

ORGANOMETALLICS

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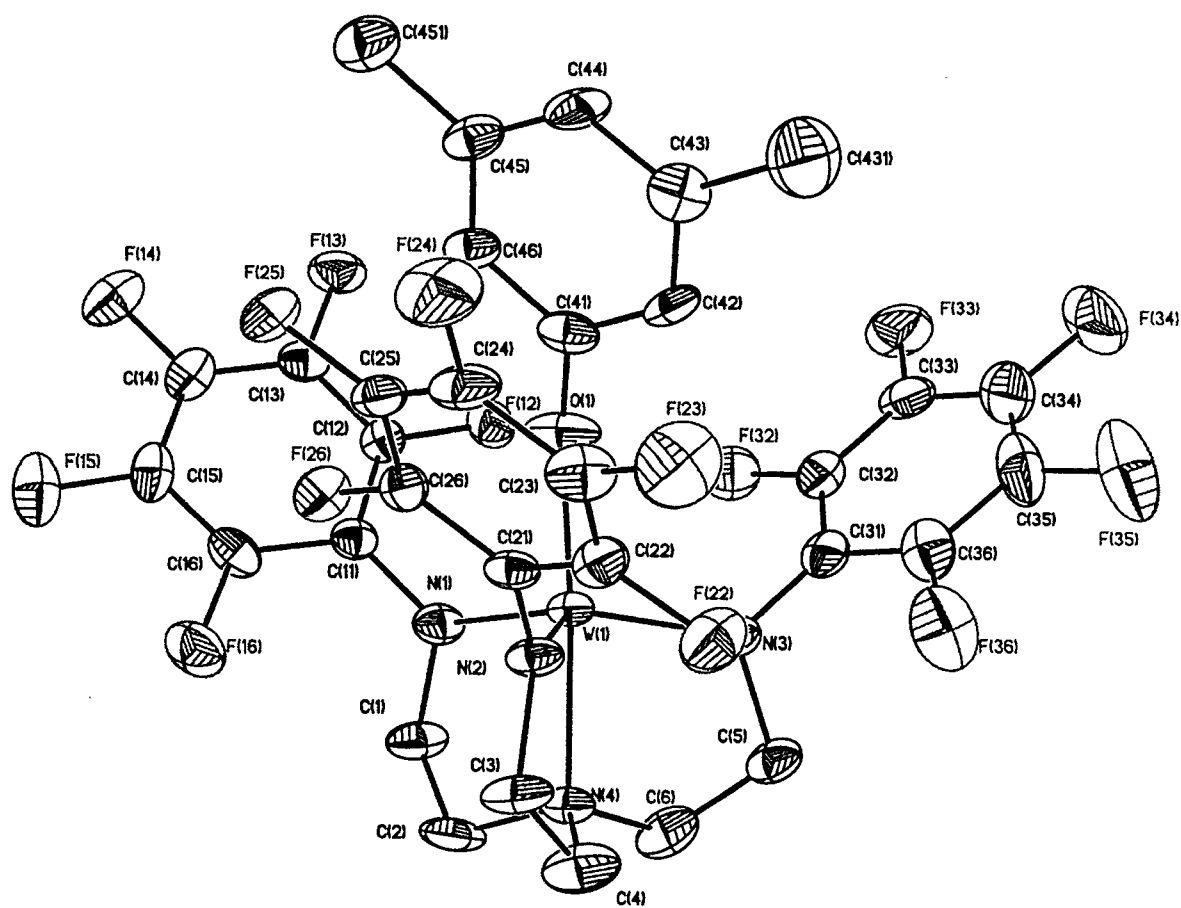


Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1b . $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W(1)	2172 (1)	1231 (1)	2045 (1)	30 (1)
F(12)	905 (3)	3094 (4)	2858 (3)	52 (1)
F(13)	-429 (3)	3217 (4)	3765 (3)	61 (2)
F(14)	-1856 (4)	2046 (5)	3410 (4)	69 (2)
F(15)	-1905 (4)	710 (5)	2120 (5)	80 (2)
F(16)	-526 (4)	496 (4)	1271 (4)	67 (2)
F(22)	3916 (4)	-1120 (4)	2703 (4)	66 (2)
F(23)	4023 (4)	-2332 (5)	4058 (5)	86 (2)
F(24)	2579 (4)	-2653 (5)	4847 (4)	77 (2)
F(25)	1053 (3)	-1698 (4)	4296 (3)	59 (1)
F(26)	923 (3)	-521 (4)	2908 (3)	51 (1)
F(32)	2721 (4)	3675 (5)	2775 (5)	71 (2)
F(33)	3853 (5)	4587 (6)	3998 (5)	100 (3)
F(34)	5520 (5)	3887 (6)	4500 (5)	110 (3)
F(35)	6043 (5)	2301 (6)	3732 (7)	119 (3)
F(36)	4925 (4)	1379 (5)	2516 (6)	88 (2)
O(1)	2050 (5)	1412 (5)	3289 (4)	59 (2)
N(1)	964 (4)	1692 (5)	1561 (4)	41 (2)
N(2)	2361 (4)	-171 (5)	2026 (4)	38 (2)
N(3)	3211 (4)	2037 (5)	1928 (4)	41 (2)
N(4)	2213 (5)	1039 (5)	653 (5)	37 (2)
C(1)	751 (6)	1769 (8)	603 (5)	53 (2)
C(2)	1290 (7)	1076 (9)	191 (6)	62 (3)
C(3)	2384 (7)	-633 (6)	1183 (5)	49 (2)
C(4)	2624 (8)	84 (7)	544 (7)	65 (3)
C(5)	3511 (6)	2072 (7)	1055 (6)	49 (2)
C(6)	2740 (7)	1862 (8)	374 (7)	64 (3)
C(11)	250 (5)	1777 (6)	2035 (5)	37 (2)
C(12)	234 (5)	2458 (5)	2681 (5)	36 (2)
C(13)	-454 (5)	2536 (6)	3140 (5)	41 (2)
C(14)	-1175 (5)	1960 (7)	2966 (6)	48 (2)
C(15)	-1202 (6)	1275 (6)	2314 (7)	50 (2)
C(16)	-497 (6)	1199 (6)	1868 (7)	46 (2)
C(21)	2409 (5)	-791 (6)	2760 (5)	34 (2)
C(22)	3187 (6)	-1267 (6)	3075 (6)	44 (2)
C(23)	3250 (6)	-1889 (7)	3771 (6)	52 (2)
C(24)	2524 (6)	-2037 (7)	4178 (6)	50 (2)
C(25)	1754 (5)	-1555 (6)	3893 (5)	39 (2)
C(26)	1694 (5)	-958 (6)	3193 (6)	36 (2)
C(31)	3781 (6)	2495 (7)	2585 (6)	46 (2)
C(32)	3537 (6)	3312 (8)	2998 (7)	54 (2)
C(33)	4100 (8)	3794 (8)	3633 (7)	64 (3)
C(34)	4949 (8)	3442 (10)	3894 (8)	76 (3)
C(35)	5212 (7)	2632 (10)	3505 (8)	74 (3)
C(36)	4634 (6)	2171 (7)	2867 (7)	56 (3)
C(41)	2223 (6)	1032 (6)	4086 (6)	42 (2)
C(42)	3073 (6)	790 (6)	4474 (5)	44 (2)
C(43)	3230 (6)	423 (7)	5309 (6)	51 (2)

C(44)	2530(6)	301(7)	5752(6)	53(2)
C(45)	1684(6)	541(6)	5390(6)	45(2)
C(46)	1533(6)	916(6)	4559(5)	39(2)
C(431)	4168(8)	169(12)	5738(10)	96(4)
C(451)	934(7)	433(8)	5902(7)	64(3)

Table 3. Bond lengths [Å] and angles [°] for 1b.

