Electronic Supplementary Information for Dalton Transactions

4,6-Bis-Supermesitylphosphanylidenemethyl-Dibenzofurane.

Synthesis, X-ray Structure and Reactivity towards Group 11 metals.

Eliane Deschamps, Bernard Deschamps, Jeanne Laure Dormieux, Louis Ricard,

Nicolas Mézailles and Pascal Le Floch*

X-Ray structural data for 3

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Data for the theoretical structure I.

Data for the theoretical structure II.

X-Ray structural data for 3.

Table 1. Crystal data for **3**

Compound	**3**
Molecular formula	$C_{50}H_{66}OP_2$
Molecular weight	744.97
Crystal habit	pale yellow plate
Crystal dimensions(mm)	0.20x0.18x0.12
Crystal system	monoclinic
Space group	C2/c
a(Å)	15.9660(10)
b(Å)	10.4070(10)
c(Å)	14.0990(10)
α(°)	90.00
β(°)	105.2600(10)
γ(°)	90.00
V(Å^3)	2260.1(3)
Z	2
d(g-cm^{-3})	1.095
F(000)	808
μ(cm^{-1})	0.130
Absorption corrections	multi-scan ; 0.9745 min, 0.9846 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	30.03
HKL ranges	-15 22 ; -14 13 ; -19 19
Reflections measured	7551
Unique data	5849
Rint	0.0193
Reflections used	5376
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	249
Reflections / parameter	21
wR2	0.0924
R1	0.0349
Flack's parameter	0.26(6)
Weights a, b	0.0488 ; 0.1741
GoF	1.056
difference peak / hole (e Å^{-3})	0.197(0.036) / -0.209(0.036)

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

atom	x	y	z	U(eq)
P(1)	-4038(1)	2162(1)	-3818(1)	26(1)
O(2)	-5000	-124(1)	-5000	23(1)
C(3)	-3513(1)	3348(1)	-2868(1)	23(1)
C(4)	-2628(1)	3708(1)	-2726(1)	24(1)
C(5)	-4436(1)	-923(1)	-4354(1)	23(1)
C(6)	-2219(1)	4357(1)	-1861(1)	27(1)
C(7)	-3980(1)	3817(1)	-2208(1)	25(1)
C(8)	-4623(1)	-2219(1)	-4581(1)	26(1)
C(9)	-3765(1)	-505(1)	-3554(1)	26(1)
C(10)	-2643(1)	4730(1)	-1165(1)	26(1)
C(11)	-2093(1)	3486(2)	-3484(1)	30(1)
C(12)	-3528(1)	4487(1)	-1374(1)	27(1)
C(13)	-3589(1)	822(1)	-3246(1)	27(1)
C(14)	-4979(1)	3663(2)	-2373(1)	32(1)
C(15)	-2149(1)	5451(2)	-235(1)	33(1)
C(16)	-3426(1)	-2790(2)	-3243(1)	35(1)
C(17)	-2744(1)	5861(2)	408(1)	45(1)
C(18)	-4106(1)	-3168(1)	-4027(1)	32(1)
C(19)	-5468(1)	4133(2)	-3394(1)	41(1)
C(20)	-2638(1)	3647(2)	-4545(1)	49(1)
C(21)	-3270(1)	-1502(2)	-3013(1)	34(1)
C(22)	-1428(1)	4597(2)	374(1)	49(1)
C(23)	-1662(1)	2168(2)	-3364(1)	53(1)
C(24)	-5316(1)	4472(2)	-1643(1)	45(1)
C(25)	-1750(1)	6677(2)	-534(1)	46(1)
C(26)	-5228(1)	2268(2)	-2222(1)	47(1)
C(27)	-1368(1)	4492(2)	-3353(1)	56(1)

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

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

P(1)-C(13)	1.674(2)	P(1)-C(3)	1.852(1)
O(2)-C(5)	1.379(1)	O(2)-C(5)#2	1.379(1)
C(3)-C(4)	1.423(2)	C(3)-C(7)	1.424(2)
C(4)-C(6)	1.397(2)	C(4)-C(11)	1.551(2)
C(5)-C(8)	1.399(2)	C(5)-C(9)	1.405(2)
C(6)-C(10)	1.387(2)	C(6)-H(6)	0.9500
C(7)-C(12)	1.394(2)	C(7)-C(14)	1.559(2)
C(8)-C(18)	1.388(2)	C(8)-C(8)#2	1.449(3)
C(9)-C(21)	1.401(2)	C(9)-C(13)	1.454(2)
C(10)-C(12)	1.389(2)	C(10)-C(15)	1.536(2)
C(11)-C(23)	1.524(2)	C(11)-C(20)	1.528(2)
C(11)-C(27)	1.535(2)	C(12)-H(12)	0.9500
C(13)-H(13)	0.9500	C(14)-C(19)	1.526(2)
C(14)-C(24)	1.533(2)	C(14)-C(26)	1.534(2)
C(15)-C(22)	1.526(2)	C(15)-C(25)	1.534(2)
C(15)-C(17)	1.536(2)	C(16)-C(21)	1.386(2)
C(16)-C(18)	1.387(2)	C(16)-H(16)	0.9500
C(17)-H(17A)	0.9800	C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800	C(18)-H(18)	0.9500
C(19)-H(19A)	0.9800	C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800	C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800	C(20)-H(20C)	0.9800
C(21)-H(21)	0.9500	C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800	C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800	C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800	C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800	C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800	C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800	C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800	C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800	C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800		

C(13)-P(1)-C(3)	98.72(7)	C(5)-O(2)-C(5)#2	105.8(1)
C(4)-C(3)-C(7)	119.3(1)	C(4)-C(3)-P(1)	121.4(1)
C(7)-C(3)-P(1)	119.1(1)	C(6)-C(4)-C(3)	118.0(1)
C(6)-C(4)-C(11)	117.2(1)	C(3)-C(4)-C(11)	124.8(1)
O(2)-C(5)-C(8)	111.5(1)	O(2)-C(5)-C(9)	124.8(1)
C(8)-C(5)-C(9)	123.6(1)	C(10)-C(6)-C(4)	123.4(1)
C(10)-C(6)-H(6)	118.3	C(4)-C(6)-H(6)	118.3
C(12)-C(7)-C(3)	118.6(1)	C(12)-C(7)-C(14)	117.4(1)
C(3)-C(7)-C(14)	124.0(1)	C(18)-C(8)-C(5)	119.8(1)
C(18)-C(8)-C(8)#2	134.6(1)	C(5)-C(8)-C(8)#2	105.55(8)
C(21)-C(9)-C(5)	114.2(1)	C(21)-C(9)-C(13)	120.2(1)
C(5)-C(9)-C(13)	125.5(1)	C(6)-C(10)-C(12)	117.2(1)
C(6)-C(10)-C(15)	120.3(1)	C(12)-C(10)-C(15)	122.3(1)
C(23)-C(11)-C(20)	109.4(1)	C(23)-C(11)-C(27)	107.2(1)
C(20)-C(11)-C(27)	105.1(1)	C(23)-C(11)-C(4)	111.9(1)
C(20)-C(11)-C(4)	112.5(1)	C(27)-C(11)-C(4)	110.4(1)
C(10)-C(12)-C(7)	122.8(1)	C(10)-C(12)-H(12)	118.6
C(7)-C(12)-H(12)	118.6	C(9)-C(13)-P(1)	128.5(1)
C(9)-C(13)-H(13)	115.7	P(1)-C(13)-H(13)	115.7
C(19)-C(14)-C(24)	105.9(1)	C(19)-C(14)-C(26)	110.3(1)
C(24)-C(14)-C(26)	106.1(1)	C(19)-C(14)-C(7)	110.9(1)
C(24)-C(14)-C(7)	111.7(1)	C(26)-C(14)-C(7)	111.6(1)
C(22)-C(15)-C(25)	109.4(1)	C(22)-C(15)-C(17)	108.8(1)
C(25)-C(15)-C(17)	107.3(1)	C(22)-C(15)-C(10)	109.7(1)
C(25)-C(15)-C(10)	109.1(1)	C(17)-C(15)-C(10)	112.4(1)
C(21)-C(16)-C(18)	121.0(1)	C(21)-C(16)-H(16)	119.5
C(18)-C(16)-H(16)	119.5	C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5	H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5	H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5	C(16)-C(18)-C(8)	118.1(1)
C(16)-C(18)-H(18)	120.9	C(8)-C(18)-H(18)	120.9
C(14)-C(19)-H(19A)	109.5	C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5	C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5	H(19B)-C(19)-H(19C)	109.5
C(11)-C(20)-H(20A)	109.5	C(11)-C(20)-H(20B)	109.5

H(20A)-C(20)-H(20B)	109.5	C(11)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(20B)-C(20)-H(20C)	109.5
C(16)-C(21)-C(9)	123.2(1)	C(16)-C(21)-H(21)	118.4
C(9)-C(21)-H(21)	118.4	C(15)-C(22)-H(22A)	109.5
C(15)-C(22)-H(22B)	109.5	H(22A)-C(22)-H(22B)	109.5
C(15)-C(22)-H(22C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5	C(11)-C(23)-H(23A)	109.5
C(11)-C(23)-H(23B)	109.5	H(23A)-C(23)-H(23B)	109.5
C(11)-C(23)-H(23C)	109.5	H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5	C(14)-C(24)-H(24A)	109.5
C(14)-C(24)-H(24B)	109.5	H(24A)-C(24)-H(24B)	109.5
C(14)-C(24)-H(24C)	109.5	H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5	C(15)-C(25)-H(25A)	109.5
C(15)-C(25)-H(25B)	109.5	H(25A)-C(25)-H(25B)	109.5
C(15)-C(25)-H(25C)	109.5	H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5	C(14)-C(26)-H(26A)	109.5
C(14)-C(26)-H(26B)	109.5	H(26A)-C(26)-H(26B)	109.5
C(14)-C(26)-H(26C)	109.5	H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5	C(11)-C(27)-H(27A)	109.5
C(11)-C(27)-H(27B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(11)-C(27)-H(27C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5		

Estimated standard deviations are given in the parenthesis.

Symmetry operators ::

1: x, y, z 2: -x, y, -z 3: x+1/2, y+1/2, z

4: -x+1/2, y+1/2, -z

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

atom	U11	U22	U33	U23	U13	U12
P(1)	29(1)	22(1)	26(1)	-2(1)	3(1)	-1(1)
O(2)	29(1)	18(1)	21(1)	0	6(1)	0
C(3)	26(1)	20(1)	23(1)	0(1)	4(1)	0(1)
C(4)	25(1)	22(1)	26(1)	1(1)	6(1)	1(1)
C(5)	28(1)	19(1)	24(1)	3(1)	10(1)	3(1)
C(6)	24(1)	28(1)	27(1)	0(1)	4(1)	-4(1)
C(7)	27(1)	22(1)	24(1)	2(1)	7(1)	-1(1)
C(8)	33(1)	21(1)	26(1)	0(1)	13(1)	2(1)
C(9)	31(1)	24(1)	24(1)	1(1)	8(1)	2(1)
C(10)	33(1)	22(1)	21(1)	0(1)	4(1)	-2(1)
C(11)	30(1)	33(1)	31(1)	-4(1)	12(1)	0(1)
C(12)	32(1)	26(1)	25(1)	0(1)	10(1)	0(1)
C(13)	30(1)	28(1)	22(1)	-2(1)	4(1)	-2(1)
C(14)	27(1)	36(1)	34(1)	0(1)	10(1)	-1(1)
C(15)	42(1)	31(1)	23(1)	-1(1)	4(1)	-8(1)
C(16)	46(1)	25(1)	32(1)	8(1)	7(1)	10(1)
C(17)	59(1)	51(1)	27(1)	-12(1)	12(1)	-10(1)
C(18)	46(1)	18(1)	35(1)	4(1)	16(1)	5(1)
C(19)	30(1)	55(1)	37(1)	2(1)	6(1)	8(1)
C(20)	45(1)	75(1)	31(1)	5(1)	16(1)	1(1)
C(21)	39(1)	32(1)	28(1)	5(1)	5(1)	6(1)
C(22)	50(1)	49(1)	37(1)	-3(1)	-7(1)	-5(1)
C(23)	54(1)	48(1)	67(1)	3(1)	35(1)	17(1)
C(24)	32(1)	62(1)	44(1)	-8(1)	16(1)	3(1)
C(25)	69(1)	35(1)	34(1)	-8(1)	13(1)	-22(1)
C(26)	37(1)	41(1)	69(1)	4(1)	24(1)	-9(1)
C(27)	56(1)	69(1)	57(1)	-21(1)	38(1)	-27(1)

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

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

atom	x	y	z	U(eq)
H(6)	-1619	4552	-1744	32
H(12)	-3838	4791	-929	32
H(13)	-3162	947	-2640.9998	33
H(16)	-3061	-3423	-2858	42
H(17A)	-2405	6338	980	68
H(17B)	-2997	5096	630	68
H(17C)	-3210	6409	24	68
H(18)	-4215	-4051	-4182	39
H(19A)	-6093.9995	4054	-3474	62
H(19B)	-5301	3612	-3894	62
H(19C)	-5321	5035	-3471	62
H(20A)	-2257	3633	-4988	74
H(20B)	-2948.0002	4469	-4612	74
H(20C)	-3058	2943	-4714	74
H(21)	-2805	-1284	-2461	40
H(22A)	-1018	4387	-11	73
H(22B)	-1681	3804	550	73
H(22C)	-1123	5053	974	73
H(23A)	-1332	2048	-2678	79
H(23B)	-1267	2108	-3790	79
H(23C)	-2108	1500	-3547	79
H(24A)	-5129	5366	-1668.0001	68
H(24B)	-5083	4133	-978	68
H(24C)	-5952	4436	-1817.9999	68
H(25A)	-1471	7172	55	69
H(25B)	-2208	7196	-964	69
H(25C)	-1318	6445	-886	69
H(26A)	-5856.9995	2208	-2321	71
H(26B)	-4933	1993	-1553.0001	71
H(26C)	-5052.0005	1712	-2697	71
H(27A)	-939	4353	-2722	84
H(27B)	-1617	5353	-3365	84
H(27C)	-1085	4410	-3888	84

X-Ray structural data for 4.

