Table 1S Crystal data and structure refinement for Re compound.

Identification code	pete12z	
Empirical formula	C_{25} H_{35} F N_3 O_3 Re S_2	
Formula weight	694.88	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.046(2) Å	α= 90°.
	b = 8.084(2) Å	β= 90°.
	c = 48.850(10) Å	γ = 90°.
Volume	2782.5(10) Å^3	
Z	4	
Density (calculated)	1.659 Mg/m^3	
Absorption coefficient	10.256 mm^{-1}	
F(000)	1384	
Crystal size	0.42 x 0.20 x 0.06 mm^3	
Theta range for data collection	1.81 to 58.22°.	
Index ranges	-7<=h<=1, -1<=k<=8, 0<=l<=53	
Reflections collected	2896	
Independent reflections	2642 [R(int) = 0.0224]	
Completeness to theta = 58.22°	99.9 %	
Absorption correction	Integration	
Max. and min. transmission	0.5409 and 0.1380	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2642 / 0 / 317	
Goodness-of-fit on F^2	1.144	
Final R indices [I>2sigma(I)]	R1 = 0.0339, wR2 = 0.0961	
R indices (all data)	R1 = 0.0393, wR2 = 0.1024	
Absolute structure parameter	-0.07(2)	
Extinction coefficient	0.00046(5)	
Largest diff. peak and hole	0.895 and -0.845 e.Å^{-3}	

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

	x	y	z	U(eq)
Re(1)	2304(1)	13542(1)	8033(1)	44(1)
O(1)	3588(13)	14237(11)	8303(2)	67(2)
C(1)	-4210(20)	15191(14)	8999(3)	64(4)
C(2)	-4040(20)	13580(16)	9171(2)	63(3)
C(3)	-1960(20)	13479(16)	9295(2)	67(3)
C(1')	-1950(30)	12161(16)	9518(2)	75(4)
C(2')	-3070(30)	12050(20)	9730(3)	115(7)
C(3')	-3030(40)	10860(30)	9936(4)	145(10)
C(4')	-1560(50)	9800(20)	9921(4)	134(11)
C(5')	-300(40)	9790(20)	9718(4)	115(7)
C(6')	-500(30)	11016(19)	9514(3)	91(5)
F(1')	-1400(30)	8616(13)	10119(2)	175(6)
C(4)	-1380(30)	15160(17)	9407(3)	89(6)
C(5)	-1850(20)	16612(16)	9207(2)	70(4)
C(6)	-3600(30)	17573(19)	9299(3)	100(7)
C(7)	-5220(30)	16580(20)	9174(3)	93(6)
N(8)	-2331(19)	15846(10)	8943(2)	60(3)
C(9)	-2290(20)	17054(12)	8720(2)	54(3)
C(10)	-2431(17)	16185(11)	8440(2)	49(3)
C(11)	-555(17)	15437(13)	8368(2)	45(3)
N(12)	-603(14)	14116(10)	8148(2)	44(2)
C(13)	-1554(18)	12625(11)	8259(2)	48(3)
C(14)	-569(18)	11070(12)	8167(2)	48(3)
O(2)	-1323(14)	9733(9)	8194(2)	66(2)
N(15)	1199(12)	11314(10)	8061(2)	44(2)
C(16)	2159(19)	9814(14)	7950(3)	61(3)
C(17)	4209(19)	10147(16)	7897(3)	64(4)
S(18)	4376(5)	12224(4)	7751(1)	60(1)
S(19)	1803(5)	15414(3)	7694(1)	61(1)
C(20)	-555(18)	16125(13)	7771(2)	54(3)
C(21)	-1656(17)	14753(13)	7900(2)	49(3)

C(22)	-4430(30)	12116(19)	8989(3)	75(4)
O(3)	-3170(20)	11339(12)	8877(2)	93(3)
C(23)	-6560(30)	11790(20)	8956(4)	125(7)
C(24)	-6990(40)	10540(20)	8742(4)	160(12)

Table 3S. Bond lengths [Å] and angles [°] for Re compound.