W(1)-N(2)	1.968 (7)	W(1)-N(3)	1.975 (7)
W(1)-N(1)	1.990 (6)	W(1)-O(1)	1.991 (7)
W(1)-N(4)	2.195 (7)	F(12)-C(12)	1.349 (9)
F(13)-C(13)	1.353 (10)	F(14)-C(14)	1.341 (10)
F(15)-C(15)	1.328 (10)	F(16)-C(16)	1.344 (10)
F(22)-C(22)	1.349 (11)	F(23)-C(23)	1.345 (10)
F(24)-C(24)	1.341 (10)	F(25)-C(25)	1.338 (9)
F(26)-C(26)	1.339 (10)	F(32)-C(32)	1.341 (11)
F(33)-C(33)	1.322 (13)	F(34)-C(34)	1.334 (14)
F(35)-C(35)	1.345 (13)	F(36)-C(36)	1.334 (12)
O(1)-C(41)	1.336 (11)	N(1)-C(11)	1.415 (10)
N(1)-C(1)	1.481 (10)	N(2)-C(21)	1.423 (10)
N(2)-C(3)	1.466 (10)	N(3)-C(31)	1.392 (11)
N(3)-C(5)	1.502 (11)	N(4)-C(2)	1.482 (12)
N(4)-C(4)	1.488 (12)	N(4)-C(6)	1.501 (12)
C(1)-C(2)	1.476 (13)	C(3)-C(4)	1.492 (13)
C(5)-C(6)	1.487 (14)	C(11)-C(12)	1.383 (11)
C(11)-C(16)	1.388 (12)	C(12)-C(13)	1.365 (12)
C(13)-C(14)	1.355 (12)	C(14)-C(15)	1.387 (14)
C(15)-C(16)	1.37 (2)	C(21)-C(22)	1.384 (13)
C(21)-C(26)	1.391 (12)	C(22)-C(23)	1.378 (13)
C(23)-C(24)	1.377 (13)	C(24)-C(25)	1.368 (13)
C(25)-C(26)	1.361 (12)	C(31)-C(32)	1.383 (14)
C(31)-C(36)	1.386 (13)	C(32)-C(33)	1.38 (2)
C(33)-C(34)	1.39 (2)	C(34)-C(35)	1.37 (2)
C(35)-C(36)	1.38 (2)	C(41)-C(46)	1.386 (13)
C(41)-C(42)	1.388 (12)	C(42)-C(43)	1.383 (13)
C(43)-C(44)	1.371 (13)	C(43)-C(431)	1.528 (14)
C(44)-C(45)	1.371 (13)	C(45)-C(46)	1.382 (12)
C(45)-C(451)	1.502 (13)		
N(2)-W(1)-N(3)	115.8 (3)	N(2)-W(1)-N(1)	116.2 (3)
N(3)-W(1)-N(1)	119.8 (3)	N(2)-W(1)-O(1)	100.1 (3)
N(3)-W(1)-O(1)	102.5 (3)	N(1)-W(1)-O(1)	96.1 (3)
N(2)-W(1)-N(4)	80.7 (3)	N(3)-W(1)-N(4)	80.3 (3)
N(1)-W(1)-N(4)	80.3 (3)	O(1)-W(1)-N(4)	176.3 (3)
C(41)-O(1)-W(1)	145.0 (6)	C(11)-N(1)-C(1)	117.0 (6)
C(11)-N(1)-W(1)	125.1 (5)	C(1)-N(1)-W(1)	116.8 (5)
C(21)-N(2)-C(3)	116.6 (6)	C(21)-N(2)-W(1)	125.1 (5)
C(3)-N(2)-W(1)	118.0 (5)	C(31)-N(3)-C(5)	114.0 (7)
C(31)-N(3)-W(1)	127.8 (6)	C(5)-N(3)-W(1)	117.7 (5)
C(2)-N(4)-C(4)	111.3 (8)	C(2)-N(4)-C(6)	110.3 (8)
C(4)-N(4)-C(6)	112.9 (7)	C(2)-N(4)-W(1)	107.7 (6)
C(4)-N(4)-W(1)	107.3 (5)	C(6)-N(4)-W(1)	106.9 (5)
C(2)-C(1)-N(1)	109.9 (7)	C(1)-C(2)-N(4)	111.5 (8)
N(2)-C(3)-C(4)	110.4 (8)	N(4)-C(4)-C(3)	111.5 (8)
C(6)-C(5)-N(3)	108.6 (7)	C(5)-C(6)-N(4)	110.3 (8)
C(12)-C(11)-C(16)	115.1 (8)	C(12)-C(11)-N(1)	122.6 (7)
C(16)-C(11)-N(1)	122.2 (8)	F(12)-C(12)-C(13)	117.8 (7)
F(12)-C(12)-C(11)	119.8 (7)	C(13)-C(12)-C(11)	122.5 (8)
C(14)-C(13)-F(13)	119.3 (8)	C(14)-C(13)-C(12)	121.2 (8)
F(13)-C(13)-C(12)	119.5 (8)	F(14)-C(14)-C(13)	121.2 (9)
F(14)-C(14)-C(15)	120.0 (8)	C(13)-C(14)-C(15)	118.8 (8)
F(15)-C(15)-C(16)	120.7 (9)	F(15)-C(15)-C(14)	120.2 (9)
C(16)-C(15)-C(14)	119.1 (8)	F(16)-C(16)-C(15)	117.5 (8)

F(16)-C(16)-C(11)	119.1(9)	C(15)-C(16)-C(11)	123.3(8)
C(22)-C(21)-C(26)	116.5(8)	C(22)-C(21)-N(2)	120.5(8)
C(26)-C(21)-N(2)	122.9(7)	F(22)-C(22)-C(23)	118.1(8)
F(22)-C(22)-C(21)	119.9(8)	C(23)-C(22)-C(21)	122.0(9)
F(23)-C(23)-C(24)	120.6(8)	F(23)-C(23)-C(22)	119.9(9)
C(24)-C(23)-C(22)	119.5(8)	F(24)-C(24)-C(25)	120.8(8)
F(24)-C(24)-C(23)	119.7(9)	C(25)-C(24)-C(23)	119.6(8)
F(25)-C(25)-C(24)	119.2(8)	F(25)-C(25)-C(26)	120.4(8)
C(24)-C(25)-C(26)	120.4(8)	F(26)-C(26)-C(25)	119.2(7)
F(26)-C(26)-C(21)	118.8(7)	C(25)-C(26)-C(21)	122.0(8)
C(32)-C(31)-N(3)	122.2(8)	C(32)-C(31)-C(36)	115.3(9)
N(3)-C(31)-C(36)	122.5(9)	F(32)-C(32)-C(33)	117.1(9)
F(32)-C(32)-C(31)	119.7(8)	C(33)-C(32)-C(31)	123.2(10)
F(33)-C(33)-C(32)	121.6(11)	F(33)-C(33)-C(34)	119.0(10)
C(32)-C(33)-C(34)	119.4(10)	F(34)-C(34)-C(35)	119.2(12)
F(34)-C(34)-C(33)	121.6(13)	C(35)-C(34)-C(33)	119.1(10)
F(35)-C(35)-C(34)	119.7(11)	F(35)-C(35)-C(36)	120.3(12)
C(34)-C(35)-C(36)	120.0(10)	F(36)-C(36)-C(35)	117.3(9)
F(36)-C(36)-C(31)	119.7(9)	C(35)-C(36)-C(31)	123.0(10)
O(1)-C(41)-C(46)	118.8(8)	O(1)-C(41)-C(42)	122.5(9)
C(46)-C(41)-C(42)	118.7(8)	C(43)-C(42)-C(41)	120.8(8)
C(42)-C(43)-C(44)	119.0(8)	C(42)-C(43)-C(431)	120.7(10)
C(44)-C(43)-C(431)	120.3(10)	C(45)-C(44)-C(43)	121.6(8)
C(44)-C(45)-C(46)	119.1(8)	C(44)-C(45)-C(451)	120.5(8)
C(46)-C(45)-C(451)	120.3(8)	C(41)-C(46)-C(45)	120.7(8)

Symmetry transformations used to generate equivalent atoms:

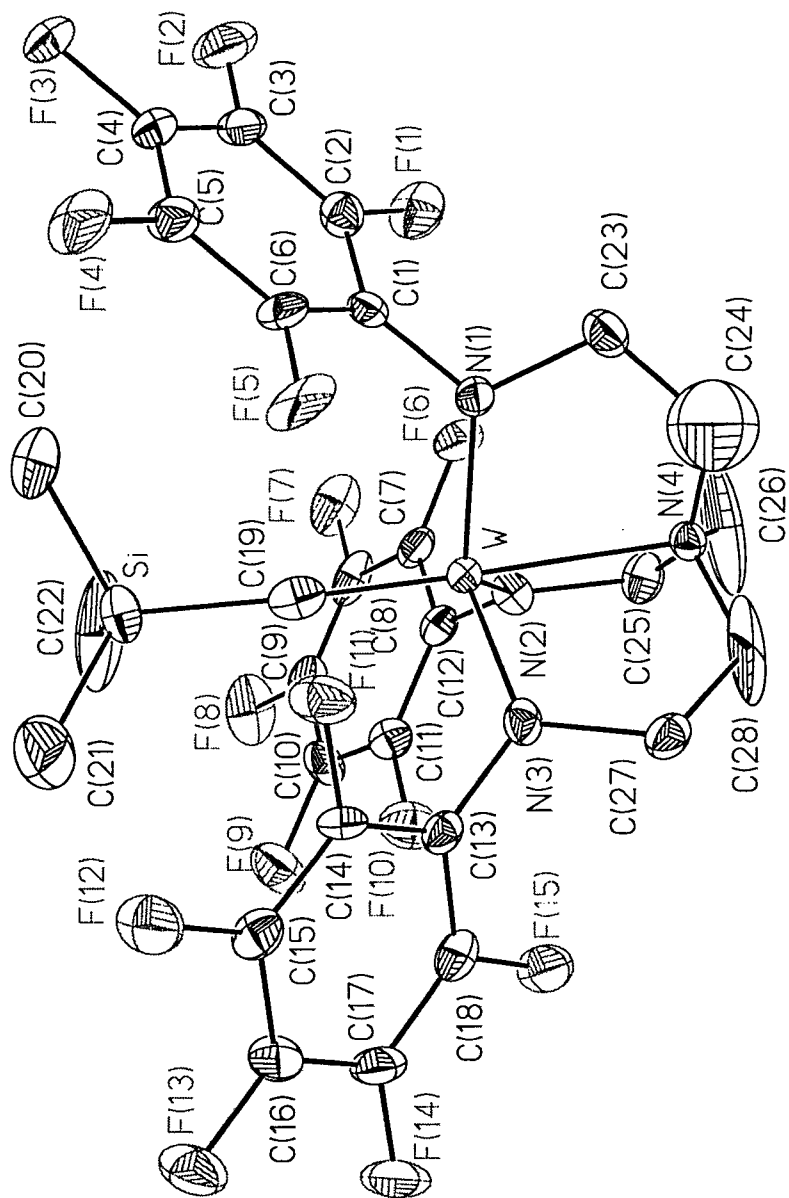
Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1b

