak
3	6	0.000E+00	-5.990E+03	-9.640E+04	-2.895E+04	-9.459E+04	-2.981E+03	0	997	0\absent peak
3	7	0.000E+00	-2.902E+04	-2.343E+04	-6.438E+04	-4.025E+04	-6.775E+04	0	997	0\absent peak
3	8	0.000E+00	-5.669E+04	-2.212E+04	-9.398E+04	-5.985E+04	-4.554E+04	0	997	0\absent peak

3	9	0.000E+00	-3.235E+02	-6.265E+04	-7.950E+04	-7.316E+04	-5.476E+04	0	997	0\absent peak
3	10	0.000E+00	-8.234E+04	-3.458E+03	-1.225E+04	-2.333E+02	-7.972E+04	0	997	0\absent peak
3	11	0.000E+00	-3.319E+04	-2.824E+04	-9.511E+04	-9.407E+04	-8.114E+04	0	997	0\absent peak
3	12	0.000E+00	-3.336E+04	-1.228E+04	-3.500E+04	-6.575E+04	-1.515E+04	0	997	0\absent peak
3	13	0.000E+00	-2.826E+04	-4.919E+03	-3.297E+03	-5.193E+04	-7.592E+04	0	997	0\absent peak
3	14	0.000E+00	-2.130E+04	-6.660E+04	-4.494E+04	-1.172E+04	-7.092E+04	0	997	0\absent peak
3	15	0.000E+00	-3.007E+04	-9.701E+04	-5.176E+04	-6.816E+04	-9.917E+04	0	997	0\absent peak
3	16	0.000E+00	-1.301E+03	-6.858E+04	-8.796E+04	-9.823E+03	-5.885E+04	0	997	0\absent peak
3	17	0.000E+00	-4.638E+04	-8.739E+03	-1.313E+04	-4.187E+04	-3.864E+04	0	997	0\absent peak
3	18	0.000E+00	-0.210E+07	-0.211E+07	-0.186E+07	-0.896E+06	-0.135E+07	0	0	0\unresolved
3	19	0.000E+00	-1.525E+05	-4.010E+05	-6.290E+05	-7.010E+05	-7.335E+05	0	995	0\good peak
3	20	0.000E+00	-8.868E+04	-2.979E+04	-8.707E+04	-6.354E+04	-7.529E+03	0	997	0\absent peak
3	21	0.000E+00	-1.302E+03	-8.836E+03	-3.442E+04	-1.374E+04	-3.596E+04	0	997	0\absent peak
3	22	0.000E+00	-5.622E+04	-2.407E+03	-2.884E+04	-4.074E+04	-4.522E+04	0	997	0\absent peak
3	23	0.000E+00	-1.266E+04	-1.446E+04	-9.754E+03	-4.199E+04	-8.628E+04	0	997	0\absent peak
3	24	0.000E+00	-7.072E+04	-5.045E+04	-3.707E+04	-4.532E+04	-7.050E+04	0	997	0\absent peak
3	25	0.000E+00	-7.390E+05	-1.255E+06	-1.231E+06	-1.118E+06	-1.235E+06	0	995	0\good peak
3	26	0.000E+00	-7.896E+04	-1.375E+04	-5.757E+04	-4.283E+04	-7.964E+02	0	997	0\absent peak
3	27	0.000E+00	-1.711E+04	-6.150E+03	-1.179E+04	-7.182E+04	-3.253E+04	0	997	0\absent peak
3	28	0.000E+00	-2.840E+07	-2.880E+07	-3.145E+07	-2.800E+07	-2.280E+07	0	0	0\unresolved
3	29	0.000E+00	-0.107E+08	-0.877E+07	-0.912E+07	-0.657E+07	-0.578E+07	0	0	0\unresolved
3	30	0.000E+00	-0.322E+07	-0.109E+07	-0.237E+07	-0.730E+06	-0.893E+06	0	0	0\unresolved
3	31	0.000E+00	-3.894E+04	-6.752E+04	-6.084E+03	-1.214E+04	-7.241E+04	0	997	0\absent peak
4	4	8.459E+08	4.760E+08	3.250E+08	2.540E+08	1.380E+08	7.480E+07	0	0	0\Diagonal,
4	5	0.000E+00	-2.484E+04	-8.865E+04	-5.961E+04	-9.577E+04	-8.744E+03	0	997	0\absent peak
4	6	0.000E+00	-8.788E+04	-5.774E+04	-6.461E+04	-4.148E+04	-1.951E+04	0	997	0\absent peak
4	7	0.000E+00	-1.074E+07	-7.890E+06	-1.002E+07	-7.885E+06	-6.885E+06	0	995	0\good peak
4	8	0.000E+00	-6.491E+04	-7.466E+04	-3.163E+04	-6.307E+04	-6.302E+04	0	997	0\absent peak
4	9	0.000E+00	-7.397E+04	-9.124E+04	-7.891E+04	-5.500E+04	-8.302E+04	0	997	0\absent peak
4	10	0.000E+00	-5.669E+04	-2.212E+04	-9.398E+04	-5.985E+04	-4.554E+04	0	997	0\absent peak
4	11	0.000E+00	-5.044E+04	-2.427E+04	-1.618E+04	-3.353E+04	-4.558E+04	0	997	0\absent peak
4	12	0.000E+00	-3.837E+04	-5.263E+04	-3.113E+04	-6.609E+04	-5.279E+03	0	997	0\absent peak
4	13	0.000E+00	-4.007E+04	-7.826E+04	-7.479E+04	-6.741E+04	-8.898E+04	0	997	0\absent peak
4	14	0.000E+00	-5.006E+04	-8.358E+04	-6.482E+04	-5.017E+04	-5.378E+04	0	997	0\absent peak
4	15	0.000E+00	-6.615E+04	-5.363E+04	-4.884E+04	-5.590E+04	-6.604E+04	0	997	0\absent peak
4	16	0.000E+00	-1.046E+04	-2.131E+04	-2.529E+04	-6.125E+04	-6.658E+04	0	997	0\absent peak
4	17	0.000E+00	-9.879E+04	-1.881E+04	-3.076E+04	-4.563E+03	-3.460E+03	0	997	0\absent peak
4	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
4	19	0.000E+00	-6.679E+04	-8.706E+04	-9.860E+04	-7.964E+04	-9.995E+03	0	997	0\absent peak
4	20	0.000E+00	-9.750E+04	-3.983E+04	-7.116E+04	-2.002E+04	-8.506E+04	0	997	0\absent peak
4	21	0.000E+00	-5.143E+04	-6.473E+04	-6.244E+04	-7.368E+04	-2.133E+04	0	997	0\absent peak
4	22	0.000E+00	-3.995E+04	-1.332E+04	-6.372E+04	-5.448E+04	-1.576E+04	0	997	0\absent peak
4	23	0.000E+00	-9.256E+04	-9.975E+04	-7.983E+04	-9.937E+02	-3.730E+04	0	997	0\absent peak
4	24	0.000E+00	-2.396E+04	-5.512E+04	-5.708E+04	-6.948E+03	-4.077E+04	0	997	0\absent peak
4	25	0.000E+00	-1.041E+03	-2.032E+04	-9.197E+04	-6.885E+04	-2.601E+04	0	997	0\absent peak
4	26	0.000E+00	-6.979E+04	-3.752E+03	-7.859E+03	-7.816E+04	-9.316E+04	0	997	0\absent peak
4	27	0.000E+00	-9.219E+04	-4.367E+04	-5.575E+04	-3.516E+03	-1.404E+04	0	997	0\absent peak