Table 6. Crystal data for **4**

Compound	**4**
Molecular formula	$C_{50}H_{66}AuOP_2,C_4H_{10}O,BF_4$
Molecular weight	1102.86
Crystal habit	pale yellow block
Crystal dimensions(mm)	0.20x0.18x0.16
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a(Å)	11.6470(10)
b(Å)	16.8950(10)
c(Å)	27.3290(10)
α(°)	90.00
β(°)	90.00
γ(°)	90.00
V(Å^3)	5377.7(6)
Z	4
d(g-cm^{-3})	1.362
F(000)	2264
μ(cm^{-1})	2.846
Absorption corrections	multi-scan ; 0.5999 min, 0.6588 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	30.03
HKL ranges	-16 16 ; -21 23 ; -38 38
Reflections measured	27925
Unique data	15461
Rint	0.0302
Reflections used	13250
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	597
Reflections / parameter	22
wR2	0.0701
R1	0.0340
Flack's parameter	-0.021(3)
Weights a, b	0.0330 ; 0.0000
GoF	0.996
difference peak / hole (e Å^{-3})	1.488(0.096) / -1.468(0.096)

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

atom	x	y	z	U(eq)
Au(1)	144(1)	8625(1)	3998(1)	30(1)
P(1)	-763(1)	7460(1)	4141(1)	28(1)
P(2)	690(1)	9860(1)	3773(1)	29(1)
O(1)	-1713(2)	8921(1)	3437(1)	29(1)
C(1)	-1987(3)	7223(2)	3859(1)	31(1)
C(2)	-2683(3)	7623(2)	3496(1)	27(1)
C(3)	-3612(3)	7199(2)	3299(1)	34(1)
C(4)	-4337(3)	7514(2)	2943(1)	36(1)
C(5)	-4185(3)	8266(2)	2762(1)	34(1)
C(6)	-3278(2)	8709(2)	2948(1)	28(1)
C(7)	-2558(2)	8388(2)	3304(1)	27(1)
C(8)	-1910(3)	9606(2)	3164(1)	28(1)
C(9)	-2867(3)	9507(2)	2862(1)	30(1)
C(10)	-3225(3)	10129(2)	2568(1)	34(1)
C(11)	-2639(3)	10843(2)	2602(1)	36(1)
C(12)	-1691(3)	10922(2)	2900(1)	36(1)
C(13)	-1254(3)	10291(2)	3190(1)	30(1)
C(14)	-186(3)	10427(2)	3444(1)	31(1)
C(15)	-258(3)	6679(2)	4536(1)	27(1)
C(16)	366(3)	6030(2)	4328(1)	30(1)
C(17)	761(3)	5451(2)	4650(1)	32(1)
C(18)	612(3)	5488(2)	5153(1)	31(1)
C(19)	45(2)	6131(2)	5340(1)	30(1)
C(20)	-398(2)	6742(2)	5055(1)	29(1)
C(21)	624(3)	5892(2)	3778(1)	40(1)
C(22)	1055(4)	6633(3)	3507(2)	64(1)
C(23)	1596(5)	5282(3)	3711(2)	73(2)
C(24)	-424(4)	5562(3)	3525(2)	77(2)
C(25)	1130(3)	4831(2)	5477(1)	37(1)
C(26)	2434(3)	4950(3)	5482(2)	60(1)
C(27)	852(4)	4017(3)	5271(2)	56(1)
C(28)	678(3)	4866(3)	6002(1)	52(1)
C(29)	-976(3)	7446(2)	5327(1)	34(1)
C(30)	-1158(4)	7263(3)	5875(1)	52(1)
C(31)	-2176(3)	7645(3)	5129(2)	49(1)
C(32)	-191(4)	8168(2)	5309(1)	52(1)
C(33)	1943(3)	10468(2)	3877(1)	26(1)
C(34)	2097(3)	10856(2)	4336(1)	27(1)
C(35)	2712(3)	11564(2)	4331(1)	34(1)
C(36)	3165(3)	11891(2)	3903(1)	36(1)
C(37)	3126(3)	11429(2)	3484(1)	35(1)
C(38)	2563(3)	10709(2)	3459(1)	29(1)
C(39)	1663(3)	10518(2)	4827(1)	31(1)
C(40)	2096(3)	9678(2)	4897(1)	38(1)
C(41)	343(3)	10533(2)	4864(1)	43(1)
C(42)	2115(4)	10999(3)	5267(1)	48(1)
C(43)	3686(4)	12722(2)	3882(1)	49(1)
C(44)	3660(7)	13127(3)	4373(2)	121(3)
C(45)	3002(4)	13225(2)	3521(2)	50(1)
C(46)	4940(4)	12660(3)	3692(2)	79(2)
C(47)	2720(3)	10223(2)	2981(1)	36(1)
C(48)	1967(4)	10544(3)	2568(1)	63(1)
C(49)	3976(3)	10295(3)	2815(2)	58(1)
C(50)	2489(5)	9342(3)	3036(2)	70(2)
C(51)	-267(6)	7963(4)	2460(2)	102(2)
C(52)	356(8)	8253(4)	2045(2)	128(3)
O(2)	434(3)	7700(2)	1677(1)	76(1)
C(53)	1030(10)	7923(4)	1256(2)	166(5)
C(54)	970(10)	7360(4)	880(2)	173(5)
B(1)	4780(5)	10189(3)	1390(2)	53(1)
F(1)	3757(2)	10462(2)	1205(1)	75(1)
F(2)	5313(2)	10795(1)	1652(1)	61(1)
F(3)	5489(3)	9968(2)	1003(1)	76(1)

F(4)	4653(3)	9552(2)	1693(1)	86(1)

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

Table 8. Bond lengths (A) and angles (deg) for **4**

Au(1)-P(1)	2.267(1)	Au(1)-P(2)	2.267(1)
P(1)-C(1)	1.669(3)	P(1)-C(15)	1.804(3)
P(2)-C(14)	1.663(3)	P(2)-C(33)	1.807(3)
O(1)-C(7)	1.383(4)	O(1)-C(8)	1.396(4)
C(1)-C(2)	1.449(4)	C(2)-C(7)	1.403(5)
C(2)-C(3)	1.405(4)	C(3)-C(4)	1.394(5)
C(4)-C(5)	1.375(5)	C(5)-C(6)	1.390(4)
C(6)-C(7)	1.395(4)	C(6)-C(9)	1.451(5)
C(8)-C(13)	1.388(5)	C(8)-C(9)	1.397(4)
C(9)-C(10)	1.386(5)	C(10)-C(11)	1.388(5)
C(11)-C(12)	1.379(5)	C(12)-C(13)	1.421(5)
C(13)-C(14)	1.443(4)	C(15)-C(20)	1.431(4)
C(15)-C(16)	1.433(5)	C(16)-C(17)	1.393(4)
C(16)-C(21)	1.550(4)	C(17)-C(18)	1.388(4)
C(18)-C(19)	1.371(5)	C(18)-C(25)	1.542(5)
C(19)-C(20)	1.394(4)	C(20)-C(29)	1.555(5)
C(21)-C(24)	1.510(6)	C(21)-C(22)	1.540(6)
C(21)-C(23)	1.543(5)	C(25)-C(27)	1.522(6)
C(25)-C(28)	1.530(5)	C(25)-C(26)	1.532(5)
C(29)-C(32)	1.525(5)	C(29)-C(31)	1.536(5)
C(29)-C(30)	1.545(5)	C(33)-C(38)	1.410(4)
C(33)-C(34)	1.427(4)	C(34)-C(35)	1.394(5)
C(34)-C(39)	1.545(4)	C(35)-C(36)	1.397(4)
C(36)-C(37)	1.389(5)	C(36)-C(43)	1.530(5)
C(37)-C(38)	1.382(5)	C(38)-C(47)	1.554(5)
C(39)-C(40)	1.518(5)	C(39)-C(41)	1.540(5)
C(39)-C(42)	1.544(5)	C(43)-C(44)	1.508(6)
C(43)-C(45)	1.527(6)	C(43)-C(46)	1.553(6)
C(47)-C(50)	1.519(6)	C(47)-C(48)	1.529(5)
C(47)-C(49)	1.536(5)	C(51)-C(52)	1.433(8)
C(52)-O(2)	1.376(6)	O(2)-C(53)	1.396(7)
C(53)-C(54)	1.404(8)	B(1)-F(4)	1.366(5)
B(1)-F(1)	1.374(5)	B(1)-F(3)	1.393(5)
B(1)-F(2)	1.395(5)		

P(1)-Au(1)-P(2)	167.56(3)	C(1)-P(1)-C(15)	112.3(2)
C(1)-P(1)-Au(1)	121.8(1)	C(15)-P(1)-Au(1)	125.9(1)
C(14)-P(2)-C(33)	104.7(2)	C(14)-P(2)-Au(1)	120.3(1)
C(33)-P(2)-Au(1)	135.1(1)	C(7)-O(1)-C(8)	106.4(2)
C(2)-C(1)-P(1)	133.0(3)	C(7)-C(2)-C(3)	114.0(3)
C(7)-C(2)-C(1)	128.9(3)	C(3)-C(2)-C(1)	117.1(3)
C(4)-C(3)-C(2)	122.6(3)	C(5)-C(4)-C(3)	121.7(3)
C(4)-C(5)-C(6)	117.7(3)	C(5)-C(6)-C(7)	120.1(3)
C(5)-C(6)-C(9)	133.8(3)	C(7)-C(6)-C(9)	106.0(3)
O(1)-C(7)-C(6)	111.0(3)	O(1)-C(7)-C(2)	125.2(3)
C(6)-C(7)-C(2)	123.8(3)	C(13)-C(8)-O(1)	125.0(3)
C(13)-C(8)-C(9)	124.7(3)	O(1)-C(8)-C(9)	110.4(3)
C(10)-C(9)-C(8)	119.4(3)	C(10)-C(9)-C(6)	134.4(3)
C(8)-C(9)-C(6)	106.2(3)	C(9)-C(10)-C(11)	118.2(3)
C(12)-C(11)-C(10)	121.1(3)	C(11)-C(12)-C(13)	122.9(3)
C(8)-C(13)-C(12)	113.5(3)	C(8)-C(13)-C(14)	129.1(3)
C(12)-C(13)-C(14)	117.2(3)	C(13)-C(14)-P(2)	134.3(3)
C(20)-C(15)-C(16)	120.5(3)	C(20)-C(15)-P(1)	120.1(2)
C(16)-C(15)-P(1)	119.2(2)	C(17)-C(16)-C(15)	117.0(3)
C(17)-C(16)-C(21)	116.2(3)	C(15)-C(16)-C(21)	126.7(3)
C(18)-C(17)-C(16)	123.6(3)	C(19)-C(18)-C(17)	117.7(3)
C(19)-C(18)-C(25)	123.0(3)	C(17)-C(18)-C(25)	119.2(3)
C(18)-C(19)-C(20)	123.8(3)	C(19)-C(20)-C(15)	117.2(3)
C(19)-C(20)-C(29)	117.3(3)	C(15)-C(20)-C(29)	125.4(3)
C(24)-C(21)-C(22)	110.1(4)	C(24)-C(21)-C(23)	106.9(4)
C(22)-C(21)-C(23)	104.2(3)	C(24)-C(21)-C(16)	110.0(3)
C(22)-C(21)-C(16)	114.1(3)	C(23)-C(21)-C(16)	111.1(3)
C(27)-C(25)-C(28)	108.0(3)	C(27)-C(25)-C(26)	109.5(4)
C(28)-C(25)-C(26)	109.1(3)	C(27)-C(25)-C(18)	110.8(3)
C(28)-C(25)-C(18)	112.1(3)	C(26)-C(25)-C(18)	107.4(3)
C(32)-C(29)-C(31)	111.1(3)	C(32)-C(29)-C(30)	105.9(3)