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
W(1)	43 (1)	25 (1)	24 (1)	-1 (1)	10 (1)	0 (1)
F(12)	52 (3)	50 (3)	53 (3)	-13 (3)	6 (2)	-5 (2)
F(13)	63 (3)	76 (4)	44 (3)	-17 (3)	13 (2)	12 (3)
F(14)	63 (3)	81 (4)	71 (4)	18 (3)	33 (3)	16 (3)
F(15)	60 (3)	72 (4)	105 (5)	7 (4)	7 (3)	-23 (3)
F(16)	82 (4)	51 (3)	66 (4)	-20 (3)	6 (3)	-10 (3)
F(22)	58 (3)	77 (4)	68 (4)	6 (3)	23 (3)	8 (3)
F(23)	78 (4)	93 (5)	86 (5)	33 (4)	8 (3)	32 (4)
F(24)	104 (4)	74 (4)	55 (4)	34 (3)	17 (3)	-3 (3)
F(25)	66 (3)	70 (4)	45 (3)	12 (3)	22 (3)	-20 (3)
F(26)	51 (3)	49 (3)	54 (3)	5 (2)	14 (2)	3 (2)
F(32)	70 (4)	71 (5)	76 (4)	-29 (3)	22 (3)	1 (3)
F(33)	118 (5)	106 (6)	88 (5)	-59 (5)	50 (4)	-44 (5)
F(34)	110 (5)	131 (7)	84 (6)	-10 (5)	-3 (4)	-78 (5)
F(35)	73 (4)	112 (6)	154 (8)	23 (6)	-39 (5)	-14 (4)
F(36)	78 (4)	59 (4)	120 (7)	3 (4)	-12 (4)	11 (3)
O(1)	115 (6)	37 (3)	29 (4)	-3 (3)	20 (3)	5 (4)
N(1)	48 (4)	46 (4)	30 (4)	5 (3)	3 (3)	7 (3)
N(2)	62 (4)	25 (4)	32 (4)	-6 (3)	18 (3)	0 (3)
N(3)	53 (4)	33 (4)	38 (4)	-4 (3)	15 (3)	-2 (3)
N(4)	58 (4)	29 (3)	25 (4)	0 (3)	11 (3)	2 (3)
C(1)	65 (6)	67 (6)	27 (5)	4 (4)	11 (4)	18 (5)
C(2)	76 (7)	84 (8)	24 (5)	-18 (5)	5 (4)	10 (5)
C(3)	88 (6)	35 (5)	30 (5)	2 (4)	25 (4)	7 (4)
C(4)	105 (8)	44 (6)	52 (6)	2 (5)	32 (5)	12 (5)
C(5)	66 (5)	41 (5)	45 (5)	2 (4)	29 (4)	-10 (4)
C(6)	77 (7)	69 (7)	52 (6)	15 (5)	32 (5)	-2 (6)
C(11)	39 (4)	39 (5)	33 (4)	1 (4)	3 (3)	5 (3)
C(12)	42 (4)	28 (4)	39 (5)	2 (4)	9 (4)	0 (4)
C(13)	47 (5)	42 (5)	32 (5)	5 (4)	2 (3)	10 (4)
C(14)	45 (5)	41 (5)	59 (6)	9 (5)	17 (4)	8 (4)
C(15)	39 (5)	44 (6)	67 (7)	12 (5)	6 (4)	-5 (4)
C(16)	57 (5)	28 (5)	50 (6)	-10 (4)	-2 (4)	2 (4)
C(21)	53 (5)	24 (4)	26 (4)	-4 (3)	9 (3)	1 (4)
C(22)	48 (5)	43 (6)	44 (6)	-2 (4)	15 (4)	-1 (4)
C(23)	64 (6)	48 (5)	44 (5)	7 (4)	8 (4)	15 (4)
C(24)	81 (6)	42 (5)	30 (5)	7 (4)	18 (4)	-6 (5)
C(25)	54 (5)	35 (4)	30 (5)	-3 (4)	16 (4)	-9 (4)
C(26)	44 (4)	27 (4)	39 (5)	-3 (4)	9 (4)	-8 (4)
C(31)	52 (5)	44 (5)	45 (5)	7 (4)	18 (4)	-14 (4)
C(32)	52 (5)	65 (7)	49 (6)	-3 (5)	18 (4)	-12 (5)
C(33)	82 (7)	67 (8)	53 (7)	-25 (5)	39 (6)	-36 (6)
C(34)	72 (8)	81 (8)	76 (8)	-2 (7)	13 (6)	-39 (7)
C(35)	51 (6)	79 (8)	86 (9)	13 (7)	-8 (6)	-24 (6)
C(36)	58 (6)	42 (6)	67 (7)	14 (5)	6 (5)	-10 (5)
C(41)	69 (6)	25 (4)	33 (5)	-7 (4)	7 (4)	2 (4)
C(42)	61 (5)	40 (5)	37 (5)	-1 (4)	30 (4)	-8 (4)
C(43)	59 (5)	37 (5)	56 (6)	-2 (4)	8 (4)	13 (4)

C(44)	70(6)	65(6)	27(5)	21(4)	16(4)	5(5)
C(45)	70(6)	29(4)	40(5)	4(4)	23(4)	-3(4)
C(46)	62(5)	27(4)	32(5)	-3(4)	14(4)	0(4)
C(431)	68(7)	122(12)	97(11)	11(9)	5(7)	23(8)
C(451)	75(6)	63(7)	55(6)	9(5)	19(5)	-3(5)



Positional parameters and B(eq) for 94046 Seidel/RRS (2d)

atom	x	y	z	B(eq)
W	0.21121(2)	0.136131(8)	0.20137(2)	1.58(1)
Si	0.5036(2)	0.12205(7)	0.4442(2)	3.29(8)
F(1)	0.1951(4)	0.2744(1)	0.2875(3)	3.9(2)
F(2)	0.4038(5)	0.3346(1)	0.3843(3)	4.9(2)
F(3)	0.6861(4)	0.3236(1)	0.3515(3)	4.7(2)
F(4)	0.7523(4)	0.2529(1)	0.2204(4)	5.0(2)
F(5)	0.5440(4)	0.1937(1)	0.1201(4)	4.6(2)
F(6)	-0.0359(4)	0.1925(1)	0.4334(3)	3.4(2)
F(7)	-0.0408(4)	0.1681(1)	0.6485(3)	4.9(2)
F(8)	0.0401(4)	0.0798(2)	0.7223(3)	5.2(2)
F(9)	0.1298(4)	0.0169(1)	0.5794(3)	4.7(2)
F(10)	0.1257(4)	0.0395(1)	0.3636(3)	4.0(2)
F(11)	0.5365(4)	0.0941(1)	0.0970(3)	3.7(2)
F(12)	0.7255(4)	0.0222(1)	0.1454(4)	4.2(2)
F(13)	0.6283(4)	-0.0643(1)	0.1905(3)	4.2(2)
F(14)	0.3386(4)	-0.0790(1)	0.1858(4)	4.9(2)
F(15)	0.1488(4)	-0.0070(1)	0.1418(3)	3.8(2)
N(1)	0.2519(5)	0.2004(1)	0.1505(4)	2.1(2)
N(2)	0.0431(5)	0.1296(2)	0.2786(4)	2.1(2)
N(3)	0.2350(5)	0.0841(2)	0.0980(4)	2.2(2)
N(4)	0.0157(5)	0.1485(1)	0.0548(4)	1.8(2)
C(1)	0.3632(6)	0.2313(2)	0.2021(5)	2.0(2)
C(2)	0.3333(7)	0.2685(2)	0.2701(5)	2.5(3)
C(3)	0.4391(7)	0.2995(2)	0.3191(5)	2.9(3)
C(4)	0.5802(7)	0.2936(2)	0.3038(5)	3.1(3)
C(5)	0.6136(7)	0.2580(2)	0.2362(6)	3.1(3)
C(6)	0.5061(7)	0.2274(2)	0.1855(5)	2.5(3)
C(7)	0.0019(7)	0.1485(2)	0.4678(5)	2.7(3)
C(8)	0.0005(7)	0.1361(3)	0.5776(5)	3.2(3)
C(9)	0.0416(7)	0.0922(3)	0.6154(5)	3.2(3)
C(10)	0.0849(7)	0.0603(2)	0.5434(5)	3.0(3)
C(11)	0.0840(7)	0.0719(2)	0.4327(5)	2.6(3)
C(12)	0.0441(6)	0.1168(2)	0.3913(5)	2.1(2)
C(13)	0.3365(6)	0.0461(2)	0.1197(4)	2.1(3)
C(14)	0.4841(6)	0.0517(2)	0.1209(5)	2.2(3)
C(15)	0.5816(7)	0.0156(2)	0.1446(5)	2.6(3)
C(16)	0.5342(7)	-0.0288(2)	0.1680(5)	3.0(3)
C(17)	0.3869(7)	-0.0361(2)	0.1649(5)	3.1(3)
C(18)	0.2915(7)	0.0012(2)	0.1416(5)	2.8(3)
C(19)	0.3550(7)	0.1279(2)	0.3174(5)	2.7(3)
C(20)	0.6144(9)	0.1777(3)	0.4605(7)	6.0(4)
C(21)	0.627(1)	0.0726(3)	0.4287(8)	7.8(5)
C(22)	0.426(1)	0.1151(4)	0.5719(6)	9.6(6)
C(23)	0.1500(7)	0.2224(2)	0.0574(5)	3.0(3)
C(24)	0.047(1)	0.1896(3)	-0.002(1)	12.7(7)
C(25)	-0.1086(6)	0.1355(2)	0.2129(5)	2.9(3)
C(26)	-0.1097(9)	0.1544(5)	0.1021(6)	10.0(6)
C(27)	0.1332(7)	0.0797(2)	-0.0104(5)	2.7(3)
C(28)	0.008(1)	0.1091(4)	-0.0158(8)	11.7(6)