4	28	0.000E+00	-0.385E+07	-0.648E+07	-0.651E+07	-0.714E+07	-0.789E+07	0	0	0\unresolved
4	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
4	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
4	31	0.000E+00	-9.065E+04	-1.959E+04	-5.815E+04	-5.656E+04	-7.557E+04	0	997	0\absent peak
5	5	8.505E+08	6.730E+08	6.010E+08	5.360E+08	4.290E+08	3.340E+08	0	0	0\Diagonal
5	6	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved

5	7	0.000E+00	-9.158E+04	-2.675E+03	-7.253E+04	-6.846E+04	-1.885E+04	0	997	0\absent peak
5	8	0.000E+00	-7.514E+04	-7.141E+04	-4.072E+04	-7.046E+04	-7.509E+03	0	997	0\absent peak
5	9	0.000E+00	-1.298E+04	-4.347E+03	-9.461E+04	-4.917E+04	-2.628E+04	0	997	0\absent peak
5	10	0.000E+00	-7.228E+04	-7.145E+04	-5.462E+04	-1.635E+04	-4.409E+04	0	997	0\absent peak
5	11	0.000E+00	-9.686E+03	-5.232E+04	-4.317E+04	-8.280E+04	-4.726E+04	0	997	0\absent peak
5	12	0.000E+00	-6.133E+04	-4.928E+04	-5.027E+04	-6.365E+04	-1.158E+04	0	997	0\absent peak
5	13	0.000E+00	-3.660E+06	-6.425E+06	-7.665E+06	-9.850E+06	-1.030E+07	0	995	0\good peak
5	14	0.000E+00	-3.900E+06	-6.155E+06	-7.635E+06	-9.995E+06	-1.025E+07	0	995	0\good peak
5	15	0.000E+00	-5.225E+04	-9.262E+04	-5.250E+04	-8.653E+04	-4.743E+04	0	997	0\absent peak
5	16	0.000E+00	-5.669E+04	-2.212E+04	-9.398E+04	-5.985E+04	-4.554E+04	0	997	0\absent peak
5	17	0.000E+00	-4.117E+04	-7.253E+04	-9.667E+04	-7.821E+04	-2.144E+03	0	997	0\absent peak
5	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
5	19	0.000E+00	-5.667E+04	-3.917E+04	-7.455E+03	-9.226E+04	-2.678E+04	0	997	0\absent peak
5	20	0.000E+00	-9.364E+04	-2.817E+04	-9.754E+04	-8.660E+04	-4.716E+04	0	997	0\absent peak
5	21	0.000E+00	-5.563E+04	-5.985E+04	-5.130E+04	-6.143E+03	-8.222E+04	0	997	0\absent peak
5	22	0.000E+00	-3.859E+04	-1.566E+04	-9.573E+04	-2.753E+04	-2.252E+04	0	997	0\absent peak
5	23	0.000E+00	-8.515E+04	-8.765E+04	-2.287E+04	-7.501E+04	-5.587E+04	0	997	0\absent peak
5	24	0.000E+00	-6.239E+04	-1.101E+04	-4.877E+04	-7.019E+04	-3.095E+04	0	997	0\absent peak
5	25	0.000E+00	-2.721E+04	-3.537E+04	-4.170E+04	-6.812E+04	-8.757E+04	0	997	0\absent peak
5	26	0.000E+00	-4.194E+04	-9.501E+04	-6.738E+03	-4.764E+03	-8.871E+04	0	997	0\absent peak
5	27	0.000E+00	-2.128E+04	-4.420E+04	-6.453E+04	-9.592E+04	-6.534E+04	0	997	0\absent peak
5	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
5	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
5	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
5	31	0.000E+00	-2.540E+06	-4.510E+06	-5.075E+06	-7.230E+06	-6.340E+06	0	995	0\good peak
6	6	2.773E+08	2.220E+08	1.980E+08	1.800E+08	1.460E+08	1.140E+08	+2.2358	0	0\Diagonal
6	7	0.000E+00	-8.125E+04	-5.138E+03	-7.491E+04	-3.846E+04	-6.910E+04	0	997	0\absent peak
6	8	0.000E+00	-8.504E+04	-3.761E+04	-6.996E+04	-2.133E+03	-7.647E+04	0	997	0\absent peak
6	9	0.000E+00	-5.736E+04	-6.901E+04	-1.737E+04	-8.203E+04	-1.437E+04	0	997	0\absent peak
6	10	0.000E+00	-8.393E+04	-1.860E+04	-9.489E+04	-5.220E+04	-2.410E+04	0	997	0\absent peak
6	11	0.000E+00	1.320E+08	1.235E+08	1.090E+08	9.065E+07	7.155E+07	-2.2358	995	0\good peak
6	12	0.000E+00	-2.721E+04	-3.537E+04	-4.170E+04	-6.812E+04	-8.757E+04	0	997	0\absent peak
6	13	0.000E+00	5.260E+05	-1.300E+06	-1.810E+06	-3.240E+06	-3.010E+06	0	995	0\good peak
6	14	0.000E+00	-4.350E+05	-1.620E+06	-2.480E+06	-3.840E+06	-3.440E+06	0	995	0\good peak
6	15	0.000E+00	-4.445E+04	-5.401E+04	-7.053E+04	-7.786E+04	-8.722E+03	0	997	0\absent peak
6	16	0.000E+00	-3.471E+03	-9.662E+04	-8.702E+04	-2.537E+04	-2.692E+04	0	997	0\absent peak
6	17	0.000E+00	-6.700E+05	-1.350E+06	-1.180E+06	-1.860E+06	-1.540E+06	0	995	0\good peak
6	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
6	19	0.000E+00	-8.047E+04	-1.512E+04	-4.544E+04	-2.943E+04	-6.452E+04	0	997	0\absent peak
6	20	0.000E+00	-7.569E+04	-1.657E+04	-4.204E+04	-5.816E+04	-3.676E+04	0	997	0\absent peak
6	21	0.000E+00	-6.160E+04	-1.832E+04	-1.497E+03	-7.140E+04	-3.518E+03	0	997	0\absent peak
6	22	0.000E+00	-9.656E+04	-1.039E+04	-4.212E+04	-9.381E+04	-1.863E+04	0	997	0\absent peak
6	23	0.000E+00	-8.300E+04	-9.858E+04	-4.916E+03	-5.194E+04	-4.915E+04	0	997	0\absent peak
6	24	0.000E+00	-7.616E+04	-6.934E+04	-2.057E+04	-3.631E+04	-3.174E+04	0	997	0\absent peak
6	25	0.000E+00	-0.262E+06	-0.341E+06	-0.344E+06	-0.592E+06	-0.616E+06	0	997	0\noisy peak
6	26	0.000E+00	-1.425E+06	-4.490E+06	-5.160E+06	-7.390E+06	-8.080E+06	0	995	0\good peak