C(31)-C(29)-C(30)	105.1(3)	C(32)-C(29)-C(20)	109.7(3)
C(31)-C(29)-C(20)	113.1(3)	C(30)-C(29)-C(20)	111.7(3)
C(38)-C(33)-C(34)	121.0(3)	C(38)-C(33)-P(2)	116.8(2)
C(34)-C(33)-P(2)	120.0(2)	C(35)-C(34)-C(33)	116.8(3)
C(35)-C(34)-C(39)	119.6(3)	C(33)-C(34)-C(39)	123.6(3)
C(34)-C(35)-C(36)	122.8(3)	C(37)-C(36)-C(35)	117.1(3)
C(37)-C(36)-C(43)	119.8(3)	C(35)-C(36)-C(43)	123.0(3)
C(38)-C(37)-C(36)	123.4(3)	C(37)-C(38)-C(33)	117.2(3)
C(37)-C(38)-C(47)	116.8(3)	C(33)-C(38)-C(47)	126.0(3)
C(40)-C(39)-C(41)	109.8(3)	C(40)-C(39)-C(42)	106.4(3)
C(41)-C(39)-C(42)	106.3(3)	C(40)-C(39)-C(34)	110.3(3)
C(41)-C(39)-C(34)	112.2(3)	C(42)-C(39)-C(34)	111.7(3)
C(44)-C(43)-C(45)	108.2(4)	C(44)-C(43)-C(36)	112.0(3)
C(45)-C(43)-C(36)	109.2(3)	C(44)-C(43)-C(46)	110.3(5)
C(45)-C(43)-C(46)	108.2(3)	C(36)-C(43)-C(46)	108.9(4)
C(50)-C(47)-C(48)	108.6(4)	C(50)-C(47)-C(49)	106.0(4)
C(48)-C(47)-C(49)	107.4(3)	C(50)-C(47)-C(38)	114.5(3)
C(48)-C(47)-C(38)	111.4(3)	C(49)-C(47)-C(38)	108.6(3)
O(2)-C(52)-C(51)	112.3(5)	C(52)-O(2)-C(53)	116.8(5)
O(2)-C(53)-C(54)	113.1(6)	F(4)-B(1)-F(1)	113.2(5)
F(4)-B(1)-F(3)	108.3(3)	F(1)-B(1)-F(3)	108.9(3)
F(4)-B(1)-F(2)	108.3(3)	F(1)-B(1)-F(2)	109.2(3)
F(3)-B(1)-F(2)	108.8(4)		

Table 9. Anisotropic displacement parameters (A^2 x 10^3) for **4**

atom	U11	U22	U33	U23	U13	U12
Au(1)	28(1)	26(1)	35(1)	4(1)	-5(1)	-5(1)
P(1)	29(1)	23(1)	31(1)	3(1)	-4(1)	-4(1)
P(2)	26(1)	26(1)	33(1)	2(1)	-1(1)	-6(1)
O(1)	28(1)	26(1)	32(1)	4(1)	-4(1)	-6(1)
C(1)	34(2)	27(2)	31(2)	2(1)	-1(1)	-3(1)
C(2)	24(1)	26(2)	32(2)	0(1)	0(1)	-4(1)
C(3)	27(2)	32(2)	43(2)	-6(2)	-3(1)	-6(2)
C(4)	27(2)	39(2)	41(2)	-7(2)	-8(1)	-7(2)
C(5)	28(2)	41(2)	32(2)	-1(2)	-5(1)	-1(2)
C(6)	25(1)	31(2)	26(1)	0(1)	-1(1)	1(1)
C(7)	22(1)	27(2)	31(2)	-3(1)	-1(1)	-4(1)
C(8)	27(2)	28(2)	29(2)	6(1)	1(1)	1(1)
C(9)	25(2)	37(2)	27(2)	5(1)	1(1)	2(1)
C(10)	26(2)	43(2)	32(2)	9(2)	0(1)	1(2)
C(11)	32(2)	38(2)	38(2)	16(2)	1(1)	1(2)
C(12)	33(2)	31(2)	45(2)	14(2)	2(1)	-1(2)
C(13)	26(2)	32(2)	31(2)	5(1)	2(1)	-3(1)
C(14)	31(2)	29(2)	33(1)	3(1)	0(1)	-6(2)
C(15)	27(2)	25(2)	28(1)	4(1)	-3(1)	-4(1)
C(16)	29(2)	31(2)	29(1)	3(1)	-6(1)	-4(1)
C(17)	32(2)	26(2)	37(2)	2(1)	-3(1)	3(1)
C(18)	25(1)	35(2)	32(2)	8(1)	-4(1)	-2(1)
C(19)	27(2)	37(2)	27(1)	3(1)	0(1)	-1(1)
C(20)	24(2)	34(2)	31(2)	-2(1)	-1(1)	-8(1)
C(21)	54(2)	35(2)	30(2)	-1(2)	0(2)	10(2)
C(22)	90(3)	62(3)	38(2)	11(2)	25(2)	15(3)
C(23)	101(4)	85(4)	34(2)	14(2)	21(2)	58(3)
C(24)	83(4)	90(4)	57(3)	-39(3)	-18(3)	-6(3)
C(25)	39(2)	39(2)	34(2)	13(2)	-2(1)	3(2)
C(26)	38(2)	86(4)	56(2)	31(2)	-11(2)	7(2)
C(27)	78(3)	38(3)	52(2)	18(2)	-1(2)	11(2)
C(28)	56(2)	60(3)	40(2)	23(2)	0(2)	5(2)
C(29)	36(2)	34(2)	33(2)	-2(2)	5(1)	-2(2)
C(30)	62(2)	59(3)	35(2)	3(2)	10(2)	11(2)
C(31)	40(2)	56(3)	52(2)	-6(2)	4(2)	18(2)
C(32)	65(3)	43(2)	47(2)	-14(2)	15(2)	-9(2)
C(33)	26(1)	24(2)	28(2)	1(1)	-2(1)	-2(1)
C(34)	28(2)	24(2)	30(2)	1(1)	2(1)	-2(1)
C(35)	41(2)	29(2)	31(2)	-2(1)	-4(1)	-5(2)
C(36)	41(2)	30(2)	36(2)	7(2)	-8(1)	-12(2)
C(37)	32(2)	39(2)	34(2)	6(2)	0(1)	-10(2)
C(38)	29(2)	32(2)	28(2)	3(1)	-2(1)	-2(1)
C(39)	33(2)	31(2)	29(2)	1(1)	5(1)	-6(2)
C(40)	38(2)	38(2)	37(2)	5(2)	-1(2)	-2(2)
C(41)	38(2)	53(3)	38(2)	3(2)	12(2)	3(2)
C(42)	61(2)	50(3)	33(2)	-2(2)	5(2)	-16(2)
C(43)	63(2)	38(2)	46(2)	11(2)	-11(2)	-26(2)
C(44)	252(9)	58(4)	52(3)	1(3)	-16(4)	-91(5)
C(45)	56(2)	31(2)	64(3)	5(2)	-1(2)	-6(2)
C(46)	52(3)	56(3)	129(4)	45(3)	-24(3)	-27(3)
C(47)	36(2)	44(2)	28(2)	-2(2)	0(1)	-5(2)
C(48)	55(2)	101(4)	34(2)	-9(2)	-9(2)	17(3)
C(49)	42(2)	87(4)	44(2)	-16(2)	10(2)	0(2)
C(50)	105(4)	45(3)	60(3)	-16(2)	36(3)	-15(3)
C(51)	113(5)	132(6)	60(3)	-12(3)	23(3)	47(5)
C(52)	202(8)	104(5)	78(4)	-39(4)	38(5)	-37(6)
O(2)	115(3)	65(2)	50(2)	-8(2)	14(2)	11(2)
C(53)	320(10)	102(6)	73(4)	-26(4)	89(6)	-90(7)
C(54)	340(10)	108(6)	69(4)	-32(4)	92(6)	-87(7)
B(1)	78(3)	43(3)	39(2)	-9(2)	-17(2)	27(3)
F(1)	76(2)	64(2)	85(2)	-30(2)	-37(2)	17(2)
F(2)	76(2)	49(1)	57(1)	-16(1)	-31(1)	32(1)
F(3)	114(2)	73(2)	40(1)	-13(1)	-5(2)	35(2)
F(4)	154(3)	47(2)	57(2)	-4(1)	13(2)	20(2)

The anisotropic displacement factor exponent takes the form 2 pi^2

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[h^2a*^2U(11) +...+ 2hka*b*U(12)]
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Table 10. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**

atom	x	y	z	U(eq)
H(1)	-2289	6725	3957	37
H(3)	-3752	6676	3413	41
H(4)	-4952	7201	2822	43
H(5)	-4683	8476	2518	40
H(10)	-3854	10069	2350	40
H(11)	-2896.0002	11284	2416	44
H(12)	-1314	11420	2913	44
H(14)	74	10958	3418	37
H(17)	1154	5008	4517	38
H(19)	-52	6161	5685	36
H(22A)	402	6973	3425	95
H(22B)	1447	6473	3204	95
H(22C)	1592	6924	3716	95
H(23A)	2303	5484	3860	110
H(23B)	1724	5191	3361	110
H(23C)	1379	4783	3868	110
H(24A)	-700	5096	3704	115
H(24B)	-224.0000	5409	3190	115
H(24C)	-1028	5965	3517	115
H(26A)	2611	5490	5590	90
H(26B)	2740	4869	5152	90
H(26C)	2785	4569	5707	90
H(27A)	1140	3978	4935	84
H(27B)	18	3937	5272	84
H(27C)	1218	3609	5473	84
H(28A)	1010	4432	6193	78
H(28B)	-161	4817	6000	78
H(28C)	894	5373	6150	78
H(30A)	-413	7173	6032	78
H(30B)	-1635	6789	5909	78
H(30C)	-1542	7712	6032	78
H(31A)	-2585	7975	5367	74
H(31B)	-2606	7154	5074	74
H(31C)	-2103	7934	4819	74
H(32A)	-530	8598	5502	78
H(32B)	-100	8341	4969	78
H(32C)	562	8029	5445	78
H(35)	2828	11835	4632	41
H(37)	3504	11617	3198	42
H(40A)	1823	9472	5211	56
H(40B)	2937	9676	4892	56
H(40C)	1807	9343	4631	56
H(41A)	13	10194	4609	64
H(41B)	69	11077	4820	64
H(41C)	107	10338	5187	64
H(42A)	1869	10746	5572	72
H(42B)	1806	11538	5252	72
H(42C)	2955	11019	5255	72
H(44A)	2861	13206	4475	181
H(44B)	4045	13642	4349	181
H(44C)	4057	12798	4615	181
H(45A)	2219	13297	3644	75
H(45B)	2977	12958	3203	75
H(45C)	3371	13742	3484	75
H(46A)	5278	13190	3673	119
H(46B)	4942	12417	3366	119
H(46C)	5392	12333	3917	119
H(48A)	2175	10285	2260	95
H(48B)	2084	11116	2538	95
H(48C)	1158	10437	2643	95
H(49A)	4485	10115	3077	86
H(49B)	4146	10849	2737	86
H(49C)	4097	9968	2523	86

H(50A)	1665	9255	3084	105
H(50B)	2913	9138	3319	105
H(50C)	2742	9065	2739	105
H(51A)	-978	7709	2349	153
H(51B)	-455	8406	2676	153
H(51C)	204	7577	2636	153
H(52A)	-30	8732	1917	154
H(52B)	1139	8406	2149	154
H(53A)	1851	8007	1342	199
H(53B)	723	8433	1136	199
H(54A)	712	6852	1015	260
H(54B)	1723	7296	729	260
H(54C)	414	7539	632	260

X-Ray structural data for 5.