Positional parameters and B(eq) for 94046 Seidel/RRS

atom	x	y	z	B(eq)
H(1)	0.329	0.095	0.324	3.0
H(2)	0.427	0.129	0.268	3.0
H(3)	0.690	0.177	0.525	6.6
H(4)	0.658	0.183	0.395	6.6
H(5)	0.553	0.205	0.469	6.6
H(6)	0.575	0.043	0.419	8.7
H(7)	0.672	0.076	0.362	8.7
H(8)	0.704	0.069	0.492	8.7
H(9)	0.363	0.141	0.582	10.9
H(10)	0.366	0.087	0.568	10.9
H(11)	0.500	0.113	0.638	10.9
H(12)	0.096	0.248	0.087	3.6
H(13)	0.205	0.238	0.007	3.6
H(14)	0.087	0.180	-0.069	13.9
H(15)	-0.042	0.206	-0.030	13.9
H(16)	-0.156	0.105	0.203	3.3
H(17)	-0.165	0.155	0.257	3.3
H(18)	-0.120	0.191	0.112	11.7
H(19)	-0.196	0.146	0.053	11.7
H(20)	0.183	0.090	-0.071	3.3
H(21)	0.109	0.047	-0.025	3.3
H(22)	-0.069	0.087	0.009	11.8
H(23)	-0.032	0.117	-0.091	11.8

U values for 94046 Seidel/RRS

ATOM	U11	U22	U33	U12	U13	U23
W	0.0203 (1)	0.0201 (1)	0.0198 (1)	-0.0003 (1)	0.0037 (1)	-0.0006 (1)
Si	0.036 (1)	0.056 (1)	0.031 (1)	0.006 (1)	-0.0010 (9)	0.0056 (9)
F1	0.041 (2)	0.059 (2)	0.052 (2)	0.004 (2)	0.016 (2)	-0.017 (2)
F2	0.077 (3)	0.043 (2)	0.063 (3)	-0.000 (2)	0.009 (2)	-0.028 (2)
F3	0.053 (3)	0.034 (2)	0.079 (3)	-0.013 (2)	-0.020 (2)	-0.011 (2)
F4	0.026 (2)	0.056 (2)	0.109 (4)	-0.006 (2)	0.013 (2)	-0.015 (2)
F5	0.038 (2)	0.046 (2)	0.093 (3)	-0.002 (2)	0.019 (2)	-0.036 (2)
F6	0.050 (2)	0.034 (2)	0.047 (2)	-0.004 (2)	0.010 (2)	-0.011 (2)
F7	0.061 (3)	0.089 (3)	0.037 (2)	-0.004 (2)	0.013 (2)	-0.025 (2)
F8	0.066 (3)	0.113 (4)	0.022 (2)	-0.011 (3)	0.014 (2)	0.015 (2)
F9	0.068 (3)	0.058 (3)	0.054 (3)	0.003 (2)	0.009 (2)	0.028 (2)
F10	0.068 (3)	0.039 (2)	0.046 (2)	0.007 (2)	0.020 (2)	0.001 (2)
F11	0.036 (2)	0.031 (2)	0.079 (3)	-0.000 (2)	0.020 (2)	0.005 (2)
F12	0.033 (2)	0.044 (2)	0.086 (3)	0.004 (2)	0.018 (2)	0.001 (2)
F13	0.053 (3)	0.031 (2)	0.077 (3)	0.017 (2)	0.013 (2)	0.004 (2)
F14	0.062 (3)	0.023 (2)	0.099 (3)	-0.007 (2)	0.012 (2)	0.007 (2)
F15	0.034 (2)	0.038 (2)	0.071 (3)	-0.009 (2)	0.009 (2)	-0.000 (2)
N1	0.026 (3)	0.024 (3)	0.027 (3)	-0.005 (2)	0.001 (2)	0.003 (2)
N2	0.026 (3)	0.033 (3)	0.025 (3)	0.002 (2)	0.011 (2)	0.005 (2)
N3	0.030 (3)	0.033 (3)	0.021 (3)	0.006 (2)	-0.000 (2)	-0.003 (2)
N4	0.020 (3)	0.025 (3)	0.024 (3)	-0.000 (2)	0.003 (2)	0.002 (2)
C1	0.024 (4)	0.020 (3)	0.032 (3)	0.003 (3)	0.003 (3)	0.005 (3)
C2	0.028 (4)	0.033 (4)	0.034 (4)	0.001 (3)	0.006 (3)	0.002 (3)
C3	0.051 (5)	0.023 (4)	0.034 (4)	0.001 (3)	0.000 (3)	-0.006 (3)
C4	0.039 (4)	0.023 (4)	0.050 (4)	-0.007 (3)	-0.008 (4)	-0.002 (3)
C5	0.027 (4)	0.028 (4)	0.063 (5)	-0.001 (3)	0.007 (4)	-0.001 (3)
C6	0.034 (4)	0.022 (3)	0.041 (4)	-0.000 (3)	0.009 (3)	-0.009 (3)
C7	0.028 (4)	0.033 (4)	0.039 (4)	-0.011 (3)	0.000 (3)	-0.006 (3)
C8	0.037 (4)	0.065 (5)	0.022 (3)	-0.010 (4)	0.010 (3)	-0.022 (4)
C9	0.034 (4)	0.063 (5)	0.025 (4)	-0.010 (4)	0.009 (3)	-0.002 (4)
C10	0.034 (4)	0.042 (4)	0.038 (4)	-0.002 (3)	0.005 (3)	0.017 (3)
C11	0.031 (4)	0.033 (4)	0.035 (4)	-0.001 (3)	0.010 (3)	-0.003 (3)
C12	0.026 (4)	0.031 (3)	0.025 (3)	-0.006 (3)	0.006 (3)	-0.004 (3)
C13	0.033 (4)	0.026 (3)	0.019 (3)	-0.001 (3)	0.002 (3)	-0.006 (3)
C14	0.035 (4)	0.014 (3)	0.035 (4)	-0.000 (3)	0.008 (3)	-0.002 (3)

U values for 94046 Seidel/RPS

ATOM	U11	U22	U33	U12	U13	U23
C(15)	0.028(4)	0.034(4)	0.039(4)	-0.003(3)	0.011(3)	-0.009(3)
C(16)	0.043(4)	0.026(4)	0.043(4)	0.016(3)	0.006(3)	-0.007(3)
C(17)	0.046(5)	0.021(4)	0.051(4)	-0.003(3)	0.008(4)	-0.005(3)
C(18)	0.028(4)	0.039(4)	0.038(4)	-0.004(3)	0.002(3)	-0.011(3)
C(19)	0.040(4)	0.032(4)	0.038(4)	-0.009(3)	0.025(3)	-0.001(3)
C(20)	0.067(6)	0.083(6)	0.064(5)	-0.011(5)	-0.026(5)	-0.008(5)
C(21)	0.095(7)	0.083(6)	0.100(7)	0.034(6)	-0.033(6)	-0.009(6)
C(22)	0.060(6)	0.27(1)	0.034(5)	-0.052(7)	-0.003(5)	0.012(7)
C(23)	0.041(4)	0.034(4)	0.036(4)	-0.000(3)	-0.001(3)	0.012(3)
C(24)	0.125(9)	0.107(7)	0.19(1)	-0.092(7)	-0.131(9)	0.113(8)
C(25)	0.026(3)	0.049(4)	0.037(4)	-0.003(3)	0.007(3)	-0.006(3)
C(26)	0.032(5)	0.32(2)	0.034(5)	0.027(7)	0.008(4)	0.048(7)
C(27)	0.047(4)	0.031(3)	0.024(3)	-0.000(3)	0.001(3)	-0.010(3)
C(28)	0.128(9)	0.18(1)	0.101(8)	0.128(8)	-0.088(7)	-0.102(8)
H(1)	0.038					
H(2)	0.038					
H(3)	0.084					
H(4)	0.084					
H(5)	0.084					
H(6)	0.110					
H(7)	0.110					
H(8)	0.110					
H(9)	0.137					
H(10)	0.137					
H(11)	0.137					
H(12)	0.046					
H(13)	0.046					
H(14)	0.177					
H(15)	0.177					
H(16)	0.042					
H(17)	0.042					
H(18)	0.148					
H(19)	0.148					
H(20)	0.041					
H(21)	0.041					
H(22)	0.149					
H(23)	0.149					