6	27	0.000E+00	-9.570E+05	-1.102E+06	-1.295E+06	-1.450E+06	-1.775E+06	0	995	0\good peak
6	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
6	29	0.000E+00	-2.363E+04	-4.386E+04	-7.425E+04	-5.424E+04	-3.949E+04	0	997	0\absent peak
6	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
6	31	0.000E+00	-1.389E+04	-8.371E+04	-7.888E+04	-4.873E+04	-6.152E+04	0	997	0\absent peak
7	7	8.459E+08	4.760E+08	3.250E+08	2.540E+08	1.380E+08	7.480E+07	0	0	0\Diagonal
7	8	0.000E+00	-1.270E+04	-2.995E+04	-7.528E+04	-2.792E+04	-8.525E+04	0	997	0\absent peak

7	9	0.000E+00	-5.921E+04	-2.397E+04	-4.853E+04	-7.726E+04	-3.118E+04	0	997	0\absent peak
7	10	0.000E+00	-4.818E+04	-3.900E+04	-8.178E+04	-3.631E+03	-1.488E+04	0	997	0\absent peak
7	11	0.000E+00	-9.212E+04	-8.087E+04	-5.627E+04	-5.173E+04	-2.694E+04	0	997	0\absent peak
7	12	0.000E+00	-6.788E+04	-2.998E+04	-8.380E+04	-4.344E+03	-7.134E+04	0	997	0\absent peak
7	13	0.000E+00	-3.938E+04	-6.082E+04	-4.069E+04	-1.342E+04	-9.462E+02	0	997	0\absent peak
7	14	0.000E+00	-9.531E+04	-3.439E+03	-8.637E+02	-3.826E+04	-6.879E+04	0	997	0\absent peak
7	15	0.000E+00	-5.947E+04	-5.249E+04	-5.329E+03	-9.830E+04	-3.020E+04	0	997	0\absent peak
7	16	0.000E+00	-2.589E+04	-9.643E+03	-5.276E+04	-4.640E+04	-8.444E+04	0	997	0\absent peak
7	17	0.000E+00	-7.222E+04	-8.056E+04	-7.859E+04	-8.108E+04	-4.903E+04	0	997	0\absent peak
7	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
7	19	0.000E+00	-1.762E+04	-3.065E+03	-8.806E+03	-8.109E+04	-5.223E+04	0	997	0\absent peak
7	20	0.000E+00	-6.303E+04	-6.987E+04	-1.422E+04	-4.123E+03	-9.605E+04	0	997	0\absent peak
7	21	0.000E+00	-2.582E+04	-4.051E+04	-7.509E+04	-9.797E+04	-3.562E+04	0	997	0\absent peak
7	22	0.000E+00	-1.313E+04	-1.812E+03	-4.680E+04	-6.221E+04	-8.016E+04	0	997	0\absent peak
7	23	0.000E+00	-5.669E+04	-2.212E+04	-9.398E+04	-5.985E+04	-4.554E+04	0	997	0\absent peak
7	24	0.000E+00	-4.331E+04	-5.578E+04	-8.751E+04	-2.512E+04	-8.037E+04	0	997	0\absent peak
7	25	0.000E+00	-9.644E+04	-4.331E+04	-5.461E+04	-5.579E+04	-1.619E+04	0	997	0\absent peak
7	26	0.000E+00	-2.942E+04	-3.506E+04	-5.687E+04	-4.886E+04	-3.917E+04	0	997	0\absent peak
7	27	0.000E+00	-8.181E+04	-1.010E+04	-4.629E+04	-3.318E+04	-7.014E+04	0	997	0\absent peak
7	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
7	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
7	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
7	31	0.000E+00	-3.615E+04	-1.571E+04	-7.677E+04	-5.898E+04	-5.543E+04	0	997	0\absent peak
8	8	8.682E+08	6.590E+08	4.630E+08	4.080E+08	2.820E+08	2.090E+08	0	0	0\Diagonal
8	9	0.000E+00	-7.312E+04	-1.526E+04	-7.219E+04	-7.187E+04	-8.385E+03	0	997	0\absent peak
8	10	0.000E+00	-3.460E+05	-2.060E+06	-3.470E+06	-6.240E+06	-6.400E+06	0	995	0\good peak
8	11	0.000E+00	-1.415E+04	-2.594E+04	-6.405E+04	-1.012E+04	-8.734E+04	0	997	0\absent peak
8	12	0.000E+00	-7.150E+04	-6.707E+04	-7.805E+04	-7.635E+04	-7.159E+04	0	997	0\absent peak
8	13	0.000E+00	-2.841E+04	-4.209E+04	-1.630E+04	-5.104E+04	-4.215E+04	0	997	0\absent peak
8	14	0.000E+00	-5.159E+04	-9.777E+04	-4.213E+03	-1.559E+04	-2.188E+04	0	997	0\absent peak
8	15	0.000E+00	-9.802E+04	-6.639E+04	-4.260E+04	-7.926E+04	-4.420E+04	0	997	0\absent peak
8	16	0.000E+00	-5.031E+04	-6.483E+04	-2.638E+04	-6.812E+04	-6.185E+03	0	997	0\absent peak
8	17	0.000E+00	-6.485E+03	-9.273E+04	-3.621E+04	-5.263E+04	-2.984E+04	0	997	0\absent peak
8	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
8	19	0.000E+00	-7.091E+04	-6.055E+04	-1.841E+04	-9.099E+04	-3.432E+04	0	997	0\absent peak
8	20	0.000E+00	-9.589E+04	-2.184E+04	-6.243E+04	-9.849E+04	-9.296E+04	0	997	0\absent peak
8	21	0.000E+00	-1.895E+04	-4.328E+04	-3.302E+04	-5.021E+04	-3.294E+04	0	997	0\absent peak
8	22	0.000E+00	-4.096E+04	-1.368E+04	-7.395E+04	-8.705E+04	-1.198E+04	0	997	0\absent peak
8	23	0.000E+00	-6.145E+04	-6.743E+04	-2.783E+04	-7.727E+04	-4.758E+04	0	997	0\absent peak
8	24	0.000E+00	-2.933E+04	-8.163E+04	-4.937E+04	-5.151E+04	-3.498E+04	0	997	0\absent peak
8	25	0.000E+00	-3.663E+04	-8.126E+04	-5.650E+04	-3.639E+03	-2.951E+04	0	997	0\absent peak
8	26	0.000E+00	-7.550E+06	-1.094E+07	-1.320E+07	-1.780E+07	-1.910E+07	0	995	0\good peak
8	27	0.000E+00	-2.870E+06	-3.370E+06	-4.050E+06	-5.090E+06	-5.800E+06	0	995	0\good peak
8	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
8	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
8	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