Table 11. Crystal data for **5**

Compound	**5**
Molecular formula	$C_{50}H_{66}AgO_2P_2,BF_4,1/2CH_2Cl_2$
Molecular weight	1040.57
Crystal habit	colorless block
Crystal dimensions(mm)	0.24x0.24x0.16
Crystal system	monoclinic
Space group	C2/c
a(Å)	35.058(3)
b(Å)	11.0840(10)
c(Å)	30.013(3)
α(°)	90.00
β(°)	116.700(2)
γ(°)	90.00
V(Å^3)	10419.0(17)
Z	8
d(g-cm^{-3})	1.327
F(000)	4336
μ(cm^{-1})	0.602
Absorption corrections	multi-scan ; 0.8690 min, 0.9098 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	27.48
HKL ranges	-30 44 ; -13 14 ; -38 37
Reflections measured	17591
Unique data	9900
Rint	0.0322
Reflections used	7576
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	559
Reflections / parameter	13
wR2	0.2282
R1	0.0724
Weights a, b	0.1431 ; 17.644
GoF	1.086
difference peak / hole (e Å^{-3})	1.645(0.101) / -1.209(0.101)

Note: The unit cell contains two disordered CH2Cl2 molecules; one is located near a symmetry center, the second near a twofold axis.Since they could not be resolved with the data at hand, they were accounted for using the Platon SQUEEZE function. We were unable to determine wether the large thermal displacements observed for the BF4 anion are due to disorder or must be attributed to libration.

Table 12. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**

atom	x	y	z	U(eq)
Ag(1)	2486(1)	1010(1)	6287(1)	49(1)
P(1)	3212(1)	455(1)	6539(1)	45(1)
P(2)	1754(1)	576(1)	5725(1)	46(1)
O(1)	2496(1)	-410(3)	5405(1)	48(1)
O(2)	2436(2)	2104(4)	6916(1)	74(1)
C(1)	2852(2)	-701(4)	5341(2)	52(1)
C(2)	3279(2)	-619(4)	5710(2)	52(1)
C(3)	3586(2)	-976(5)	5554(2)	66(2)
C(4)	3462(3)	-1380(5)	5055(2)	77(2)
C(5)	3050(2)	-1405(5)	4712(2)	69(2)
C(6)	2741(2)	-1078(4)	4854(2)	60(2)
C(7)	2277(2)	-1046(4)	4596(2)	61(2)
C(8)	1965(3)	-1326(5)	4110(2)	79(2)
C(9)	1553(3)	-1214(6)	3996(2)	77(2)
C(10)	1424(2)	-805(5)	4349(2)	67(2)
C(11)	1718(2)	-497(4)	4840(2)	52(1)
C(12)	2146(2)	-631(4)	4950(2)	52(1)
C(13)	3444(2)	-226(4)	6227(2)	53(1)
C(14)	1538(2)	-90(4)	5162(1)	48(1)
C(15)	3662(2)	729(4)	7147(2)	46(1)
C(16)	3911(2)	1793(5)	7216(2)	55(1)
C(17)	4294(2)	1854(6)	7633(2)	66(1)
C(18)	4449(2)	977(6)	7987(2)	70(2)
C(19)	4190(2)	-32(5)	7929(2)	58(1)
C(20)	3792(1)	-173(4)	7524(2)	46(1)
C(21)	3767(2)	2914(5)	6871(2)	66(1)
C(22)	3330(2)	3369(5)	6804(2)	66(1)
C(23)	3765(3)	2681(7)	6362(3)	87(2)
C(24)	4075(3)	4014(6)	7114(4)	94(2)
C(25)	3530(2)	-1313(4)	7519(2)	49(1)
C(26)	3639(2)	-1715(7)	8045(2)	86(2)
C(27)	3049(2)	-1093(5)	7267(2)	58(1)
C(28)	3625(2)	-2352(6)	7244(2)	75(2)
C(29)	4888(2)	1062(8)	8447(3)	96(3)
C(30)	5073(3)	2340(10)	8484(4)	144(4)
C(31)	5185(3)	230(10)	8396(5)	185(7)
C(32)	4812(3)	990(10)	8900(3)	149(5)
C(33)	1285(2)	840(4)	5834(2)	47(1)
C(34)	1150(1)	-65(4)	6065(1)	45(1)
C(35)	749(2)	51(5)	6040(2)	50(1)
C(36)	477(2)	1036(5)	5809(2)	56(1)
C(37)	636(2)	1937(5)	5635(2)	59(1)
C(38)	1033(2)	1905(4)	5639(2)	51(1)
C(39)	1412(2)	-1194(4)	6340(2)	47(1)
C(40)	1328(2)	-2212(5)	5959(2)	71(2)
C(41)	1899(2)	-977(5)	6616(3)	79(2)
C(42)	1278(2)	-1636(8)	6732(2)	93(2)
C(43)	32(2)	1070(6)	5793(2)	73(2)
C(44)	87(3)	1110(10)	6326(3)	106(3)
C(45)	-211(2)	-114(8)	5551(3)	92(2)
C(46)	-237(3)	2080(10)	5470(5)	145(5)
C(47)	1174(2)	3034(5)	5445(2)	61(1)
C(48)	907(2)	4155(6)	5428(3)	82(2)
C(49)	1115(2)	2827(6)	4911(2)	82(2)
C(50)	1637(2)	3405(5)	5789(2)	65(1)
B(1)	2544(3)	671(6)	8111(2)	64(2)
F(1)	2863(4)	989(7)	8027(5)	269(7)
F(2)	2552(2)	-518(4)	8181(2)	135(2)
F(3)	2531(2)	1382(4)	8470(1)	105(1)
F(4)	2199(3)	846(7)	7676(2)	218(5)

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

Table 13. Bond lengths (A) and angles (deg) for **5**

Ag(1)-O(2)	2.316(3)	Ag(1)-P(1)	2.388(1)
Ag(1)-P(2)	2.403(1)	P(1)-C(13)	1.672(5)
P(1)-C(15)	1.825(5)	P(2)-C(14)	1.681(4)
P(2)-C(33)	1.840(5)	O(1)-C(1)	1.383(6)
O(1)-C(12)	1.387(6)	C(1)-C(6)	1.398(6)
C(1)-C(2)	1.410(8)	C(2)-C(3)	1.409(7)
C(2)-C(13)	1.456(6)	C(3)-C(4)	1.432(8)
C(4)-C(5)	1.35(1)	C(5)-C(6)	1.378(8)
C(6)-C(7)	1.46(1)	C(7)-C(8)	1.409(9)
C(7)-C(12)	1.411(6)	C(8)-C(9)	1.33(1)
C(9)-C(10)	1.402(9)	C(10)-C(11)	1.409(7)
C(11)-C(12)	1.393(8)	C(11)-C(14)	1.441(7)
C(15)-C(20)	1.423(7)	C(15)-C(16)	1.425(7)
C(16)-C(17)	1.366(8)	C(16)-C(21)	1.549(8)
C(17)-C(18)	1.361(9)	C(18)-C(19)	1.402(8)
C(18)-C(29)	1.540(8)	C(19)-C(20)	1.385(6)
C(20)-C(25)	1.560(7)	C(21)-C(22)	1.537(9)
C(21)-C(23)	1.547(8)	C(21)-C(24)	1.572(9)
C(25)-C(26)	1.515(8)	C(25)-C(27)	1.527(7)
C(25)-C(28)	1.540(8)	C(29)-C(31)	1.45(1)
C(29)-C(32)	1.50(1)	C(29)-C(30)	1.54(1)
C(33)-C(34)	1.414(7)	C(33)-C(38)	1.433(6)
C(34)-C(35)	1.381(7)	C(34)-C(39)	1.552(6)
C(35)-C(36)	1.410(7)	C(36)-C(37)	1.354(8)
C(36)-C(43)	1.543(9)	C(37)-C(38)	1.387(8)
C(38)-C(47)	1.552(8)	C(39)-C(42)	1.529(7)
C(39)-C(40)	1.538(7)	C(39)-C(41)	1.545(8)
C(43)-C(46)	1.50(1)	C(43)-C(44)	1.52(1)
C(43)-C(45)	1.55(1)	C(47)-C(50)	1.537(7)
C(47)-C(49)	1.538(8)	C(47)-C(48)	1.544(8)
B(1)-F(1)	1.30(1)	B(1)-F(2)	1.332(8)
B(1)-F(4)	1.34(1)	B(1)-F(3)	1.351(7)

O(2)-Ag(1)-P(1)	109.8(1)	O(2)-Ag(1)-P(2)	103.3(1)
P(1)-Ag(1)-P(2)	145.14(4)	C(13)-P(1)-C(15)	102.5(2)
C(13)-P(1)-Ag(1)	131.1(2)	C(15)-P(1)-Ag(1)	126.4(2)
C(14)-P(2)-C(33)	102.4(2)	C(14)-P(2)-Ag(1)	130.6(2)
C(33)-P(2)-Ag(1)	126.9(1)	C(1)-O(1)-C(12)	106.0(3)
O(1)-C(1)-C(6)	111.9(5)	O(1)-C(1)-C(2)	125.6(4)
C(6)-C(1)-C(2)	122.5(5)	C(3)-C(2)-C(1)	114.9(5)
C(3)-C(2)-C(13)	116.1(5)	C(1)-C(2)-C(13)	129.0(4)
C(2)-C(3)-C(4)	121.2(7)	C(5)-C(4)-C(3)	121.5(6)
C(4)-C(5)-C(6)	118.7(5)	C(5)-C(6)-C(1)	121.1(6)
C(5)-C(6)-C(7)	133.4(5)	C(1)-C(6)-C(7)	105.5(5)
C(8)-C(7)-C(12)	119.2(7)	C(8)-C(7)-C(6)	135.0(5)
C(12)-C(7)-C(6)	105.8(5)	C(9)-C(8)-C(7)	119.6(5)
C(8)-C(9)-C(10)	121.0(6)	C(9)-C(10)-C(11)	122.6(7)
C(12)-C(11)-C(10)	115.1(5)	C(12)-C(11)-C(14)	128.6(4)
C(10)-C(11)-C(14)	116.3(5)	O(1)-C(12)-C(11)	126.6(4)
O(1)-C(12)-C(7)	110.8(5)	C(11)-C(12)-C(7)	122.5(5)
C(2)-C(13)-P(1)	132.1(4)	C(11)-C(14)-P(2)	132.6(4)
C(20)-C(15)-C(16)	120.6(4)	C(20)-C(15)-P(1)	120.2(3)
C(16)-C(15)-P(1)	118.7(4)	C(17)-C(16)-C(15)	117.4(5)
C(17)-C(16)-C(21)	117.5(5)	C(15)-C(16)-C(21)	125.0(5)
C(18)-C(17)-C(16)	124.3(5)	C(17)-C(18)-C(19)	117.6(5)
C(17)-C(18)-C(29)	122.9(6)	C(19)-C(18)-C(29)	119.5(6)
C(20)-C(19)-C(18)	122.7(5)	C(19)-C(20)-C(15)	117.0(5)
C(19)-C(20)-C(25)	117.2(4)	C(15)-C(20)-C(25)	125.8(4)
C(22)-C(21)-C(23)	111.2(5)	C(22)-C(21)-C(16)	110.8(4)
C(23)-C(21)-C(16)	112.5(5)	C(22)-C(21)-C(24)	104.0(5)
C(23)-C(21)-C(24)	106.6(6)	C(16)-C(21)-C(24)	111.3(6)
C(26)-C(25)-C(27)	105.6(5)	C(26)-C(25)-C(28)	109.0(5)
C(27)-C(25)-C(28)	108.2(4)	C(26)-C(25)-C(20)	110.9(4)
C(27)-C(25)-C(20)	113.0(4)	C(28)-C(25)-C(20)	110.0(4)
C(31)-C(29)-C(32)	119(1)	C(31)-C(29)-C(18)	110.1(7)
C(32)-C(29)-C(18)	107.2(6)	C(31)-C(29)-C(30)	107(1)
C(32)-C(29)-C(30)	102.9(8)	C(18)-C(29)-C(30)	109.8(7)