Intramolecular Distances Involving the Nonhydrogen Atoms ($\sim 2\sigma$)

atom	atom	distance	atom	atom	distance
W	N(1)	1.973(4)	N(2)	C(12)	1.403(7)
W	N(2)	1.963(5)	N(2)	C(25)	1.498(7)
W	N(3)	1.968(4)	N(3)	C(13)	1.422(7)
W	N(4)	2.323(4)	N(3)	C(27)	1.475(6)
W	C(19)	1.768(6)	N(4)	C(24)	1.406(9)
Si	C(19)	1.876(6)	N(4)	C(26)	1.40(1)
Si	C(20)	1.871(8)	N(4)	C(28)	1.397(9)
Si	C(21)	1.839(9)	C(1)	C(2)	1.392(8)
Si	C(22)	1.820(9)	C(1)	C(6)	1.381(8)
F(1)	C(2)	1.347(7)	C(2)	C(3)	1.370(8)
F(2)	C(3)	1.343(7)	C(3)	C(4)	1.365(9)
F(3)	C(4)	1.348(6)	C(4)	C(5)	1.365(9)
F(4)	C(5)	1.343(7)	C(5)	C(6)	1.378(8)
F(5)	C(6)	1.326(7)	C(7)	C(8)	1.371(9)
F(6)	C(7)	1.338(6)	C(7)	C(12)	1.393(8)
F(7)	C(8)	1.347(7)	C(8)	C(9)	1.354(9)
F(8)	C(9)	1.338(7)	C(9)	C(10)	1.361(9)
F(9)	C(10)	1.344(7)	C(10)	C(11)	1.371(8)
F(10)	C(11)	1.341(7)	C(11)	C(12)	1.391(8)
F(11)	C(14)	1.343(6)	C(13)	C(14)	1.377(8)
F(12)	C(15)	1.347(7)	C(13)	C(18)	1.376(8)
F(13)	C(16)	1.327(6)	C(14)	C(15)	1.362(8)
F(14)	C(17)	1.330(7)	C(15)	C(16)	1.375(8)
F(15)	C(18)	1.345(7)	C(16)	C(17)	1.377(9)
N(1)	C(1)	1.411(7)	C(17)	C(18)	1.375(8)
N(1)	C(23)	1.471(7)	C(23)	C(24)	1.431(9)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Nonhydrogen Atoms (cont)

atom	atom	distance	atom	atom	distance
C(25)	C(26)	1.44(1)			
C(27)	C(28)	1.42(1)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intermolecular Distances Involving the Nonhydrogen Atoms (2d).

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
F(1)	F(7)	2.992(5)	55404	F(8)	F(15)	3.316(5)	55603
F(1)	C(24)	3.26(1)	4	F(8)	C(28)	3.33(1)	55601
F(1)	C(23)	3.355(7)	4	F(9)	F(9)	2.958(8)	55603
F(2)	F(13)	2.995(5)	65502	F(9)	F(10)	3.035(6)	55603
F(2)	F(5)	3.016(5)	4	F(9)	C(10)	3.143(7)	55603
F(2)	F(11)	3.322(5)	4	F(9)	C(11)	3.184(7)	55603
F(3)	F(14)	2.793(5)	65502	F(9)	C(21)	3.408(9)	65603
F(3)	C(26)	3.327(8)	65504	F(9)	F(13)	3.509(5)	65603
F(3)	C(24)	3.518(8)	65504	F(9)	F(12)	3.526(5)	65603
F(4)	F(7)	3.163(6)	65404	F(11)	C(25)	3.540(7)	65501
F(4)	F(6)	3.402(5)	65501	F(12)	C(18)	3.500(7)	65503
F(4)	C(26)	3.48(1)	65501	F(12)	C(25)	3.583(7)	65501
F(4)	C(25)	3.570(7)	65501	F(13)	C(22)	3.32(1)	65603
F(5)	C(26)	3.446(9)	65501	F(13)	C(27)	3.395(8)	65503
F(5)	C(3)	3.590(7)	55404	F(13)	C(9)	3.597(7)	65603
F(6)	C(23)	3.174(6)	4	F(14)	C(22)	3.474(9)	65603
F(6)	C(20)	3.35(1)	45501	F(14)	C(28)	3.60(1)	3
F(6)	C(24)	3.476(9)	4	F(15)	C(28)	3.46(1)	3
F(7)	C(20)	3.588(8)	45501	F(15)	C(27)	3.479(6)	3
F(8)	F(13)	3.103(5)	65603	C(14)	C(16)	3.518(9)	65503
F(8)	C(27)	3.183(6)	55601				

Contacts out to 3.60 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (2d).

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	W	N(2)	116.4(2)	W	N(4)	C(26)	107.7(4)
N(1)	W	N(3)	116.3(2)	W	N(4)	C(28)	106.9(4)
N(1)	W	N(4)	78.0(2)	C(24)	N(4)	C(26)	111.1(8)
N(1)	W	C(19)	102.0(2)	C(24)	N(4)	C(28)	110.6(9)
N(2)	W	N(3)	114.8(2)	C(26)	N(4)	C(28)	113.1(8)
N(2)	W	N(4)	78.2(2)	N(1)	C(1)	C(2)	121.4(5)
N(2)	W	C(19)	99.5(2)	N(1)	C(1)	C(6)	122.2(5)
N(3)	W	N(4)	78.0(2)	C(2)	C(1)	C(6)	116.4(5)
N(3)	W	C(19)	104.4(2)	F(1)	C(2)	C(1)	118.8(5)
N(4)	W	C(19)	177.3(2)	F(1)	C(2)	C(3)	118.9(6)
C(19)	Si	C(20)	108.8(3)	C(1)	C(2)	C(3)	122.3(6)
C(19)	Si	C(21)	111.4(3)	F(2)	C(3)	C(2)	119.6(6)
C(19)	Si	C(22)	110.8(3)	F(2)	C(3)	C(4)	120.8(6)
C(20)	Si	C(21)	108.1(4)	C(2)	C(3)	C(4)	119.6(6)
C(20)	Si	C(22)	107.0(4)	F(3)	C(4)	C(3)	120.5(6)
C(21)	Si	C(22)	110.5(5)	F(3)	C(4)	C(5)	119.5(6)
W	N(1)	C(1)	126.8(3)	C(3)	C(4)	C(5)	119.9(6)
W	N(1)	C(23)	119.6(3)	F(4)	C(5)	C(4)	119.4(6)
C(1)	N(1)	C(23)	113.2(4)	F(4)	C(5)	C(6)	120.3(6)
W	N(2)	C(12)	127.8(4)	C(4)	C(5)	C(6)	120.2(6)
W	N(2)	C(25)	119.5(3)	F(5)	C(6)	C(1)	120.5(5)
C(12)	N(2)	C(25)	112.6(5)	F(5)	C(6)	C(5)	117.9(6)
W	N(3)	C(13)	126.5(3)	C(1)	C(6)	C(5)	121.6(6)
W	N(3)	C(27)	119.8(3)	F(6)	C(7)	C(8)	119.2(6)
C(13)	N(3)	C(27)	113.5(4)	F(6)	C(7)	C(12)	118.9(6)
W	N(4)	C(24)	107.2(4)	C(8)	C(7)	C(12)	121.8(6)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
F(7)	C(8)	C(7)	119.6(6)	C(15)	C(16)	C(17)	118.9(6)
F(7)	C(8)	C(9)	119.9(6)	F(14)	C(17)	C(16)	119.8(6)
C(7)	C(8)	C(9)	120.5(6)	F(14)	C(17)	C(18)	120.8(6)
F(8)	C(9)	C(8)	120.7(6)	C(16)	C(17)	C(18)	119.5(6)
F(8)	C(9)	C(10)	119.9(6)	F(15)	C(18)	C(13)	119.4(5)
C(8)	C(9)	C(10)	119.4(6)	F(15)	C(18)	C(17)	117.9(6)
F(9)	C(10)	C(9)	120.6(6)	C(13)	C(18)	C(17)	122.7(6)
F(9)	C(10)	C(11)	118.6(6)	W	C(19)	Si	176.9(4)
C(9)	C(10)	C(11)	120.8(6)	N(1)	C(23)	C(24)	112.9(5)
F(10)	C(11)	C(10)	119.4(5)	N(4)	C(24)	C(23)	117.8(7)
F(10)	C(11)	C(12)	119.2(5)	N(2)	C(25)	C(26)	112.6(6)
C(10)	C(11)	C(12)	121.4(6)	N(4)	C(26)	C(25)	117.8(7)
N(2)	C(12)	C(7)	121.5(5)	N(3)	C(27)	C(28)	112.4(5)
N(2)	C(12)	C(11)	122.4(5)	N(4)	C(28)	C(27)	119.3(7)
C(7)	C(12)	C(11)	116.1(6)				
N(3)	C(13)	C(14)	122.9(5)				
N(3)	C(13)	C(18)	121.1(5)				
C(14)	C(13)	C(18)	116.0(5)				
F(11)	C(14)	C(13)	119.7(5)				
F(11)	C(14)	C(15)	117.5(5)				
C(13)	C(14)	C(15)	122.8(6)				
F(12)	C(15)	C(14)	121.3(6)				
F(12)	C(15)	C(16)	118.6(5)				
C(14)	C(15)	C(16)	120.1(6)				
F(13)	C(16)	C(15)	120.6(6)				
F(13)	C(16)	C(17)	120.5(6)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Torsion or Conformation Angles (2d).