8	31	0.000E+00	-4.982E+04	-9.400E+04	-1.560E+04	-5.862E+04	-3.875E+04	0	997	0\absent peak
9	9	3.783E+08	3.130E+08	2.500E+08	2.270E+08	1.820E+08	1.450E+08	0	0	0\Diagonal
9	10	0.000E+00	5.380E+05	-9.540E+05	-3.020E+06	-5.320E+06	-4.950E+06	0	995	0\good peak
9	11	0.000E+00	-9.326E+04	-3.999E+04	-6.258E+04	-7.807E+04	-8.807E+04	0	997	0\absent peak
9	12	0.000E+00	-5.669E+04	-2.212E+04	-9.398E+04	-5.985E+04	-4.554E+04	0	997	0\absent peak
9	13	0.000E+00	-3.296E+04	-6.465E+04	-4.214E+04	-3.044E+04	-7.641E+04	0	997	0\absent peak
9	14	0.000E+00	-2.247E+04	-6.690E+04	-5.066E+04	-4.978E+04	-3.670E+04	0	997	0\absent peak

9	15	0.000E+00	-7.386E+04	-2.897E+04	-6.012E+04	-4.253E+04	-6.433E+04	0	997	0\absent peak
9	16	0.000E+00	-9.189E+03	-2.816E+04	-3.692E+04	-4.598E+04	-1.265E+03	0	997	0\absent peak
9	17	0.000E+00	-1.480E+04	-2.702E+04	-8.372E+04	-6.196E+04	-4.351E+04	0	997	0\absent peak
9	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
9	19	0.000E+00	-9.748E+04	-2.710E+04	-3.397E+04	-1.354E+04	-9.061E+04	0	997	0\absent peak
9	20	0.000E+00	-5.538E+04	-7.667E+04	-9.445E+03	-2.922E+04	-7.885E+04	0	997	0\absent peak
9	21	0.000E+00	-8.272E+04	-2.756E+04	-3.899E+04	-7.553E+04	-8.200E+04	0	997	0\absent peak
9	22	0.000E+00	-2.587E+04	-4.624E+04	-2.446E+03	-9.661E+03	-7.796E+04	0	997	0\absent peak
9	23	0.000E+00	-6.628E+04	-6.820E+04	-4.319E+04	-2.975E+03	-8.905E+04	0	997	0\absent peak
9	24	0.000E+00	-5.733E+04	-4.175E+04	-1.239E+04	-4.605E+04	-6.885E+04	0	997	0\absent peak
9	25	0.000E+00	-1.770E+06	-3.830E+06	-4.470E+06	-5.750E+06	-6.350E+06	0	995	0\good peak
9	26	0.000E+00	-1.932E+04	-3.919E+04	-2.806E+04	-6.874E+03	-1.500E+04	0	997	0\absent peak
9	27	0.000E+00	-3.683E+04	-8.850E+04	-9.689E+04	-5.557E+04	-2.309E+04	0	997	0\absent peak
9	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
9	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
9	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
9	31	0.000E+00	-7.690E+04	-6.347E+04	-2.092E+04	-3.386E+04	-8.220E+04	0	997	0\absent peak
10	10	6.747E+08	5.620E+08	5.190E+08	4.780E+08	4.070E+08	3.350E+08	0	0	0\Diagonal
10	11	0.000E+00	-7.543E+04	-4.592E+04	-7.100E+03	-5.365E+04	-1.297E+04	0	997	0\absent peak
10	12	0.000E+00	-4.498E+04	-3.118E+04	-4.428E+04	-7.438E+04	-3.515E+04	0	997	0\absent peak
10	13	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
10	14	0.000E+00	-3.657E+04	-6.908E+04	-5.443E+04	-4.782E+04	-7.334E+03	0	997	0\absent peak
10	15	0.000E+00	-9.080E+04	-7.715E+03	-3.840E+04	-4.362E+04	-9.842E+04	0	997	0\absent peak
10	16	0.000E+00	-8.379E+04	-1.945E+04	-4.642E+04	-2.342E+04	-6.634E+04	0	997	0\absent peak
10	17	0.000E+00	-3.683E+04	-8.850E+04	-9.689E+04	-5.557E+04	-2.309E+04	0	997	0\absent peak
10	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
10	19	0.000E+00	-6.476E+04	-4.089E+04	-8.024E+04	-4.119E+04	-2.024E+04	0	997	0\absent peak
10	20	0.000E+00	-6.347E+04	-6.910E+04	-3.036E+04	-1.878E+04	-1.953E+04	0	997	0\absent peak
10	21	0.000E+00	-7.893E+04	-4.376E+04	-7.551E+04	-1.741E+04	-6.580E+04	0	997	0\absent peak
10	22	0.000E+00	-6.812E+04	-2.852E+04	-7.685E+04	-8.784E+04	-6.138E+04	0	997	0\absent peak
10	23	0.000E+00	-5.820E+04	-1.338E+03	-2.483E+04	-8.394E+04	-2.073E+04	0	997	0\absent peak
10	24	0.000E+00	-9.856E+03	-2.163E+04	-7.666E+04	-8.640E+03	-5.121E+04	0	997	0\absent peak
10	25	0.000E+00	-6.168E+04	-1.765E+04	-2.842E+04	-7.734E+04	-2.221E+04	0	997	0\absent peak
10	26	0.000E+00	-5.945E+04	-2.866E+04	-3.217E+04	-3.448E+04	-6.011E+04	0	997	0\absent peak
10	27	0.000E+00	-5.644E+04	-9.592E+04	-9.948E+04	-5.312E+04	-9.046E+04	0	997	0\absent peak
10	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
10	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
10	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
10	31	0.000E+00	-9.183E+04	-1.280E+03	-9.645E+04	-4.188E+04	-5.579E+04	0	997	0\absent peak
11	11	2.773E+08	2.220E+08	1.980E+08	1.800E+08	1.460E+08	1.140E+08	+2.2358	0	0\Diagonal
11	12	0.000E+00	-4.172E+04	-3.510E+04	-1.479E+04	-9.567E+04	-6.590E+04	0	997	0\absent peak
11	13	0.000E+00	-2.975E+06	-4.135E+06	-5.620E+06	-8.715E+06	-9.785E+06	0	995	0\good peak
11	14	0.000E+00	-5.749E+05	-1.230E+06	-1.350E+06	-2.515E+06	-2.660E+06	0	995	0\good peak
11	15	0.000E+00	-3.098E+04	-9.806E+04	-5.016E+04	-5.010E+04	-9.539E+04	0	997	0\absent peak
11	16	0.000E+00	-1.994E+04	-9.183E+04	-9.501E+04	-3.937E+04	-5.153E+04	0	997	0\absent peak
11	17	0.000E+00	-4.840E+05	-8.370E+05	-1.415E+06	-1.805E+06	-1.720E+06	0	995	0\good peak