C(34)-C(33)-C(38)	120.4(5)	C(34)-C(33)-P(2)	119.7(3)
C(38)-C(33)-P(2)	119.6(4)	C(35)-C(34)-C(33)	117.6(4)
C(35)-C(34)-C(39)	116.6(4)	C(33)-C(34)-C(39)	125.8(4)
C(34)-C(35)-C(36)	123.0(5)	C(37)-C(36)-C(35)	117.2(5)
C(37)-C(36)-C(43)	123.7(5)	C(35)-C(36)-C(43)	119.0(5)
C(36)-C(37)-C(38)	124.2(5)	C(37)-C(38)-C(33)	117.1(5)
C(37)-C(38)-C(47)	117.7(4)	C(33)-C(38)-C(47)	125.2(5)
C(42)-C(39)-C(40)	108.4(5)	C(42)-C(39)-C(41)	106.5(5)
C(40)-C(39)-C(41)	108.0(5)	C(42)-C(39)-C(34)	110.8(4)
C(40)-C(39)-C(34)	109.0(4)	C(41)-C(39)-C(34)	114.0(4)
C(46)-C(43)-C(44)	113.6(8)	C(46)-C(43)-C(36)	111.8(7)
C(44)-C(43)-C(36)	108.6(5)	C(46)-C(43)-C(45)	105.9(7)
C(44)-C(43)-C(45)	107.6(7)	C(36)-C(43)-C(45)	109.1(5)
C(50)-C(47)-C(49)	110.3(5)	C(50)-C(47)-C(48)	104.4(5)
C(49)-C(47)-C(48)	107.0(5)	C(50)-C(47)-C(38)	112.4(4)
C(49)-C(47)-C(38)	110.8(4)	C(48)-C(47)-C(38)	111.7(5)
F(1)-B(1)-F(2)	110.0(8)	F(1)-B(1)-F(4)	104(1)
F(2)-B(1)-F(4)	104.0(7)	F(1)-B(1)-F(3)	109.6(6)
F(2)-B(1)-F(3)	117.2(6)	F(4)-B(1)-F(3)	110.7(6)

Table 14. Anisotropic displacement parameters (A^2 x 10^3) for **5**

atom	U11	U22	U33	U23	U13	U12
Ag(1)	51(1)	52(1)	40(1)	-8(1)	17(1)	4(1)
P(1)	51(1)	46(1)	44(1)	-4(1)	26(1)	0(1)
P(2)	54(1)	47(1)	32(1)	-5(1)	14(1)	0(1)
O(1)	84(2)	34(2)	38(1)	1(1)	36(2)	0(1)
O(2)	120(4)	56(2)	62(2)	-10(2)	54(2)	5(2)
C(1)	97(4)	30(2)	47(2)	6(2)	49(3)	10(2)
C(2)	87(4)	36(2)	52(2)	10(2)	47(3)	13(2)
C(3)	106(5)	48(3)	67(3)	19(2)	61(3)	26(3)
C(4)	140(7)	54(3)	77(4)	17(3)	84(5)	31(4)
C(5)	134(6)	44(3)	51(3)	12(2)	62(3)	24(3)
C(6)	123(5)	29(2)	45(2)	5(2)	51(3)	7(2)
C(7)	124(6)	30(2)	49(2)	-4(2)	56(3)	-11(2)
C(8)	169(8)	38(3)	48(3)	-4(2)	63(4)	-17(4)
C(9)	123(6)	71(4)	40(2)	-15(2)	38(3)	-38(4)
C(10)	111(5)	51(3)	39(2)	-10(2)	33(3)	-25(3)
C(11)	83(4)	41(2)	36(2)	-2(2)	29(2)	-14(2)
C(12)	102(4)	29(2)	34(2)	-5(2)	39(2)	-12(2)
C(13)	75(3)	43(2)	49(2)	5(2)	35(2)	13(2)
C(14)	62(3)	43(2)	34(2)	0(2)	17(2)	-10(2)
C(15)	43(2)	50(2)	50(2)	-9(2)	25(2)	-7(2)
C(16)	57(3)	59(3)	66(3)	-14(2)	41(2)	-13(2)
C(17)	62(3)	72(4)	69(3)	-14(3)	34(3)	-27(3)
C(18)	50(3)	91(5)	63(3)	-19(3)	20(2)	-20(3)
C(19)	43(3)	64(3)	58(3)	-10(2)	15(2)	-2(2)
C(20)	38(2)	51(2)	50(2)	-9(2)	20(2)	0(2)
C(21)	82(4)	58(3)	75(3)	-2(3)	50(3)	-11(3)
C(22)	80(4)	49(3)	76(3)	-3(2)	42(3)	-10(3)
C(23)	119(6)	85(5)	92(4)	16(4)	77(4)	-3(4)
C(24)	89(5)	68(4)	129(7)	-7(4)	53(5)	-28(4)
C(25)	43(2)	48(2)	48(2)	-1(2)	13(2)	-1(2)
C(26)	75(4)	95(5)	65(3)	14(3)	12(3)	-28(4)
C(27)	39(3)	56(3)	75(3)	11(2)	23(2)	-2(2)
C(28)	83(4)	51(3)	84(4)	-15(3)	31(3)	3(3)
C(29)	55(4)	113(6)	88(5)	1(4)	5(3)	-36(4)
C(30)	98(6)	170(10)	115(7)	-38(7)	6(5)	-70(7)
C(31)	58(5)	200(10)	210(10)	-80(10)	-14(6)	42(7)
C(32)	100(7)	210(10)	75(5)	15(6)	-13(4)	-62(7)
C(33)	46(2)	51(2)	31(2)	-5(2)	7(2)	2(2)
C(34)	48(2)	45(2)	33(2)	-6(2)	11(2)	5(2)
C(35)	50(3)	50(3)	43(2)	-5(2)	14(2)	-2(2)
C(36)	44(3)	59(3)	49(2)	-10(2)	7(2)	3(2)
C(37)	51(3)	55(3)	49(2)	-3(2)	2(2)	6(2)
C(38)	50(3)	51(3)	32(2)	-3(2)	1(2)	6(2)
C(39)	49(3)	48(2)	44(2)	3(2)	21(2)	5(2)
C(40)	97(4)	49(3)	64(3)	-3(2)	34(3)	3(3)
C(41)	60(4)	58(3)	80(4)	21(3)	-4(3)	-2(3)
C(42)	101(5)	122(6)	73(4)	52(4)	55(4)	56(5)
C(43)	47(3)	86(4)	70(3)	-8(3)	14(2)	9(3)
C(44)	68(5)	148(9)	103(6)	-46(5)	40(4)	-2(4)
C(45)	55(4)	116(6)	88(4)	-15(4)	16(3)	-9(4)
C(46)	70(5)	150(10)	210(10)	73(8)	54(6)	57(6)
C(47)	63(3)	50(3)	46(2)	6(2)	3(2)	6(2)
C(48)	77(4)	58(4)	94(5)	9(3)	22(3)	16(3)
C(49)	116(5)	62(4)	44(3)	13(2)	15(3)	-3(3)
C(50)	61(3)	52(3)	65(3)	5(2)	12(2)	-1(2)
B(1)	93(5)	51(3)	53(3)	1(3)	39(3)	1(3)
F(1)	370(10)	186(7)	440(20)	-229(9)	360(10)	-198(8)
F(2)	160(5)	54(2)	145(4)	31(3)	28(4)	-6(3)
F(3)	159(4)	108(3)	68(2)	-17(2)	69(3)	-11(3)
F(4)	300(10)	171(6)	81(3)	-21(4)	-6(5)	143(7)

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

Table 15. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**

atom	x	y	z	U(eq)
H(3)	3880	-948	5784	79
H(4)	3676	-1636	4964	93
H(5)	2973	-1643	4378	82
H(8)	2048	-1593	3865	95
H(9)	1342	-1415	3669	93
H(10)	1128	-732	4254	81
H(13)	3739	-386	6423	63
H(14)	1240	-224.0000	5030	58
H(17)	4464	2554	7677	79
H(19)	4291	-644.9999	8176	69
H(22A)	3264	4138	6624	99
H(22B)	3338	3484	7131	99
H(22C)	3110	2773	6614	99
H(23A)	3534	2117	6167	131
H(23B)	4039	2336	6416	131
H(23C)	3718	3444	6179	131
H(24A)	3934	4759	6944	141
H(24B)	4338	3898	7081	141
H(24C)	4143	4069	7468	141
H(26A)	3586	-1052	8226	129
H(26B)	3941	-1945	8217	129
H(26C)	3462	-2410	8033	129
H(27A)	2904	-1761	7343	87
H(27B)	2945	-1040	6906	87
H(27C)	2986	-336	7390	87
H(28A)	3456	-3061	7238	113
H(28B)	3930	-2552.9998	7416	113
H(28C)	3551	-2103	6901	113
H(30A)	5316	2454	8813	216
H(30B)	4852	2942	8436	216
H(30C)	5169	2448	8226	216
H(31A)	5475	548	8575	278
H(31B)	5113	134	8042	278
H(31C)	5168	-555	8536	278
H(32A)	4534	617	8810	223
H(32B)	4816	1804	9029	223
H(32C)	5037	502	9156	223
H(35)	652	-561	6187	60
H(37)	464	2634	5503	71
H(40A)	1525	-2883	6120	106
H(40B)	1374	-1908	5680	106
H(40C)	1033	-2493	5834	106
H(41A)	2035	-1634	6854	119
H(41B)	1956	-208	6796	119
H(41C)	2015	-952	6373	119
H(42A)	983	-1923.9999	6566	139
H(42B)	1300	-970	6957	139
H(42C)	1465	-2296	6924	139
H(44A)	226	1873	6483	159
H(44B)	264	434	6515	159
H(44C)	-193	1065	6322	159
H(45A)	-473	-158	5590	138
H(45B)	-29	-809	5716	138
H(45C)	-283	-120	5195	138
H(46A)	-183	2168	5177	218
H(46B)	-165	2832	5661	218
H(46C)	-540	1894	5359	218
H(48A)	882	4211	5740	123
H(48B)	621	4084	5147	123
H(48C)	1047	4882	5388	123
H(49A)	1148	3595	4770	123
H(49B)	829	2500	4705	123
H(49C)	1331	2253	4918	123
H(50A)	1829	2733	5820	98

H(50B)	1663	3614	6118	98
H(50C)	1713	4106	5647	98

X-Ray structural data for 6.

Table 16. Crystal data for **6**

Compound	**6**
Molecular formula	$C_{52}H_{69}CuNOP_2$,2($CHCl_3$),BF_4
Molecular weight	1175.11
Crystal habit	lemon yellow plate
Crystal dimensions(mm)	0.22x0.22x0.08
Crystal system	triclinic
Space group	Pbar1
a(Å)	11.9310(10)
b(Å)	14.5270(10)
c(Å)	19.1690(10)
α(°)	107.9200(10)
β(°)	92.0300(10)
γ(°)	109.7100(10)
V(Å^3)	2939.9(4)
Z	2
d(g-cm^{-3})	1.327
F(000)	1224
μ(cm^{-1})	0.748
Absorption corrections	multi-scan ; 0.8527 min, 0.9426 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	23.81
HKL ranges	-13 13 ; -16 16 ; -21 21
Reflections measured	16842
Unique data	16843
Rint	0.0000
Reflections used	13870
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	651
Reflections / parameter	21
wR2	0.1806
R1	0.0628
Weights a, b	0.0746 ; 9.0853
GoF	1.069
difference peak / hole (e Å^{-3})	0.941(0.097) / -0.835(0.097)

Note: Crystals were found to be twinned by twofold rotation about de (0 1 0) reciprocal lattice direction; BASF=0.519. Disorder of the solvate molecules apparent in their large thermal displacement parameters could not be accounted for.