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
W	N(1)	C(1)	C(2)	-101.0(6)	F(3)	C(4)	C(3)	C(2)	-179.8(5)
W	N(1)	C(1)	C(6)	81.0(7)	F(3)	C(4)	C(5)	F(4)	1.5(9)
W	N(1)	C(23)	C(24)	-13(1)	F(3)	C(4)	C(5)	C(6)	-179.1(6)
W	N(2)	C(12)	C(7)	114.2(6)	F(4)	C(5)	C(4)	C(3)	179.0(6)
W	N(2)	C(12)	C(11)	-67.3(7)	F(4)	C(5)	C(6)	F(5)	-1.0(9)
W	N(2)	C(25)	C(26)	-11.1(8)	F(4)	C(5)	C(6)	C(1)	178.7(6)
W	N(3)	C(13)	C(14)	-73.5(7)	F(5)	C(6)	C(1)	N(1)	-0.5(9)
W	N(3)	C(13)	C(18)	106.0(6)	F(5)	C(6)	C(1)	C(2)	-178.6(5)
W	N(3)	C(27)	C(28)	-12.8(9)	F(5)	C(6)	C(5)	C(4)	179.6(6)
W	N(4)	C(24)	C(23)	-22(1)	F(6)	C(7)	C(8)	F(7)	1.0(9)
W	N(4)	C(26)	C(25)	-22(1)	F(6)	C(7)	C(8)	C(9)	-178.4(5)
W	N(4)	C(28)	C(27)	-20(1)	F(6)	C(7)	C(12)	N(2)	-2.2(8)
W	C(19)	Si	C(20)	-60(7)	F(6)	C(7)	C(12)	C(11)	179.1(5)
W	C(19)	Si	C(21)	-179(7)	F(7)	C(8)	C(7)	C(12)	179.8(5)
W	C(19)	Si	C(22)	57(7)	F(7)	C(8)	C(9)	F(8)	0.8(9)
Si	C(19)	W	N(1)	60(7)	F(7)	C(8)	C(9)	C(10)	-179.2(5)
Si	C(19)	W	N(2)	-59(7)	F(8)	C(9)	C(8)	C(7)	-179.8(5)
Si	C(19)	W	N(3)	-178(7)	F(8)	C(9)	C(10)	F(9)	-1.7(9)
Si	C(19)	W	N(4)	-28(10)	F(8)	C(9)	C(10)	C(11)	178.5(6)
F(1)	C(2)	C(1)	N(1)	0.8(8)	F(9)	C(10)	C(9)	C(8)	178.3(6)
F(1)	C(2)	C(1)	C(6)	178.9(5)	F(9)	C(10)	C(11)	F(10)	1.0(9)
F(1)	C(2)	C(3)	F(2)	0.8(9)	F(9)	C(10)	C(11)	C(12)	-177.5(5)
F(1)	C(2)	C(3)	C(4)	178.9(6)	F(10)	C(11)	C(10)	C(9)	-179.3(6)
F(2)	C(3)	C(2)	C(1)	-179.7(5)	F(10)	C(11)	C(12)	N(2)	1.3(9)
F(2)	C(3)	C(4)	F(3)	-2(1)	F(10)	C(11)	C(12)	C(7)	179.9(5)
F(2)	C(3)	C(4)	C(5)	-179.3(5)	F(11)	C(14)	C(13)	N(3)	-2.5(9)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles

(cont)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
F(11)	C(14)	C(13)	C(18)	178.0(5)	N(2)	W	N(1)	C(23)	-69.1(5)
F(11)	C(14)	C(15)	F(12)	0.9(9)	N(2)	W	N(3)	C(13)	-102.0(5)
F(11)	C(14)	C(15)	C(16)	-179.0(5)	N(2)	W	N(3)	C(27)	72.7(5)
F(12)	C(15)	C(14)	C(13)	-179.8(6)	N(2)	W	N(4)	C(24)	131.6(7)
F(12)	C(15)	C(16)	F(13)	-0.2(9)	N(2)	W	N(4)	C(26)	11.9(6)
F(12)	C(15)	C(16)	C(17)	-178.6(6)	N(2)	W	N(4)	C(28)	-109.8(7)
F(13)	C(16)	C(15)	C(14)	179.6(5)	N(2)	C(12)	C(7)	C(8)	179.0(6)
F(13)	C(16)	C(17)	F(14)	1(1)	N(2)	C(12)	C(11)	C(10)	179.7(6)
F(13)	C(16)	C(17)	C(18)	179.8(5)	N(2)	C(25)	C(26)	N(4)	23(1)
F(14)	C(17)	C(16)	C(15)	179.1(5)	N(3)	W	N(1)	C(1)	-116.7(5)
F(14)	C(17)	C(18)	F(15)	0.6(9)	N(3)	W	N(1)	C(23)	71.0(5)
F(14)	C(17)	C(18)	C(13)	179.9(6)	N(3)	W	N(2)	C(12)	104.7(5)
F(15)	C(18)	C(13)	N(3)	0.5(9)	N(3)	W	N(2)	C(25)	-71.2(4)
F(15)	C(18)	C(13)	C(14)	-180.0(5)	N(3)	W	N(4)	C(24)	-109.6(7)
F(15)	C(18)	C(17)	C(16)	-178.5(6)	N(3)	W	N(4)	C(26)	130.8(7)
N(1)	W	N(2)	C(12)	-114.6(5)	N(3)	W	N(4)	C(28)	9.0(7)
N(1)	W	N(2)	C(25)	69.5(4)	N(3)	C(13)	C(14)	C(15)	178.3(5)
N(1)	W	N(3)	C(13)	117.3(5)	N(3)	C(13)	C(18)	C(17)	-178.8(6)
N(1)	W	N(3)	C(27)	-68.0(5)	N(3)	C(27)	C(28)	N(4)	22(1)
N(1)	W	N(4)	C(24)	10.9(7)	N(4)	W	N(1)	C(1)	173.3(5)
N(1)	W	N(4)	C(26)	-108.7(7)	N(4)	W	N(1)	C(23)	1.0(4)
N(1)	W	N(4)	C(28)	129.5(7)	N(4)	W	N(2)	C(12)	175.4(5)
N(1)	C(1)	C(2)	C(3)	-178.7(5)	N(4)	W	N(2)	C(25)	-0.5(4)
N(1)	C(1)	C(6)	C(5)	179.8(5)	N(4)	W	N(3)	C(13)	-172.8(5)
N(1)	C(23)	C(24)	N(4)	24(1)	N(4)	W	N(3)	C(27)	1.9(4)
N(2)	W	N(1)	C(1)	103.2(5)	C(1)	N(1)	W	C(19)	-3.9(5)

The sign is positive if when looking from atom 2 to atom 3 a *clockwise* motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles

(cont)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
C(1)	N(1)	C(23)	C(24)	173.7(8)	C(15)	C(14)	C(13)	C(18)	-1.3(9)
C(1)	C(2)	C(3)	C(4)	-1.6(9)	C(15)	C(16)	C(17)	C(18)	-2(1)
C(1)	C(6)	C(5)	C(4)	-1(1)	C(18)	C(13)	N(3)	C(27)	-69.0(7)
C(2)	C(1)	N(1)	C(23)	71.7(7)	C(19)W	N(1)	C(23)		-176.2(5)
C(2)	C(1)	C(6)	C(5)	1.7(9)	C(19)W	N(2)	C(25)		178.1(4)
C(2)	C(3)	C(4)	C(5)	3(1)	C(19)W	N(3)	C(27)		-179.5(4)
C(3)	C(2)	C(1)	C(6)	-0.6(9)	C(19)W	N(4)	C(24)		100(4)
C(3)	C(4)	C(5)	C(6)	-2(1)	C(19)W	N(4)	C(26)		-19(5)
C(6)	C(1)	N(1)	C(23)	-106.3(6)	C(19)W	N(4)	C(28)		-141(4)
C(7)	C(8)	C(9)	C(10)	0(1)	C(23)	C(24)	N(4)	C(26)	95(1)
C(7)	C(12)	N(2)	C(25)	-69.7(7)	C(23)	C(24)	N(4)	C(28)	-138(1)
C(7)	C(12)	C(11)	C(10)	-1.7(9)	C(24)	N(4)	C(26)	C(25)	-139.3(9)
C(8)	C(7)	C(12)	C(11)	0.3(9)	C(24)	N(4)	C(28)	C(27)	97(1)
C(8)	C(9)	C(10)	C(11)	-2(1)	C(25)	C(26)	N(4)	C(28)	96(1)
C(9)	C(8)	C(7)	C(12)	0(1)	C(26)	N(4)	C(28)	C(27)	-138(1)
C(9)	C(10)	C(11)	C(12)	2(1)					
C(11)	C(12)	N(2)	C(25)	108.9(6)					
C(12)	N(2)	W	C(19)	-6.0(5)					
C(12)	N(2)	C(25)	C(26)	172.4(7)					
C(13)	N(3)	W	C(19)	5.8(5)					
C(13)	N(3)	C(27)	C(28)	162.6(8)					
C(13)	C(14)	C(15)	C(16)	0(1)					
C(13)	C(18)	C(17)	C(16)	1(1)					
C(14)	C(13)	N(3)	C(27)	111.5(6)					
C(14)	C(13)	C(18)	C(17)	0.7(9)					
C(14)	C(15)	C(16)	C(17)	1(1)					

The sign is positive if when looking from atom 2 to atom 3 a *clockwise* motion of atom 1 would superimpose it on atom 4.