11	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
11	19	0.000E+00	-3.481E+04	-5.552E+04	-7.042E+04	-2.082E+03	-2.625E+03	0	997	0\absent peak
11	20	0.000E+00	-9.373E+04	-9.216E+04	-2.725E+04	-9.460E+03	-3.950E+04	0	997	0\absent peak
11	21	0.000E+00	-9.749E+04	-3.984E+04	-9.520E+04	-4.179E+04	-1.424E+04	0	997	0\absent peak
11	22	0.000E+00	-1.916E+04	-6.255E+04	-1.023E+04	-3.370E+04	-1.203E+04	0	997	0\absent peak
11	23	0.000E+00	-1.187E+04	-5.477E+03	-9.682E+03	-7.637E+04	-5.865E+04	0	997	0\absent peak
11	24	0.000E+00	-3.683E+04	-8.850E+04	-9.689E+04	-5.557E+04	-2.309E+04	0	997	0\absent peak

11	25	0.000E+00	-7.631E+03	-7.812E+04	-4.050E+04	-2.600E+04	-6.373E+04	0	997	0\absent peak
11	26	0.000E+00	-3.625E+06	-5.745E+06	-6.420E+06	-8.355E+06	-8.170E+06	0	995	0\good peak
11	27	0.000E+00	-6.955E+06	-9.740E+06	-1.175E+07	-1.515E+07	-1.595E+07	0	995	0\good peak
11	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
11	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
11	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
11	31	0.000E+00	-9.094E+04	-8.565E+04	-1.436E+04	-8.786E+04	-6.950E+04	0	997	0\absent peak
12	12	8.459E+08	4.760E+08	3.250E+08	2.540E+08	1.380E+08	7.480E+07	0	0	0\Diagonal
12	13	0.000E+00	-1.420E+04	-3.911E+04	-8.610E+04	-1.762E+04	-6.876E+04	0	997	0\absent peak
12	14	0.000E+00	-3.176E+04	-4.833E+04	-3.116E+04	-9.416E+04	-1.032E+04	0	997	0\absent peak
12	15	0.000E+00	-4.721E+04	-8.291E+03	-7.318E+02	-8.984E+04	-7.718E+04	0	997	0\absent peak
12	16	0.000E+00	-9.056E+04	-5.575E+04	-4.193E+04	-9.005E+04	-5.113E+04	0	997	0\absent peak
12	17	0.000E+00	-4.414E+04	-2.591E+04	-7.933E+04	-8.493E+04	-3.560E+03	0	997	0\absent peak
12	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
12	19	0.000E+00	-9.390E+04	-4.299E+04	-8.724E+04	-4.667E+04	-8.780E+04	0	997	0\absent peak
12	20	0.000E+00	-6.948E+04	-2.559E+04	-8.844E+04	-1.735E+04	-8.384E+04	0	997	0\absent peak
12	21	0.000E+00	-7.546E+04	-4.730E+04	-6.587E+04	-3.019E+03	-5.606E+04	0	997	0\absent peak
12	22	0.000E+00	-5.997E+04	-1.333E+04	-6.831E+04	-4.038E+04	-1.587E+04	0	997	0\absent peak
12	23	0.000E+00	-1.913E+04	-4.609E+04	-8.800E+03	-8.881E+04	-5.696E+04	0	997	0\absent peak
12	24	0.000E+00	-1.836E+04	-1.693E+04	-7.901E+03	-9.378E+04	-9.115E+04	0	997	0\absent peak
12	25	0.000E+00	-9.953E+04	-2.099E+04	-2.494E+04	-8.872E+04	-8.278E+04	0	997	0\absent peak
12	26	0.000E+00	-9.923E+04	-8.983E+04	-5.130E+04	-4.477E+04	-4.061E+04	0	997	0\absent peak
12	27	0.000E+00	-6.637E+04	-1.685E+03	-9.071E+04	-4.480E+04	-6.183E+03	0	997	0\absent peak
12	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
12	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
12	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
12	31	0.000E+00	-9.381E+04	-9.879E+04	-6.904E+04	-8.066E+04	-2.925E+04	0	997	0\absent peak
13	13	8.297E+08	6.700E+08	6.060E+08	5.410E+08	4.420E+08	3.530E+08	+2.2358	0	0\Diagonal
13	14	0.000E+00	1.650E+08	1.500E+08	1.360E+08	1.110E+08	8.540E+07	-2.2358	995	0\good peak
13	15	0.000E+00	-8.869E+04	-1.166E+04	-4.306E+03	-1.984E+03	-3.986E+04	0	997	0\absent peak
13	16	0.000E+00	-7.826E+04	-3.498E+04	-5.897E+03	-2.241E+04	-6.371E+04	0	997	0\absent peak
13	17	0.000E+00	-6.948E+04	-2.559E+04	-8.844E+04	-1.735E+04	-8.384E+04	0	997	0\absent peak
13	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
13	19	0.000E+00	-2.367E+04	-9.455E+04	-3.333E+02	-6.881E+04	-3.090E+03	0	997	0\absent peak
13	20	0.000E+00	-1.299E+04	-9.497E+04	-6.052E+04	-4.790E+03	-3.933E+04	0	997	0\absent peak
13	21	0.000E+00	-4.406E+04	-6.070E+04	-4.729E+03	-5.664E+04	-6.836E+03	0	997	0\absent peak
13	22	0.000E+00	-2.428E+04	-4.368E+04	-5.725E+03	-9.606E+04	-8.294E+04	0	997	0\absent peak
13	23	0.000E+00	-4.614E+04	-4.557E+04	-2.917E+04	-2.433E+04	-4.101E+04	0	997	0\absent peak
13	24	0.000E+00	-1.446E+02	-3.642E+04	-9.830E+04	-2.919E+04	-8.556E+04	0	997	0\absent peak
13	25	0.000E+00	-1.220E+06	-2.660E+06	-4.380E+06	-5.470E+06	-5.150E+06	0	995	0\good peak
13	26	0.000E+00	-2.490E+06	-4.570E+06	-5.540E+06	-6.210E+06	-6.190E+06	0	995	0\good peak
13	27	0.000E+00	-2.425E+05	-5.960E+05	-7.395E+05	-9.995E+05	-9.905E+05	0	995	0\good peak
13	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
13	29	0.000E+00	-0.117E+07	-0.622E+06	-0.116E+07	-0.598E+06	-0.963E+06	0	0	0\unresolved
13	30	0.000E+00	-0.102E+07	-0.404E+06	-0.150E+07	-0.692E+06	-0.166E+06	0	0	0\unresolved