Table 17 Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6**

atom	x	y	z	U(eq)
Cu(1)	309(1)	1970(1)	3437(1)	29(1)
Cl(1)	-1372(2)	1977(2)	148(1)	121(1)
Cl(2)	-3222(2)	2833(1)	564(1)	113(1)
Cl(3)	-3856(1)	726(1)	-310(1)	73(1)
Cl(4)	-5189(2)	2672(1)	-1094(1)	90(1)
Cl(5)	-6949(2)	759(2)	-1102(1)	113(1)
Cl(6)	-6553(2)	1134(2)	-2463(1)	109(1)
P(1)	968(1)	2763(1)	4646(1)	26(1)
P(2)	-141(1)	2528(1)	2542(1)	25(1)
O(1)	-1646(2)	2038(2)	3751(1)	25(1)
N(1)	-66(4)	469(3)	3109(2)	38(1)
C(1)	-46(4)	2574(3)	5204(2)	30(1)
C(2)	-1353(4)	2069(3)	5040(2)	24(1)
C(3)	-2003(4)	1807(3)	5593(2)	31(1)
C(4)	-3255(4)	1339(3)	5480(2)	33(1)
C(5)	-3922(4)	1108(3)	4801(2)	31(1)
C(6)	-3323(4)	1352(3)	4244(2)	26(1)
C(7)	-2077(4)	1817(3)	4370(2)	23(1)
C(8)	-2664(4)	1717(3)	3232(2)	25(1)
C(9)	-3712(4)	1279(3)	3495(2)	25(1)
C(10)	-4831(4)	919(3)	3049(3)	34(1)
C(11)	-4840(4)	1020(3)	2360(3)	36(1)
C(12)	-3785(4)	1467(3)	2108(3)	36(1)
C(13)	-2638(4)	1813(3)	2528(2)	26(1)
C(14)	-1576(4)	2267(3)	2222(2)	27(1)
C(15)	-238(5)	-383(4)	2857(3)	50(1)
C(16)	-488(6)	-1510(4)	2498(5)	93(3)
C(17)	2376(4)	3412(3)	5307(2)	24(1)
C(18)	2924(4)	4514(3)	5561(2)	25(1)
C(19)	3589(4)	5001(3)	6268(2)	29(1)
C(20)	3778(4)	4474(3)	6722(2)	32(1)
C(21)	3404(4)	3399(3)	6402(2)	32(1)
C(22)	2737(4)	2843(3)	5693(2)	29(1)
C(23)	2837(4)	5177(3)	5083(2)	30(1)
C(24)	1649(4)	5374(3)	5108(3)	36(1)
C(25)	2990(4)	4677(3)	4281(2)	35(1)
C(26)	3863(4)	6250(3)	5369(3)	48(1)
C(27)	4436(4)	5016(4)	7522(2)	43(1)
C(28)	5695(4)	4975(5)	7541(3)	69(2)
C(29)	4530(5)	6154(4)	7818(3)	66(2)
C(30)	3742(5)	4479(4)	8031(3)	50(1)
C(31)	2511(4)	1665(3)	5363(3)	38(1)
C(32)	3539(7)	1459(5)	5672(4)	84(2)
C(33)	1390(8)	1018(6)	5550(10)	223(8)
C(34)	2570(10)	1338(6)	4540(3)	150(5)
C(35)	749(4)	3105(3)	1923(2)	26(1)
C(36)	1311(4)	2520(3)	1415(2)	27(1)
C(37)	1728(4)	2864(3)	842(2)	32(1)
C(38)	1628(4)	3741(3)	746(2)	31(1)
C(39)	1179(4)	4333(3)	1279(2)	30(1)
C(40)	755(4)	4066(3)	1891(2)	26(1)
C(41)	1491(4)	1536(3)	1475(2)	33(1)
C(42)	2182(4)	1773(4)	2232(3)	38(1)
C(43)	280(4)	617(3)	1299(3)	44(1)
C(44)	2266(5)	1164(4)	911(3)	50(1)
C(45)	2080(4)	4072(4)	85(2)	41(1)
C(46)	1612(6)	3151(5)	-628(3)	81(2)
C(47)	1682(8)	4917(7)	-6(4)	106(3)
C(48)	3442(5)	4459(5)	212(3)	70(2)
C(49)	452(4)	4925(3)	2480(2)	34(1)
C(50)	-575(6)	5120(5)	2138(3)	78(2)
C(51)	1634(6)	5913(4)	2719(3)	69(2)
C(52)	150(6)	4758(4)	3204(3)	61(2)

C(53)	-2801(5)	1948(4)	-126(3)	55(2)
C(54)	-5873(5)	1343(4)	-1571(3)	52(1)
B(1)	-2357(6)	1504(5)	-2135(4)	49(2)
F(1)	-3423(4)	1497(3)	-1926(3)	110(2)
F(2)	-2354(5)	1379(4)	-2850(2)	115(2)
F(3)	-1482(3)	2414(3)	-1720(2)	95(1)
F(4)	-2164(4)	711(3)	-1991(3)	112(2)

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

Table 18 Bond lengths (A) and angles (deg) for **6**

Cu(1)-N(1)	1.958(4)	Cu(1)-P(1)	2.221(1)
Cu(1)-P(2)	2.230(1)	Cl(1)-C(53)	1.749(6)
Cl(2)-C(53)	1.758(6)	Cl(3)-C(53)	1.714(5)
Cl(4)-C(54)	1.740(5)	Cl(5)-C(54)	1.729(6)
Cl(6)-C(54)	1.758(6)	P(1)-C(1)	1.654(5)
P(1)-C(17)	1.834(4)	P(2)-C(14)	1.671(4)
P(2)-C(35)	1.827(4)	O(1)-C(8)	1.389(4)
O(1)-C(7)	1.393(4)	N(1)-C(15)	1.122(6)
C(1)-C(2)	1.456(6)	C(2)-C(7)	1.397(5)
C(2)-C(3)	1.406(6)	C(3)-C(4)	1.393(6)
C(4)-C(5)	1.385(6)	C(5)-C(6)	1.376(6)
C(6)-C(7)	1.386(6)	C(6)-C(9)	1.454(6)
C(8)-C(9)	1.389(6)	C(8)-C(13)	1.398(6)
C(9)-C(10)	1.399(6)	C(10)-C(11)	1.373(7)
C(11)-C(12)	1.387(7)	C(12)-C(13)	1.408(6)
C(13)-C(14)	1.453(6)	C(15)-C(16)	1.486(8)
C(17)-C(22)	1.417(6)	C(17)-C(18)	1.420(5)
C(18)-C(19)	1.386(6)	C(18)-C(23)	1.544(6)
C(19)-C(20)	1.382(6)	C(20)-C(21)	1.391(6)
C(20)-C(27)	1.531(6)	C(21)-C(22)	1.397(6)
C(22)-C(31)	1.553(6)	C(23)-C(25)	1.532(6)
C(23)-C(24)	1.537(6)	C(23)-C(26)	1.539(6)
C(27)-C(28)	1.523(7)	C(27)-C(30)	1.528(7)
C(27)-C(29)	1.535(7)	C(31)-C(33)	1.478(8)
C(31)-C(32)	1.500(7)	C(31)-C(34)	1.512(9)
C(35)-C(40)	1.414(6)	C(35)-C(36)	1.429(6)
C(36)-C(37)	1.381(6)	C(36)-C(41)	1.553(6)
C(37)-C(38)	1.384(6)	C(38)-C(39)	1.371(6)
C(38)-C(45)	1.542(6)	C(39)-C(40)	1.405(6)
C(40)-C(49)	1.558(6)	C(41)-C(42)	1.523(6)
C(41)-C(44)	1.537(7)	C(41)-C(43)	1.540(6)
C(45)-C(47)	1.510(8)	C(45)-C(48)	1.512(7)
C(45)-C(46)	1.512(7)	C(49)-C(52)	1.516(6)
C(49)-C(50)	1.519(7)	C(49)-C(51)	1.563(7)
B(1)-F(2)	1.325(7)	B(1)-F(1)	1.345(8)
B(1)-F(4)	1.351(7)	B(1)-F(3)	1.354(7)

N(1)-Cu(1)-P(1)	113.5(1)	N(1)-Cu(1)-P(2)	113.7(1)
P(1)-Cu(1)-P(2)	132.60(4)	C(1)-P(1)-C(17)	101.6(2)
C(1)-P(1)-Cu(1)	116.5(2)	C(17)-P(1)-Cu(1)	140.6(1)
C(14)-P(2)-C(35)	105.6(2)	C(14)-P(2)-Cu(1)	120.6(2)
C(35)-P(2)-Cu(1)	133.1(1)	C(8)-O(1)-C(7)	105.4(3)
C(15)-N(1)-Cu(1)	172.9(4)	C(2)-C(1)-P(1)	130.7(3)
C(7)-C(2)-C(3)	113.8(4)	C(7)-C(2)-C(1)	126.4(4)
C(3)-C(2)-C(1)	119.8(4)	C(4)-C(3)-C(2)	122.9(4)
C(5)-C(4)-C(3)	120.4(4)	C(6)-C(5)-C(4)	118.6(4)
C(5)-C(6)-C(7)	119.8(4)	C(5)-C(6)-C(9)	133.8(4)
C(7)-C(6)-C(9)	106.3(4)	C(6)-C(7)-O(1)	111.2(3)
C(6)-C(7)-C(2)	124.4(4)	O(1)-C(7)-C(2)	124.4(3)
O(1)-C(8)-C(9)	111.6(3)	O(1)-C(8)-C(13)	124.3(4)
C(9)-C(8)-C(13)	124.1(3)	C(8)-C(9)-C(10)	119.8(4)
C(8)-C(9)-C(6)	105.5(3)	C(10)-C(9)-C(6)	134.7(4)
C(11)-C(10)-C(9)	117.7(4)	C(10)-C(11)-C(12)	121.9(4)
C(11)-C(12)-C(13)	122.4(4)	C(8)-C(13)-C(12)	114.2(4)
C(8)-C(13)-C(14)	126.7(3)	C(12)-C(13)-C(14)	119.0(4)
C(13)-C(14)-P(2)	127.3(3)	N(1)-C(15)-C(16)	178.0(6)
C(22)-C(17)-C(18)	119.7(3)	C(22)-C(17)-P(1)	118.9(3)
C(18)-C(17)-P(1)	119.6(3)	C(19)-C(18)-C(17)	117.5(4)
C(19)-C(18)-C(23)	119.3(3)	C(17)-C(18)-C(23)	123.2(3)
C(20)-C(19)-C(18)	123.7(4)	C(19)-C(20)-C(21)	116.5(4)
C(19)-C(20)-C(27)	123.5(4)	C(21)-C(20)-C(27)	119.9(4)
C(20)-C(21)-C(22)	123.2(4)	C(21)-C(22)-C(17)	117.2(4)
C(21)-C(22)-C(31)	118.0(4)	C(17)-C(22)-C(31)	124.6(4)
C(25)-C(23)-C(24)	110.8(3)	C(25)-C(23)-C(26)	105.4(4)
C(24)-C(23)-C(26)	106.8(4)	C(25)-C(23)-C(18)	111.2(3)
C(24)-C(23)-C(18)	111.5(4)	C(26)-C(23)-C(18)	110.9(3)

C(28)-C(27)-C(30)	110.3(4)	C(28)-C(27)-C(20)	108.5(4)
C(30)-C(27)-C(20)	110.2(4)	C(28)-C(27)-C(29)	109.6(4)
C(30)-C(27)-C(29)	107.0(4)	C(20)-C(27)-C(29)	111.3(4)
C(33)-C(31)-C(32)	107.9(6)	C(33)-C(31)-C(34)	113.0(8)
C(32)-C(31)-C(34)	102.6(5)	C(33)-C(31)-C(22)	112.2(5)
C(32)-C(31)-C(22)	109.5(4)	C(34)-C(31)-C(22)	111.3(4)
C(40)-C(35)-C(36)	120.7(4)	C(40)-C(35)-P(2)	119.6(3)
C(36)-C(35)-P(2)	119.3(3)	C(37)-C(36)-C(35)	117.6(4)
C(37)-C(36)-C(41)	118.5(4)	C(35)-C(36)-C(41)	123.9(4)
C(36)-C(37)-C(38)	123.0(4)	C(39)-C(38)-C(37)	117.9(4)
C(39)-C(38)-C(45)	121.3(4)	C(37)-C(38)-C(45)	120.8(4)
C(38)-C(39)-C(40)	123.5(4)	C(39)-C(40)-C(35)	116.6(4)
C(39)-C(40)-C(49)	114.6(4)	C(35)-C(40)-C(49)	128.6(4)
C(42)-C(41)-C(44)	105.2(4)	C(42)-C(41)-C(43)	112.2(4)
C(44)-C(41)-C(43)	105.7(4)	C(42)-C(41)-C(36)	110.7(3)
C(44)-C(41)-C(36)	111.6(4)	C(43)-C(41)-C(36)	111.2(4)
C(47)-C(45)-C(48)	109.3(5)	C(47)-C(45)-C(46)	108.0(5)
C(48)-C(45)-C(46)	108.7(5)	C(47)-C(45)-C(38)	112.6(4)
C(48)-C(45)-C(38)	108.1(4)	C(46)-C(45)-C(38)	110.1(4)
C(52)-C(49)-C(50)	108.3(5)	C(52)-C(49)-C(40)	117.8(4)
C(50)-C(49)-C(40)	109.8(4)	C(52)-C(49)-C(51)	104.0(4)
C(50)-C(49)-C(51)	111.2(4)	C(40)-C(49)-C(51)	105.6(4)
Cl(3)-C(53)-Cl(1)	110.1(3)	Cl(3)-C(53)-Cl(2)	108.5(3)
Cl(1)-C(53)-Cl(2)	111.7(3)	Cl(5)-C(54)-Cl(4)	110.9(3)
Cl(5)-C(54)-Cl(6)	109.5(3)	Cl(4)-C(54)-Cl(6)	109.5(3)
F(2)-B(1)-F(1)	112.2(6)	F(2)-B(1)-F(4)	110.0(6)
F(1)-B(1)-F(4)	106.4(5)	F(2)-B(1)-F(3)	109.9(5)
F(1)-B(1)-F(3)	108.9(5)	F(4)-B(1)-F(3)	109.4(5)