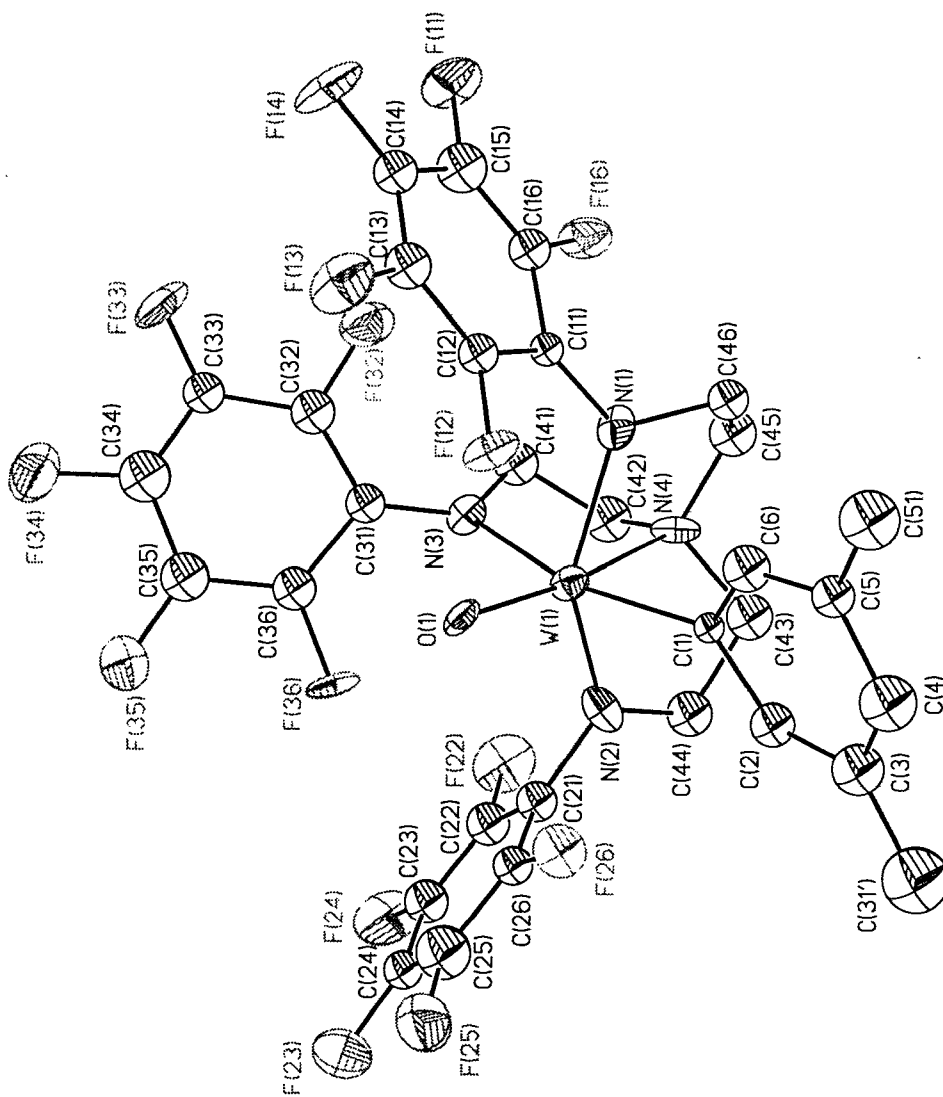


Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\frac{1}{6}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W(1)	-23 (1)	1102 (1)	2398 (1)	31 (1)
F(11)	-2805 (7)	261 (10)	1428 (6)	67 (5)
F(12)	-1045 (5)	2734 (9)	2027 (5)	46 (4)
F(13)	-2232 (6)	3150 (9)	2045 (7)	67 (4)
F(14)	-3140 (6)	1948 (11)	1711 (7)	76 (5)
F(16)	-1620 (6)	-193 (9)	1411 (6)	54 (4)
F(22)	963 (7)	-533 (10)	3625 (7)	78 (5)
F(23)	1712 (8)	1723 (15)	4879 (7)	105 (7)
F(24)	1399 (8)	-54 (13)	4647 (7)	93 (6)
F(25)	1535 (8)	2952 (12)	4074 (6)	84 (5)
F(26)	1108 (6)	2478 (9)	3041 (6)	53 (4)
F(32)	-1843 (6)	-241 (11)	2666 (6)	69 (5)
F(33)	-2594 (6)	112 (11)	3452 (6)	72 (5)
F(34)	-2158 (7)	947 (12)	4410 (7)	81 (5)
F(35)	-949 (7)	1434 (11)	4552 (6)	76 (5)
F(36)	-174 (5)	995 (9)	3803 (5)	50 (4)
O(1)	-250 (6)	1921 (10)	2815 (6)	34 (4)
N(1)	-659 (8)	1008 (13)	1717 (7)	38 (5)
N(2)	778 (9)	701 (12)	2742 (7)	39 (5)
N(3)	-580 (8)	163 (11)	2790 (7)	32 (5)
N(4)	172 (8)	-268 (12)	1980 (8)	37 (5)
C(1)	483 (9)	1927 (13)	1815 (8)	19 (5)
C(2)	1126 (11)	2014 (16)	1843 (10)	42 (7)
C(3)	1470 (13)	2585 (18)	1547 (11)	56 (8)
C(4)	1129 (13)	3107 (19)	1159 (11)	63 (8)
C(5)	499 (11)	3022 (15)	1074 (9)	35 (6)
C(6)	220 (12)	2490 (16)	1403 (10)	45 (7)
C(11)	-1264 (10)	1269 (14)	1724 (8)	24 (6)
C(12)	-1489 (11)	2098 (16)	1890 (9)	33 (6)
C(13)	-2103 (12)	2306 (18)	1874 (10)	44 (7)
C(14)	-2559 (12)	1726 (17)	1730 (9)	41 (7)
C(15)	-2371 (13)	897 (19)	1565 (11)	56 (8)
C(16)	-1766 (11)	649 (17)	1573 (9)	39 (7)
C(21)	1037 (11)	959 (17)	3293 (10)	40 (7)
C(22)	1112 (12)	351 (18)	3723 (10)	47 (7)
C(23)	1326 (12)	539 (18)	4243 (11)	50 (7)
C(24)	1483 (11)	1415 (16)	4379 (10)	37 (7)
C(25)	1388 (14)	2062 (22)	3975 (12)	70 (9)
C(26)	1160 (10)	1852 (17)	3422 (10)	36 (6)
C(31)	-962 (12)	390 (16)	3160 (10)	38 (7)
C(31')	2152 (15)	2638 (23)	1641 (13)	93 (11)
C(32)	-1580 (12)	153 (18)	3129 (11)	48 (7)
C(33)	-2020 (13)	315 (16)	3521 (10)	42 (7)
C(34)	-1795 (14)	779 (19)	3971 (12)	64 (9)
C(35)	-1176 (13)	1028 (20)	4081 (12)	57 (8)
C(36)	-775 (12)	824 (16)	3677 (10)	46 (7)
C(41)	-620 (11)	-726 (17)	2546 (11)	51 (8)
C(42)	-11 (12)	-986 (18)	2360 (11)	57 (7)

C(43)	849(12)	-230(19)	1936(10)	54(8)
C(44)	1164(12)	-1(18)	2494(10)	52(8)
C(45)	-160(12)	-341(17)	1420(10)	54(8)
C(46)	-437(11)	564(15)	1219(9)	37(7)
C(51)	153(13)	3642(19)	648(11)	66(9)

Table 4. Bond lengths [Å] and angles [°] for 1b.