13	31	0.000E+00	≈4.840E+04	-4.890E+04	-6.346E+04	-8.471E+04	-7.582E+04	0	997	0\absent peak
14	14	2.237E+08	1.810E+08	1.610E+08	1.420E+08	1.130E+08	9.360E+07	+2.2358	0	0\Diagonal
14	15	0.000E+00	-2.028E+04	-6.068E+04	-1.776E+03	-5.533E+04	-2.272E+04	0	997	0\absent peak
14	16	0.000E+00	-3.384E+04	-9.151E+04	-6.422E+03	-7.072E+04	-2.238E+04	0	997	0\absent peak
14	17	0.000E+00	-4.898E+03	-4.810E+04	-7.446E+04	-8.586E+04	-6.637E+04	0	997	0\absent peak
14	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
14	19	0.000E+00	-6.485E+04	-5.197E+04	-8.006E+04	-8.111E+04	-9.010E+04	0	997	0\absent peak
14	20	0.000E+00	-9.395E+04	-8.538E+04	-2.686E+04	-2.755E+04	-5.874E+04	0	997	0\absent peak

14	21	0.000E+00	-9.334E+04	-1.684E+04	-6.518E+04	-6.067E+04	-2.476E+04	0	997	0\absent peak
14	22	0.000E+00	-3.238E+04	-9.963E+04	-8.928E+03	-4.509E+04	-6.872E+04	0	997	0\absent peak
14	23	0.000E+00	-6.948E+04	-2.559E+04	-8.844E+04	-1.735E+04	-8.384E+04	0	997	0\absent peak
14	24	0.000E+00	-1.969E+04	-6.909E+04	-5.853E+02	-8.292E+04	-8.598E+04	0	997	0\absent peak
14	25	0.000E+00	-2.170E+06	-3.760E+06	-4.990E+06	-6.220E+06	-5.830E+06	0	995	0\good peak
14	26	0.000E+00	-2.240E+06	-2.780E+06	-4.630E+06	-5.160E+06	-5.880E+06	0	995	0\good peak
14	27	0.000E+00	-6.120E+05	-1.072E+06	-1.100E+06	-1.267E+06	-1.545E+06	0	995	0\good peak
14	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
14	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
14	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
14	31	0.000E+00	-6.197E+04	-8.838E+04	-8.385E+04	-4.050E+04	-9.865E+04	0	997	0\absent peak
15	15	3.945E+08	2.810E+08	2.320E+08	1.960E+08	1.400E+08	9.710E+07	0	0	0\Diagonal
15	16	0.000E+00	-7.632E+04	-7.701E+04	-6.319E+04	-1.888E+03	-3.538E+04	0	997	0\absent peak
15	17	0.000E+00	-7.495E+06	-9.685E+06	-1.085E+07	-1.155E+07	-1.060E+07	0	995	0\good peak
15	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
15	19	0.000E+00	-5.496E+04	-8.523E+04	-2.825E+04	-9.781E+04	-2.646E+04	0	997	0\absent peak
15	20	0.000E+00	-2.378E+04	-8.480E+04	-2.932E+04	-5.611E+03	-8.662E+04	0	997	0\absent peak
15	21	0.000E+00	-5.234E+04	-7.133E+04	-7.878E+04	-4.743E+04	-9.280E+04	0	997	0\absent peak
15	22	0.000E+00	-1.211E+04	-2.819E+04	-8.839E+04	-8.715E+04	-1.041E+04	0	997	0\absent peak
15	23	0.000E+00	-8.927E+04	-1.837E+04	-6.988E+04	-7.355E+04	-7.298E+04	0	997	0\absent peak
15	24	0.000E+00	-3.840E+04	-2.963E+04	-6.488E+04	-4.108E+03	-5.818E+04	0	997	0\absent peak
15	25	0.000E+00	-1.630E+06	-1.940E+06	-2.990E+06	-3.090E+06	-3.580E+06	0	995	0\good peak
15	26	0.000E+00	-7.165E+06	-8.945E+06	-1.002E+07	-1.153E+07	-1.162E+07	0	995	0\good peak
15	27	0.000E+00	-6.905E+04	-5.674E+04	-6.734E+03	-8.519E+04	-9.744E+04	0	997	0\absent peak
15	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
15	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
15	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
15	31	0.000E+00	-8.224E+02	-6.072E+04	-4.627E+04	-1.035E+04	-6.210E+03	0	997	0\absent peak
16	16	2.844E+08	0.241E+09	0.220E+09	0.203E+09	0.171E+09	0.142E+09	0	0	0\Diagonal
16	17	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
16	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
16	19	0.000E+00	-6.306E+04	-3.615E+04	-7.963E+04	-8.186E+04	-4.962E+04	0	997	0\absent peak
16	20	0.000E+00	-9.076E+04	-9.500E+04	-6.446E+04	-7.286E+04	-5.098E+04	0	997	0\absent peak
16	21	0.000E+00	-4.422E+04	-5.006E+04	-8.826E+04	-2.718E+04	-7.012E+04	0	997	0\absent peak
16	22	0.000E+00	-5.291E+04	-3.323E+04	-6.343E+04	-9.587E+04	-5.138E+04	0	997	0\absent peak
16	23	0.000E+00	-9.271E+04	-9.095E+04	-2.063E+04	-7.983E+03	-1.683E+04	0	997	0\absent peak
16	24	0.000E+00	-1.806E+04	-7.405E+04	-3.125E+04	-7.577E+03	-7.051E+04	0	997	0\absent peak
16	25	0.000E+00	-5.333E+04	-8.116E+04	-7.152E+04	-4.007E+03	-5.722E+04	0	997	0\absent peak
16	26	0.000E+00	-6.948E+04	-2.559E+04	-8.844E+04	-1.735E+04	-8.384E+04	0	997	0\absent peak
16	27	0.000E+00	-1.952E+04	-9.921E+04	-6.433E+03	-8.125E+04	-6.412E+04	0	997	0\absent peak
16	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
16	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
16	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
16	31	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
17	17	8.459E+08	4.760E+08	3.250E+08	2.540E+08	1.380E+08	7.480E+07	0	0	0\Diagonal
17	18	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
17	19	0.000E+00	-4.642E+04	-1.046E+04	-3.612E+04	-3.581E+04	-3.850E+03	0	997	0\absent peak