Table 19. Anisotropic displacement parameters (A^2 x 10^3) for **6**

atom	U11	U22	U33	U23	U13	U12
Cu(1)	30(1)	33(1)	22(1)	11(1)	1(1)	8(1)
Cl(1)	43(1)	213(2)	51(1)	31(1)	-7(1)	-7(1)
Cl(2)	217(3)	68(1)	53(1)	8(1)	-5(1)	64(1)
Cl(3)	62(1)	54(1)	87(1)	16(1)	17(1)	6(1)
Cl(4)	91(1)	48(1)	104(1)	1(1)	-11(1)	17(1)
Cl(5)	125(2)	83(1)	151(2)	49(1)	82(2)	47(1)
Cl(6)	153(2)	108(2)	68(1)	-4(1)	-36(1)	85(1)
P(1)	25(1)	27(1)	23(1)	9(1)	0(1)	6(1)
P(2)	24(1)	32(1)	21(1)	11(1)	4(1)	9(1)
O(1)	19(2)	32(2)	22(2)	12(1)	5(1)	7(1)
N(1)	48(3)	29(2)	32(2)	8(2)	1(2)	9(2)
C(1)	34(3)	35(2)	14(2)	1(2)	-1(2)	12(2)
C(2)	29(3)	22(2)	22(2)	9(2)	5(2)	8(2)
C(3)	40(3)	31(2)	25(2)	8(2)	8(2)	15(2)
C(4)	39(3)	29(2)	35(3)	15(2)	18(2)	11(2)
C(5)	27(3)	26(2)	37(3)	13(2)	7(2)	5(2)
C(6)	23(2)	22(2)	33(2)	12(2)	6(2)	6(2)
C(7)	30(3)	20(2)	22(2)	10(2)	10(2)	13(2)
C(8)	19(2)	30(2)	22(2)	5(2)	-3(2)	10(2)
C(9)	17(2)	30(2)	27(2)	9(2)	2(2)	9(2)
C(10)	23(3)	34(3)	42(3)	8(2)	6(2)	9(2)
C(11)	27(3)	38(3)	40(3)	8(2)	-5(2)	11(2)
C(12)	31(3)	44(3)	32(3)	15(2)	4(2)	12(2)
C(13)	21(2)	27(2)	26(2)	7(2)	-1(2)	8(2)
C(14)	34(3)	31(2)	20(2)	11(2)	4(2)	13(2)
C(15)	45(3)	45(4)	53(3)	14(3)	5(3)	11(3)
C(16)	82(5)	27(3)	143(7)	-5(4)	4(5)	16(3)
C(17)	22(2)	25(2)	23(2)	6(2)	1(2)	7(2)
C(18)	23(2)	30(2)	24(2)	9(2)	5(2)	11(2)
C(19)	25(2)	27(2)	27(2)	6(2)	1(2)	3(2)
C(20)	18(2)	44(3)	28(2)	11(2)	5(2)	6(2)
C(21)	28(3)	41(3)	29(2)	18(2)	-1(2)	12(2)
C(22)	32(3)	32(2)	27(2)	12(2)	10(2)	14(2)
C(23)	30(3)	29(2)	33(2)	14(2)	2(2)	11(2)
C(24)	42(3)	32(2)	42(3)	17(2)	10(2)	21(2)
C(25)	43(3)	40(3)	35(3)	23(2)	14(2)	21(2)
C(26)	48(3)	29(3)	60(3)	22(2)	-3(3)	1(2)
C(27)	28(3)	59(3)	28(3)	10(2)	3(2)	4(2)
C(28)	34(4)	127(6)	30(3)	17(4)	-5(3)	19(4)
C(29)	67(4)	66(4)	30(3)	2(3)	-6(3)	-4(3)
C(30)	47(3)	73(4)	27(3)	17(2)	2(2)	18(3)
C(31)	39(3)	24(2)	53(3)	14(2)	0(2)	13(2)
C(32)	119(6)	73(4)	67(4)	-8(3)	-17(4)	75(4)
C(33)	119(7)	58(5)	550(30)	144(9)	200(10)	58(5)
C(34)	340(10)	89(5)	40(4)	-23(3)	-52(6)	154(8)
C(35)	24(2)	31(2)	18(2)	8(2)	1(2)	4(2)
C(36)	23(2)	32(2)	24(2)	7(2)	2(2)	8(2)
C(37)	27(3)	39(3)	25(2)	8(2)	7(2)	10(2)
C(38)	21(2)	46(3)	22(2)	16(2)	2(2)	3(2)
C(39)	27(3)	37(2)	27(2)	16(2)	3(2)	6(2)
C(40)	21(2)	34(2)	19(2)	7(2)	-1(2)	7(2)
C(41)	37(3)	29(2)	34(3)	8(2)	14(2)	13(2)
C(42)	31(3)	43(3)	48(3)	22(2)	10(2)	18(2)
C(43)	52(3)	27(3)	39(3)	3(2)	5(2)	4(2)
C(44)	57(4)	49(3)	53(3)	19(3)	20(3)	28(3)
C(45)	31(3)	71(3)	30(3)	32(2)	10(2)	15(2)
C(46)	72(4)	113(5)	23(3)	23(3)	5(3)	-7(4)
C(47)	149(8)	166(8)	95(6)	110(6)	76(5)	106(7)
C(48)	52(4)	101(5)	39(3)	35(3)	7(3)	-3(3)
C(49)	47(3)	34(3)	25(2)	11(2)	4(2)	21(2)
C(50)	91(5)	109(5)	51(4)	7(3)	4(3)	76(4)
C(51)	78(4)	38(3)	72(4)	5(3)	15(3)	11(3)
C(52)	115(5)	51(3)	31(3)	11(2)	21(3)	49(3)
C(53)	67(4)	52(3)	28(3)	17(2)	-4(3)	-1(3)

C(54)	43(3)	49(3)	63(4)	17(3)	1(3)	19(3)
B(1)	41(4)	49(4)	56(4)	21(3)	9(3)	11(3)
F(1)	68(3)	114(3)	136(4)	36(3)	34(3)	21(2)
F(2)	159(4)	139(4)	42(2)	36(2)	19(2)	44(3)
F(3)	74(3)	75(3)	103(3)	16(2)	-16(2)	2(2)
F(4)	110(3)	94(3)	165(4)	84(3)	21(3)	40(3)

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

Table 20. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6**

atom	x	y	z	U(eq)
H(1)	277	2839	5717	36
H(3)	-1570	1956	6065	38
H(4)	-3653	1176	5871	40
H(5)	-4776	789	4722	37
H(10)	-5559	615	3218	41
H(11)	-5589	776	2048	44
H(12)	-3838	1541	1634	43
H(14)	-1712.0001	2433	1793	33
H(16A)	-1356	-1901	2429	140
H(16B)	-61	-1743	2814	140
H(16C)	-211	-1631	2014	140
H(19)	3934	5739	6450	34
H(21)	3612	3025	6681	38
H(24A)	1567	5690	5626	53
H(24B)	971	4713	4880	53
H(24C)	1650	5845	4836	53
H(25A)	3019	5150	4005	52
H(25B)	2307	4022	4046	52
H(25C)	3740	4541	4278	52
H(26A)	3739	6659	5851	72
H(26B)	3868	6614	5015	72
H(26C)	4636	6161	5423	72
H(28A)	5633	4249	7383	104
H(28B)	6138	5342	8047	104
H(28C)	6124	5309	7204	104
H(29A)	4962	6483	8328	98
H(29B)	3719	6179	7810	98
H(29C)	4969	6524	7503	98
H(30A)	3652	3746	7855	76
H(30B)	2944	4531	8026	76
H(30C)	4186	4817	8538	76
H(32A)	3509	1542	6197	126
H(32B)	4304	1952	5623	126
H(32C)	3476	748	5398	126
H(33A)	1342	1326	6071	334
H(33B)	1391	315	5450	334
H(33C)	694	982	5238	334
H(34A)	2706	681	4382	225
H(34B)	3233	1875	4439	225
H(34C)	1808	1246	4267	225
H(37)	2100	2481	499	38
H(39)	1154	4958	1232	36
H(42A)	2998	2278	2287	57
H(42B)	2230	1131	2274	57
H(42C)	1763	2062	2622	57
H(43A)	425	-5	1307	66
H(43B)	-128	485	806	66
H(43C)	-228	785	1672	66
H(44A)	3050	1724	992	76
H(44B)	1857	974	406	76
H(44C)	2383	557	974	76
H(46A)	1907	2610	-595	121
H(46B)	1898	3371	-1045	121
H(46C)	729	2874	-706	121
H(47A)	800	4675	-75	159
H(47B)	1972	5085	-440	159
H(47C)	2017	5538	439	159
H(48A)	3757	5074	662	104
H(48B)	3747	4641	-215	104
H(48C)	3703	3912	270	104
H(50A)	-1323	4516	2042	117
H(50B)	-394	5235	1670	117
H(50C)	-673	5737	2481	117

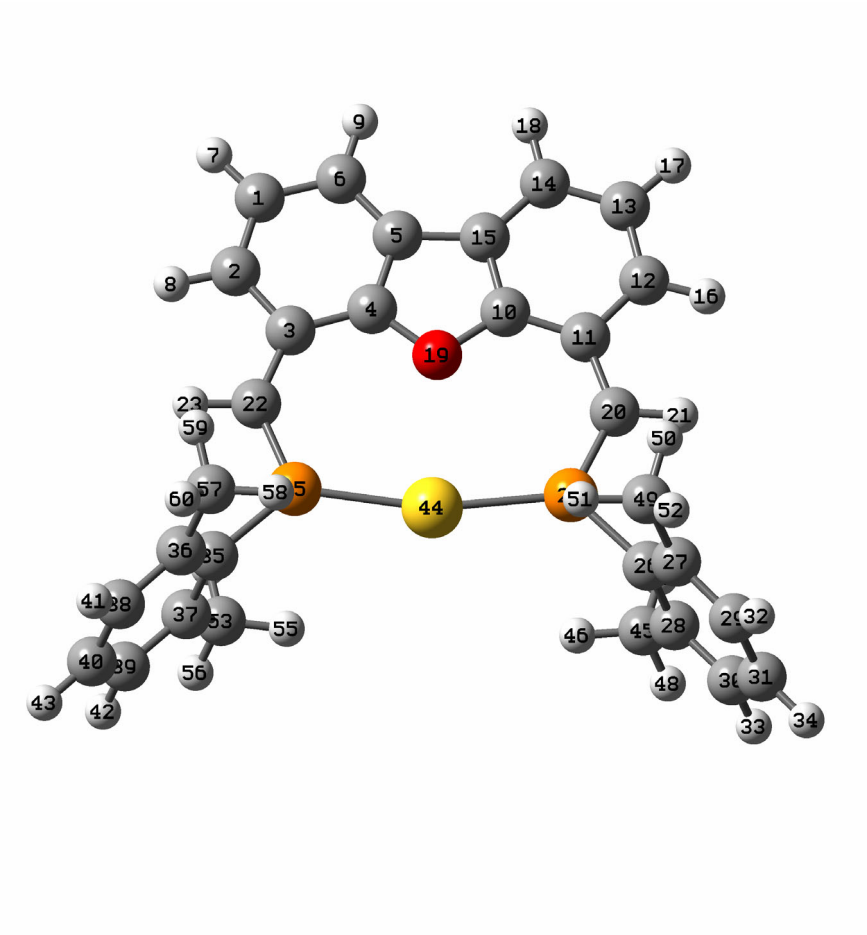
H(51A)	1502	6483	3097	103
H(51B)	1852	6118	2286	103
H(51C)	2286	5759	2922	103
H(52A)	197	5417	3571	92
H(52B)	726	4507	3388	92
H(52C)	-666.9999	4243	3122	92
H(53)	-2790.0002	2133	-587	66
H(54)	-5244	1023	-1619	62

Electronic Supplementary Information for Dalton Transactions

Data for the theoretical structure I.