W(1)-O(1)	1.685(14)	W(1)-N(2)	1.96(2)
W(1)-N(1)	2.06(2)	W(1)-N(3)	2.13(2)
W(1)-C(1)	2.23(2)	W(1)-N(4)	2.33(2)
F(11)-C(15)	1.36(3)	F(12)-C(12)	1.37(3)
F(13)-C(13)	1.36(3)	F(14)-C(14)	1.30(3)
F(16)-C(16)	1.36(3)	F(22)-C(22)	1.37(3)
F(23)-C(24)	1.35(3)	F(24)-C(23)	1.32(3)
F(25)-C(25)	1.38(3)	F(26)-C(26)	1.31(3)
F(32)-C(32)	1.35(3)	F(33)-C(33)	1.28(3)
F(34)-C(34)	1.40(3)	F(35)-C(35)	1.35(3)
F(36)-C(36)	1.34(3)	N(1)-C(11)	1.37(3)
N(1)-C(46)	1.49(3)	N(2)-C(21)	1.45(3)
N(2)-C(44)	1.50(3)	N(3)-C(31)	1.32(3)
N(3)-C(41)	1.45(3)	N(4)-C(42)	1.49(3)
N(4)-C(43)	1.48(3)	N(4)-C(45)	1.48(3)
C(1)-C(6)	1.39(3)	C(1)-C(2)	1.40(3)
C(2)-C(3)	1.37(3)	C(3)-C(4)	1.38(3)
C(3)-C(31')	1.48(4)	C(4)-C(5)	1.37(3)
C(5)-C(6)	1.31(3)	C(5)-C(51)	1.53(3)
C(11)-C(12)	1.40(3)	C(11)-C(16)	1.45(3)
C(12)-C(13)	1.37(3)	C(13)-C(14)	1.34(3)
C(14)-C(15)	1.37(3)	C(15)-C(16)	1.36(3)
C(21)-C(26)	1.39(3)	C(21)-C(22)	1.38(3)
C(22)-C(23)	1.33(3)	C(23)-C(24)	1.38(3)
C(24)-C(25)	1.38(3)	C(25)-C(26)	1.42(4)
C(31)-C(32)	1.38(3)	C(31)-C(36)	1.43(3)
C(32)-C(33)	1.42(3)	C(33)-C(34)	1.34(3)
C(34)-C(35)	1.40(4)	C(35)-C(36)	1.40(3)
C(41)-C(42)	1.49(3)	C(43)-C(44)	1.50(3)
C(45)-C(46)	1.54(3)		
O(1)-W(1)-N(2)	105.3(7)	O(1)-W(1)-N(1)	108.4(7)
N(2)-W(1)-N(1)	146.0(7)	O(1)-W(1)-N(3)	90.2(7)
N(2)-W(1)-N(3)	97.4(7)	N(1)-W(1)-N(3)	86.7(7)
O(1)-W(1)-C(1)	99.5(7)	N(2)-W(1)-C(1)	88.2(7)
N(1)-W(1)-C(1)	82.3(7)	N(3)-W(1)-C(1)	167.2(7)
O(1)-W(1)-N(4)	165.2(7)	N(2)-W(1)-N(4)	74.2(7)
N(1)-W(1)-N(4)	74.3(7)	N(3)-W(1)-N(4)	75.3(7)
C(1)-W(1)-N(4)	95.3(7)	C(11)-N(1)-C(46)	121(2)
C(11)-N(1)-W(1)	123.3(13)	C(46)-N(1)-W(1)	115.7(13)
C(21)-N(2)-C(44)	111(2)	C(21)-N(2)-W(1)	124.7(14)
C(44)-N(2)-W(1)	123.5(14)	C(31)-N(3)-C(41)	120(2)
C(31)-N(3)-W(1)	123(2)	C(41)-N(3)-W(1)	115.9(14)
C(42)-N(4)-C(43)	113(2)	C(42)-N(4)-C(45)	112(2)
C(43)-N(4)-C(45)	110(2)	C(42)-N(4)-W(1)	107.3(14)
C(43)-N(4)-W(1)	102.4(14)	C(45)-N(4)-W(1)	111.5(14)
C(6)-C(1)-C(2)	109(2)	C(6)-C(1)-W(1)	126(2)
C(2)-C(1)-W(1)	124(2)	C(3)-C(2)-C(1)	128(2)
C(2)-C(3)-C(4)	115(3)	C(2)-C(3)-C(31')	122(3)
C(4)-C(3)-C(31')	123(3)	C(5)-C(4)-C(3)	121(3)
C(6)-C(5)-C(4)	118(2)	C(6)-C(5)-C(51)	123(2)
C(4)-C(5)-C(51)	118(2)	C(5)-C(6)-C(1)	128(2)
N(1)-C(11)-C(12)	128(2)	N(1)-C(11)-C(16)	121(2)
C(12)-C(11)-C(16)	111(2)	C(13)-C(12)-F(12)	121(2)
C(13)-C(12)-C(11)	124(2)	F(12)-C(12)-C(11)	115(2)

C(14)-C(13)-F(13)	121(2)	C(14)-C(13)-C(12)	124(3)
F(13)-C(13)-C(12)	115(2)	F(14)-C(14)-C(13)	123(2)
F(14)-C(14)-C(15)	122(2)	C(13)-C(14)-C(15)	115(3)
C(16)-C(15)-F(11)	118(2)	C(16)-C(15)-C(14)	123(3)
F(11)-C(15)-C(14)	119(2)	C(15)-C(16)-F(16)	120(2)
C(15)-C(16)-C(11)	122(2)	F(16)-C(16)-C(11)	118(2)
C(26)-C(21)-C(22)	117(2)	C(26)-C(21)-N(2)	121(2)
C(22)-C(21)-N(2)	122(2)	C(23)-C(22)-C(21)	126(3)
C(23)-C(22)-F(22)	115(2)	C(21)-C(22)-F(22)	120(2)
F(24)-C(23)-C(22)	125(3)	F(24)-C(23)-C(24)	117(2)
C(22)-C(23)-C(24)	119(3)	F(23)-C(24)-C(25)	115(2)
F(23)-C(24)-C(23)	127(2)	C(25)-C(24)-C(23)	119(3)
F(25)-C(25)-C(24)	122(3)	F(25)-C(25)-C(26)	116(3)
C(24)-C(25)-C(26)	122(3)	F(26)-C(26)-C(21)	122(2)
F(26)-C(26)-C(25)	121(2)	C(21)-C(26)-C(25)	118(3)
N(3)-C(31)-C(32)	124(2)	N(3)-C(31)-C(36)	124(2)
C(32)-C(31)-C(36)	111(2)	F(32)-C(32)-C(31)	120(2)
F(32)-C(32)-C(33)	112(2)	C(31)-C(32)-C(33)	129(3)
F(33)-C(33)-C(34)	121(2)	F(33)-C(33)-C(32)	125(2)
C(34)-C(33)-C(32)	114(3)	C(35)-C(34)-F(34)	114(3)
C(35)-C(34)-C(33)	125(3)	F(34)-C(34)-C(33)	121(3)
F(35)-C(35)-C(34)	124(3)	F(35)-C(35)-C(36)	119(2)
C(34)-C(35)-C(36)	117(3)	F(36)-C(36)-C(35)	117(2)
F(36)-C(36)-C(31)	119(2)	C(35)-C(36)-C(31)	124(3)
N(3)-C(41)-C(42)	110(2)	N(4)-C(42)-C(41)	107(2)
N(4)-C(43)-C(44)	109(2)	N(2)-C(44)-C(43)	107(2)
N(4)-C(45)-C(46)	112(2)	N(1)-C(46)-C(45)	106(2)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(h a^*)^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
W(1)	26(1)	26(1)	40(1)	-3(1)	2(1)	1(1)
F(11)	48(10)	51(10)	101(12)	-9(9)	8(8)	-26(8)
F(12)	25(8)	39(9)	73(10)	0(7)	-1(7)	-1(7)
F(13)	54(10)	41(10)	104(13)	-3(9)	10(9)	10(8)
F(14)	19(9)	82(12)	128(14)	2(11)	7(8)	-5(8)
F(16)	46(9)	42(9)	73(10)	-17(8)	-4(7)	-8(7)
F(22)	84(13)	47(11)	103(13)	28(9)	3(10)	10(9)
F(23)	71(13)	183(20)	57(11)	-12(12)	-19(9)	-3(13)
F(24)	75(13)	122(16)	80(12)	54(12)	-13(9)	1(11)
F(25)	91(13)	99(15)	66(11)	-8(10)	17(9)	-20(11)
F(26)	68(11)	32(9)	57(9)	8(8)	6(8)	2(8)
F(32)	49(10)	90(12)	66(11)	19(10)	0(8)	-16(9)
F(33)	22(9)	102(13)	91(12)	16(10)	13(8)	0(9)
F(34)	62(11)	94(14)	88(12)	-1(11)	21(9)	13(10)
F(35)	75(11)	83(12)	71(11)	-18(9)	14(9)	2(10)
F(36)	22(8)	55(10)	71(10)	2(8)	-8(7)	-22(7)
O(1)	18(9)	36(10)	50(10)	-10(8)	13(7)	-8(8)
N(1)	33(13)	41(13)	40(12)	8(11)	6(9)	21(11)
N(2)	64(15)	24(12)	29(12)	0(9)	2(10)	4(11)
N(3)	33(13)	14(11)	49(13)	0(10)	8(10)	3(9)
N(4)	31(13)	30(12)	47(13)	0(10)	-18(10)	-5(10)