17	20	0.000E+00	-6.828E+04	-5.730E+04	-9.356E+04	-8.269E+04	-2.751E+04	0	997	0\absent peak
17	21	0.000E+00	-7.643E+04	-3.982E+04	-9.708E+04	-5.940E+04	-7.237E+04	0	997	0\absent peak
17	22	0.000E+00	-1.688E+04	-1.333E+04	-9.607E+04	-8.264E+04	-1.053E+04	0	997	0\absent peak
17	23	0.000E+00	-9.155E+04	-1.044E+04	-5.103E+04	-5.977E+04	-9.992E+04	0	997	0\absent peak
17	24	0.000E+00	-6.482E+04	-2.750E+04	-1.058E+04	-9.514E+04	-4.958E+04	0	997	0\absent peak
17	25	0.000E+00	-2.870E+06	-4.600E+06	-4.840E+06	-4.020E+06	-4.630E+06	0	995	0\good peak

17	26	0.000E+00	-1.820E+06	-2.210E+06	-2.730E+06	-3.820E+06	-3.510E+06	0	995	0\good peak
17	27	0.000E+00	-5.363E+04	-7.327E+04	-2.528E+04	-9.871E+04	-1.678E+03	0	997	0\absent peak
17	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
17	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
17	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
17	31	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	18	4.718E+08	0.307E+09	0.222E+09	0.179E+09	0.116E+09	0.710E+08	0	0	0\Diagonal
18	19	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	20	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	21	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	22	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	23	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	24	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	25	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	26	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	27	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
18	31	0.000E+00	-7.399E+04	-2.544E+04	-6.100E+04	-2.224E+03	-8.010E+04	0	997	0\absent peak
19	19	7.469E+08	6.260E+08	5.560E+08	5.130E+08	4.290E+08	3.510E+08	0	0	0\Diagonal
19	20	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
19	21	0.000E+00	-7.105E+04	-6.448E+04	-6.213E+04	-3.176E+04	-4.149E+04	0	997	0\absent peak
19	22	0.000E+00	-8.942E+03	-6.116E+04	-4.916E+04	-2.706E+04	-2.985E+04	0	997	0\absent peak
19	23	0.000E+00	-6.948E+04	-2.559E+04	-8.844E+04	-1.735E+04	-8.384E+04	0	997	0\absent peak
19	24	0.000E+00	-5.491E+04	-3.293E+04	-4.413E+04	-5.608E+04	-3.622E+04	0	997	0\absent peak
19	25	0.000E+00	-8.625E+06	-1.214E+07	-1.980E+07	-2.140E+07	-2.480E+07	0	995	1\tau1opt
19	26	0.000E+00	-9.206E+03	-9.239E+04	-4.436E+04	-3.343E+04	-8.732E+04	0	997	0\absent peak
19	27	0.000E+00	-7.039E+04	-6.043E+04	-3.003E+04	-7.521E+04	-4.876E+04	0	997	0\absent peak
19	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
19	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
19	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
19	31	0.000E+00	-6.396E+04	-7.621E+04	-1.942E+04	-2.316E+04	-9.969E+03	0	997	0\absent peak
20	20	4.272E+08	3.570E+08	3.640E+08	3.130E+08	2.770E+08	2.360E+08	0	0	0\Diagonal
20	21	0.000E+00	-7.487E+04	-4.608E+03	-1.303E+04	-3.706E+03	-6.848E+04	0	997	0\absent peak
20	22	0.000E+00	-6.614E+04	-8.872E+04	-4.084E+04	-6.853E+04	-9.656E+04	0	997	0\absent peak
20	23	0.000E+00	-7.685E+04	-5.011E+04	-1.411E+04	-7.503E+04	-8.302E+04	0	997	0\absent peak
20	24	0.000E+00	-4.164E+04	-2.467E+04	-2.827E+04	-3.333E+04	-1.370E+04	0	997	0\absent peak
20	25	0.000E+00	-5.887E+04	-5.728E+04	-1.012E+03	-8.611E+04	-7.563E+04	0	997	0\absent peak
20	26	0.000E+00	-1.741E+04	-1.875E+04	-1.247E+04	-5.276E+04	-8.464E+04	0	997	0\absent peak
20	27	0.000E+00	-1.341E+04	-8.283E+04	-9.915E+04	-7.136E+04	-7.998E+04	0	997	0\absent peak
20	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
20	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
20	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
20	31	0.000E+00	-1.341E+04	-8.283E+04	-9.915E+04	-7.136E+04	-7.998E+04	0	997	0\absent peak
21	21	6.025E+08	4.920E+08	4.310E+08	3.990E+08	3.220E+08	2.570E+08	0	0	0\Diagonal
21	22	0.000E+00	-1.062E+04	-5.863E+04	-2.895E+04	-7.911E+04	-2.110E+04	0	997	0\absent peak
21	23	0.000E+00	-2.845E+04	-1.495E+04	-2.506E+04	-8.020E+04	-9.661E+04	0	997	0\absent peak
21	24	0.000E+00	-1.857E+04	-9.150E+04	-2.915E+04	-4.155E+04	-6.378E+04	0	997	0\absent peak
21	25	0.000E+00	-7.206E+04	-7.503E+04	-8.256E+04	-8.607E+04	-2.862E+04	0	997	0\absent peak
21	26	0.000E+00	-5.417E+04	-6.840E+04	-8.191E+04	-7.344E+04	-6.958E+04	0	997	0\absent peak
21	27	0.000E+00	-1.131E+07	-1.355E+07	-1.625E+07	-2.025E+07	-2.265E+07	0	995	1\tau1opt
21	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved

21	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