Functional: B3PW91

Basis set: 6-31G* for C, H, O, P and LANL2DZ for Au.



Standard orientation:

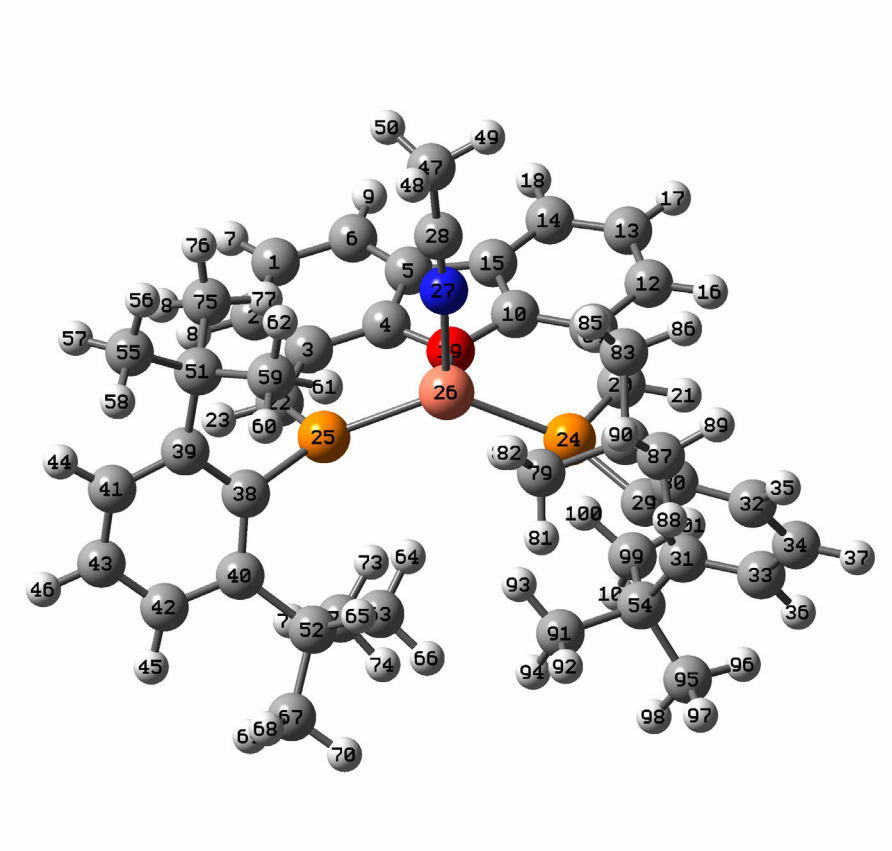
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.033262	4.861950	-0.020594
2	6	0	-3.393017	3.517490	-0.015349
3	6	0	-2.449256	2.460775	-0.010123
4	6	0	-1.105626	2.884629	-0.011012
5	6	0	-0.723818	4.234086	-0.016575
6	6	0	-1.692252	5.238876	-0.021296
7	1	0	-3.809429	5.620698	-0.024337
8	1	0	-4.447751	3.255986	-0.015225
9	1	0	-1.409646	6.287332	-0.025628
10	6	0	1.105627	2.884628	-0.011015
11	6	0	2.449257	2.460773	-0.010129
12	6	0	3.393019	3.517487	-0.015361
13	6	0	3.033265	4.861947	-0.020608
14	6	0	1.692255	5.238874	-0.021307
15	6	0	0.723821	4.234085	-0.016617
16	1	0	4.447753	3.255982	-0.015239
17	1	0	3.809431	5.620694	-0.024355
18	1	0	1.409648	6.287330	-0.025640
19	8	0	0.000000	2.074320	-0.007441
20	6	0	2.977225	1.116251	-0.005680
21	1	0	4.067499	1.081600	-0.009044
22	6	0	-2.977225	1.116254	-0.005675
23	1	0	-4.067499	1.081603	-0.009036
24	15	0	2.293993	-0.420923	0.004594
25	15	0	-2.293994	-0.420921	0.004593
26	6	0	3.605080	-1.671241	0.005906
27	6	0	4.108927	-2.137085	1.240799
28	6	0	4.052912	-2.194594	-1.227562
29	6	0	5.096284	-3.125044	1.213519
30	6	0	5.041591	-3.181051	-1.199521
31	6	0	5.560226	-3.640453	0.007203
32	1	0	5.500835	-3.494512	2.152184
33	1	0	5.404019	-3.593571	-2.137460
34	1	0	6.326793	-4.410509	0.007724
35	6	0	-3.605082	-1.671237	0.005906
36	6	0	-4.108918	-2.137092	1.240799
37	6	0	-4.052923	-2.194584	-1.227562
38	6	0	-5.096272	-3.125053	1.213521
39	6	0	-5.041598	-3.181044	-1.199520
40	6	0	-5.560223	-3.640456	0.007206
41	1	0	-5.500814	-3.494529	2.152187
42	1	0	-5.404030	-3.593561	-2.137458
43	1	0	-6.326787	-4.410516	0.007728
44	79	0	0.000000	-0.706119	0.006345
45	6	0	3.505886	-1.716027	-2.547510
46	1	0	2.412964	-1.808918	-2.595037
47	1	0	3.748481	-0.662437	-2.731751
48	1	0	3.921059	-2.299384	-3.374013
49	6	0	3.622098	-1.598340	2.561194
50	1	0	3.890044	-0.543291	2.695340
51	1	0	2.530537	-1.668510	2.654341
52	1	0	4.059352	-2.157525	3.392988
53	6	0	-3.505906	-1.716011	-2.547511
54	1	0	-3.748503	-0.662420	-2.731746
55	1	0	-2.412984	-1.808900	-2.595044
56	1	0	-3.921084	-2.299365	-3.374015

57	6	0	-3.622079	-1.598356	2.561194
58	1	0	-2.530518	-1.668526	2.654333
59	1	0	-3.890024	-0.543307	2.695350
60	1	0	-4.059328	-2.157545	3.392989

Data for the theoretical structure II.

Functional: B3PW91 MM: UFF

Basis set: 6-31G* for C, H, O, P and LANL2DZ for Cu. The methyl groups of the xylyl substituents were optimiozed at the UFF level of theory.



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	10061000	-2.973133	4.909256	-1.553524
2	6	10061000	-3.280751	3.549843	-1.507678
3	6	10061000	-2.348908	2.562670	-1.117668
4	6	10061000	-1.071419	3.059329	-.808518
5	6	10061000	-.738529	4.418601	-.853055
6	6	10061000	-1.699620	5.362832	-1.223160
7	1	10011000	-3.738521	5.617515	-1.855614
8	1	10011000	-4.284121	3.225431	-1.770450
9	1	10011000	-1.456393	6.420304	-1.264433
10	6	10061000	1.079408	3.176459	-.291275
11	6	10061000	2.409639	2.814931	-.018722
12	6	10061000	3.303911	3.903957	.077747
13	6	10061000	2.904281	5.229661	-.087305
14	6	10061000	1.582454	5.543368	-.391586
15	6	10061000	.664330	4.496161	-.503717
16	1	10011000	4.349238	3.686830	.280862
17	1	10011000	3.641099	6.022061	.001850
18	1	10011000	1.276881	6.573322	-.549616
19	8	10081000	.026844	2.300431	-.457356
20	6	10061000	2.937544	1.471789	.089073
21	1	10011000	4.025860	1.413015	.067559
22	6	10061000	-2.799188	1.187664	-1.051107
23	1	10011000	-3.788193	1.019356	-1.477424
24	15	10151004	2.106205	.005784	.143353
25	15	10151004	-2.061019	-.150185	-.344770
26	29	10291003	-.102112	.157591	.796606
27	7	10071001	-.415371	.689745	2.756109
28	6	10061001	-.656936	.912672	3.866256
29	6	10061000	3.462670	-1.240032	.126055
30	6	10061000	3.841769	-1.854647	1.369765
31	6	10061000	4.271421	-1.329260	-1.065789
32	6	10061000	5.196100	-2.221465	1.464776
33	6	10061000	5.608016	-1.703800	-.847566
34	6	10061000	6.071160	-2.076270	.403242
35	1	10011000	5.629455	-2.619532	2.375671
36	1	10011000	6.344125	-1.726611	-1.644234
37	1	10011000	7.119847	-2.327819	.534007
38	6	10061000	-3.322235	-1.477175	-.561320
39	6	10061000	-4.474082	-1.461951	.302773
40	6	10061000	-3.235971	-2.299767	-1.736513
41	6	10061000	-5.639840	-2.018090	-.251238
42	6	10061000	-4.462821	-2.814527	-2.193167
43	6	10061000	-5.643472	-2.617617	-1.499386
44	1	10011000	-6.595518	-2.006950	.262427
45	1	10011000	-4.551427	-3.384265	-3.111947
46	1	10011000	-6.574827	-3.000480	-1.906986
47	6	10061003	-.962700	1.186637	5.258996
48	1	10011000	-1.297388	.268403	5.751909
49	1	10011000	-.071888	1.562277	5.771842
50	1	10011000	-1.756998	1.936521	5.326379
51	6	10061003	-4.456177	-.967563	1.808097
52	6	10061003	-1.883057	-2.691777	-2.457857
53	6	10061003	2.861419	-2.144692	2.576597
54	6	10061003	3.724616	-1.151876	-2.544633
55	6	10061003	-5.714989	-1.422684	2.572691
56	1	10011000	-5.635467	-1.185118	3.656545

57	1	10011000	-6.622643	-.899869	2.200686
58	1	10011000	-5.858736	-2.521850	2.485626
59	6	10061003	-3.259583	-1.588946	2.545239
60	1	10011000	-3.307130	-2.698330	2.491952
61	1	10011000	-2.289089	-1.275023	2.121260
62	1	10011000	-3.252543	-1.290665	3.616588
63	6	10061003	-.829166	-3.109475	-1.418153
64	1	10011000	-.456146	-2.259904	-.817970
65	1	10011000	-1.252706	-3.865552	-.722118
66	1	10011000	.062737	-3.557285	-1.906075
67	6	10061003	-2.070949	-3.906273	-3.389307
68	1	10011000	-2.537371	-4.755789	-2.844214
69	1	10011000	-2.692136	-3.647482	-4.273598
70	1	10011000	-1.096852	-4.262140	-3.791580
71	6	10061003	-1.342857	-1.544598	-3.323464
72	1	10011000	-2.150825	-1.138127	-3.968983
73	1	10011000	-.925616	-.715539	-2.723033
74	1	10011000	-.518473	-1.896214	-3.981032
75	6	10061003	-4.396581	.563784	1.919109
76	1	10011000	-4.667094	.904300	2.942630
77	1	10011000	-3.382593	.963881	1.733660
78	1	10011000	-5.104449	1.030369	1.200833
79	6	10061003	1.495292	-2.646375	2.074696
80	1	10011000	.886158	-1.851396	1.615711
81	1	10011000	1.631371	-3.460647	1.330410
82	1	10011000	.875360	-3.040803	2.909147
83	6	10061003	2.674655	-.894347	3.442716
84	1	10011000	2.218141	-.061682	2.878175
85	1	10011000	2.015766	-1.109809	4.312214
86	1	10011000	3.656326	-.541098	3.825788
87	6	10061003	3.409384	-3.257641	3.493854
88	1	10011000	3.680310	-4.158606	2.901358
89	1	10011000	4.294045	-2.917930	4.073133
90	1	10011000	2.657078	-3.564652	4.253289
91	6	10061003	2.381886	-1.879430	-2.699230
92	1	10011000	2.477255	-2.937883	-2.373708
93	1	10011000	1.576757	-1.405741	-2.109606
94	1	10011000	2.039517	-1.869957	-3.756892
95	6	10061003	4.678416	-1.785472	-3.577436
96	1	10011000	5.621801	-1.204941	-3.666870
97	1	10011000	4.914776	-2.837728	-3.306744
98	1	10011000	4.225235	-1.796775	-4.593213
99	6	10061003	3.554125	.322353	-2.933320
100	1	10011000	2.651167	.772491	-2.479528
101	1	10011000	4.445333	.909092	-2.623370
102	1	10011000	3.428604	.435919	-4.032426