21	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
21	31	0.000E+00	-4.945E+04	-1.608E+04	-9.151E+04	-6.913E+04	-3.875E+04	0	997	0\absent peak
22	22	6.025E+08	4.920E+08	4.310E+08	3.990E+08	3.220E+08	2.570E+08	0	0	0\Diagonal
22	23	0.000E+00	-8.523E+04	-2.108E+04	-4.048E+04	-4.105E+04	-1.457E+04	0	997	0\absent peak
22	24	0.000E+00	-8.530E+04	-8.429E+04	-4.884E+03	-6.121E+04	-3.220E+04	0	997	0\absent peak
22	25	0.000E+00	-5.460E+04	-7.707E+04	-1.948E+04	-6.081E+04	-7.424E+04	0	997	0\absent peak
22	26	0.000E+00	-2.410E+06	-8.230E+06	-1.640E+07	-1.830E+07	-1.580E+07	0	995	0\good peak
22	27	0.000E+00	-9.719E+04	-9.962E+04	-7.498E+04	-3.592E+04	-1.204E+04	0	997	0\absent peak
22	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
22	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
22	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
22	31	0.000E+00	-4.660E+04	-7.549E+04	-6.175E+04	-3.921E+04	-6.546E+04	0	997	0\absent peak
23	23	1.653E+09	1.250E+09	1.120E+09	8.800E+08	6.940E+08	5.350E+08	0	0	0\Diagonal
23	24	0.000E+00	-6.530E+04	-9.429E+04	-7.884E+03	-8.121E+04	-2.220E+04	0	997	0\absent peak
23	25	0.000E+00	-1.341E+04	-8.283E+04	-9.915E+04	-7.136E+04	-7.998E+04	0	997	0\absent peak
23	26	0.000E+00	1.020E+08	1.231E+08	2.517E+07	5.800E+05	-4.185E+06	0	0	0\unresolved
23	27	0.000E+00	-7.017E+04	-9.887E+04	-1.973E+04	-4.690E+04	-7.115E+04	0	997	0\absent peak
23	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
23	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
23	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
23	31	0.000E+00	-2.368E+04	-1.522E+04	-1.760E+04	-2.735E+04	-3.884E+04	0	997	0\absent peak
24	24	4.272E+08	3.570E+08	3.640E+08	3.130E+08	2.770E+08	2.360E+08	0	0	0\Diagonal
24	25	0.000E+00	-9.033E+04	-6.426E+04	-5.757E+04	-3.765E+04	-6.970E+04	0	997	0\absent peak
24	26	0.000E+00	-4.736E+04	-4.454E+04	-7.955E+04	-9.064E+04	-7.740E+04	0	997	0\absent peak
24	27	0.000E+00	-1.230E+06	-2.610E+06	-3.050E+06	-5.210E+06	-2.980E+06	0	995	1\tau1opt
24	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
24	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
24	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
24	31	0.000E+00	-1.069E+04	-4.836E+03	-9.533E+04	-2.141E+04	-5.938E+04	0	997	0\absent peak
25	25	6.025E+08	4.920E+08	4.310E+08	3.990E+08	3.220E+08	2.570E+08	0	0	0\Diagonal
25	26	0.000E+00	-8.829E+04	-9.564E+04	-4.454E+04	-3.362E+04	-4.765E+04	0	997	0\absent peak
25	27	0.000E+00	-9.859E+03	-7.448E+04	-6.895E+04	-3.473E+04	-9.176E+04	0	997	0\absent peak
25	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
25	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
25	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
25	31	0.000E+00	-1.951E+04	-4.881E+04	-1.781E+04	-4.927E+04	-2.139E+04	0	997	0\absent peak
26	26	1.653E+09	1.250E+09	1.120E+09	8.800E+08	6.940E+08	5.350E+08	0	0	0\Diagonal
26	27	0.000E+00	-1.053E+07	-4.425E+06	-4.405E+06	-5.625E+06	-1.184E+07	0	995	0\good peak
26	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
26	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
26	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
26	31	0.000E+00	-5.501E+04	-3.396E+04	-3.556E+04	-4.381E+04	-2.719E+04	0	997	0\absent peak
27	27	6.025E+08	4.920E+08	4.310E+08	3.990E+08	3.220E+08	2.570E+08	0	0	0\Diagonal
27	28	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
27	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
27	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
27	31	0.000E+00	-9.380E+04	-7.230E+04	-7.257E+04	-7.309E+04	-4.286E+04	0	997	0\absent peak
28	28	2.408E+09	0.159E+10	0.126E+10	0.101E+10	0.659E+09	0.438E+09	0	0	0\Diagonal
28	29	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
28	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
28	31	0.000E+00	-4.727E+03	-3.766E+03	-6.109E+04	-1.568E+02	-7.150E+04	0	997	0\absent peak
29	29	1.018E+09	0.680E+09	0.526E+09	0.415E+09	0.270E+09	0.183E+09	0	0	0\Diagonal

29	30	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
29	31	0.000E+00	-6.644E+04	-5.895E+04	-6.907E+04	-7.278E+04	-8.072E+04	0	997	0\absent peak
30	30	6.432E+08	0.403E+09	0.295E+09	0.223E+09	0.140E+09	0.854E+08	0	0	0\Diagonal
30	31	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0	0	0\unresolved
31	31	3.945E+08	2.810E+08	2.320E+08	1.960E+08	1.400E+08	9.710E+07	0	0	0\Diagonal

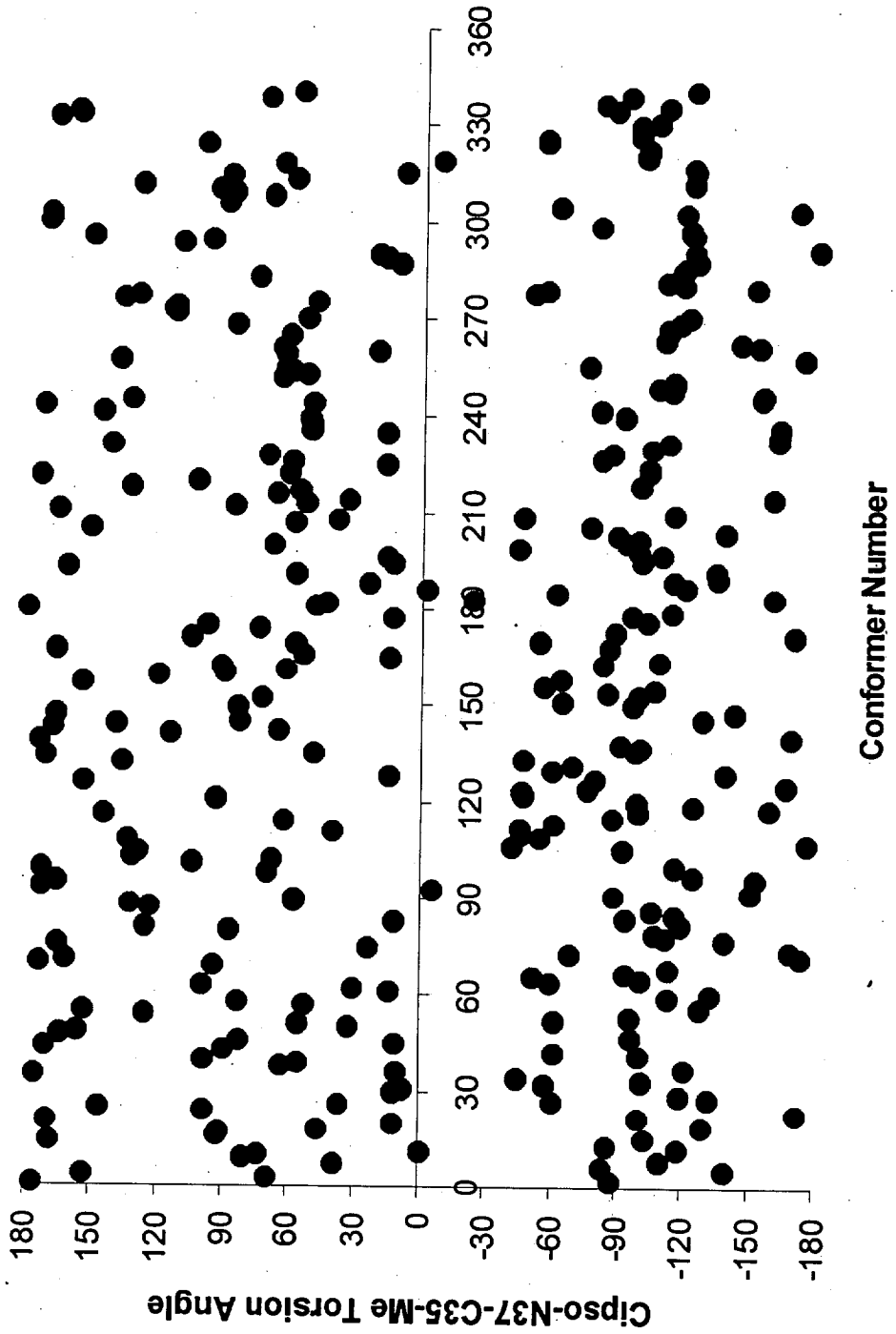

Figure 8. Conformer Distribution for 2DCPA