Re(1)-O(1)	1.694(8)	C(17)-S(18)	1.828(13)
Re(1)-N(15)	1.967(9)	S(19)-C(20)	1.798(13)
Re(1)-N(12)	2.174(10)	C(20)-C(21)	1.492(14)
Re(1)-S(18)	2.273(3)	C(22)-O(3)	1.22(2)
Re(1)-S(19)	2.273(3)	C(22)-C(23)	1.53(3)
C(1)-N(8)	1.46(2)	C(23)-C(24)	1.48(2)
C(1)-C(2)	1.556(16)		
C(1)-C(7)	1.580(19)	O(1)-Re(1)-N(15)	117.5(4)
C(2)-C(22)	1.51(2)	O(1)-Re(1)-N(12)	103.4(4)
C(2)-C(3)	1.59(2)	N(15)-Re(1)-N(12)	78.8(3)
C(3)-C(4)	1.521(18)	O(1)-Re(1)-S(18)	106.5(3)
C(3)-C(1')	1.524(16)	N(15)-Re(1)-S(18)	82.3(3)
C(1')-C(2')	1.31(2)	N(12)-Re(1)-S(18)	149.6(2)
C(1')-C(6')	1.37(2)	O(1)-Re(1)-S(19)	115.4(3)
C(2')-C(3')	1.39(2)	N(15)-Re(1)-S(19)	126.8(3)
C(3')-C(4')	1.34(3)	N(12)-Re(1)-S(19)	84.3(2)
C(4')-C(5')	1.33(3)	S(18)-Re(1)-S(19)	88.24(12)
C(4')-F(1')	1.365(18)	N(8)-C(1)-C(2)	109.6(12)
C(5')-C(6')	1.41(2)	N(8)-C(1)-C(7)	104.5(11)
C(4)-C(5)	1.563(17)	C(2)-C(1)-C(7)	109.8(11)
C(5)-N(8)	1.469(14)	C(22)-C(2)-C(1)	108.9(10)
C(5)-C(6)	1.53(2)	C(22)-C(2)-C(3)	110.7(13)
C(6)-C(7)	1.52(2)	C(1)-C(2)-C(3)	108.7(12)
N(8)-C(9)	1.465(13)	C(4)-C(3)-C(1')	111.5(10)
C(9)-C(10)	1.537(13)	C(4)-C(3)-C(2)	109.8(14)
C(10)-C(11)	1.496(16)	C(1')-C(3)-C(2)	108.4(13)
C(11)-N(12)	1.515(12)	C(2')-C(1')-C(6')	114.6(13)
N(12)-C(13)	1.482(13)	C(2')-C(1')-C(3)	127.7(15)
N(12)-C(21)	1.512(13)	C(6')-C(1')-C(3)	117.6(14)
C(13)-C(14)	1.505(15)	C(1')-C(2')-C(3')	127(2)
C(14)-O(2)	1.212(13)	C(4')-C(3')-C(2')	115(2)
C(14)-N(15)	1.363(15)	C(5')-C(4')-C(3')	123.9(17)
N(15)-C(16)	1.490(13)	C(5')-C(4')-F(1')	118(3)
C(16)-C(17)	1.492(19)	C(3')-C(4')-F(1')	118(3)

C(4')-C(5')-C(6')	117(2)	C(11)-N(12)-Re(1)	108.2(7)
C(1')-C(6')-C(5')	122.3(18)	N(12)-C(13)-C(14)	111.2(9)
C(3)-C(4)-C(5)	112.9(11)	O(2)-C(14)-N(15)	124.9(11)
N(8)-C(5)-C(6)	106.8(13)	O(2)-C(14)-C(13)	120.6(11)
N(8)-C(5)-C(4)	106.4(10)	N(15)-C(14)-C(13)	114.5(9)
C(6)-C(5)-C(4)	111.7(12)	C(14)-N(15)-C(16)	115.8(9)
C(7)-C(6)-C(5)	102.6(10)	C(14)-N(15)-Re(1)	121.3(7)
C(6)-C(7)-C(1)	104.9(14)	C(16)-N(15)-Re(1)	122.7(7)
C(1)-N(8)-C(9)	113.5(11)	N(15)-C(16)-C(17)	110.9(10)
C(1)-N(8)-C(5)	101.4(11)	C(16)-C(17)-S(18)	107.2(10)
C(9)-N(8)-C(5)	111.6(8)	C(17)-S(18)-Re(1)	98.8(5)
N(8)-C(9)-C(10)	110.8(8)	C(20)-S(19)-Re(1)	101.7(4)
C(11)-C(10)-C(9)	109.8(10)	C(21)-C(20)-S(19)	109.4(8)
C(10)-C(11)-N(12)	115.6(9)	C(20)-C(21)-N(12)	109.7(9)
C(13)-N(12)-C(21)	110.4(9)	O(3)-C(22)-C(2)	122.6(16)
C(13)-N(12)-C(11)	108.9(8)	O(3)-C(22)-C(23)	125.2(16)
C(21)-N(12)-C(11)	109.9(8)	C(2)-C(22)-C(23)	112.1(17)
C(13)-N(12)-Re(1)	110.3(7)	C(24)-C(23)-C(22)	113(2)
C(21)-N(12)-Re(1)	109.1(6)		

Symmetry transformations used to generate equivalent atoms:

Table 4S. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Re compound. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	38(1)	40(1)	54(1)	-6(1)	0(1)	-13(1)
O(1)	58(5)	66(5)	77(5)	-12(4)	-9(5)	-19(5)
C(1)	85(11)	40(6)	66(8)	9(6)	0(8)	0(7)
C(2)	83(9)	53(7)	52(7)	8(6)	22(6)	7(9)
C(3)	89(10)	56(7)	56(6)	1(6)	9(7)	-6(9)
C(1')	118(13)	63(7)	43(6)	5(5)	-12(8)	6(10)
C(2')	170(20)	111(12)	67(9)	22(8)	17(12)	51(15)
C(3')	230(30)	134(16)	72(10)	48(12)	13(16)	30(20)
C(4')	250(30)	95(13)	60(9)	29(10)	-53(16)	-22(18)
C(5')	170(20)	87(12)	91(12)	28(11)	-40(14)	12(14)
C(6')	100(13)	86(12)	88(10)	30(9)	-13(9)	8(11)
F(1')	294(19)	127(8)	105(7)	63(6)	-51(10)	-7(11)
C(4)	133(16)	75(9)	59(7)	0(7)	-12(9)	-18(10)
C(5)	100(11)	58(7)	52(6)	-4(6)	2(7)	-22(9)
C(6)	180(20)	55(8)	69(8)	-16(7)	21(11)	14(12)
C(7)	117(14)	77(10)	83(10)	18(9)	49(10)	29(12)
N(8)	89(8)	37(4)	54(5)	-5(4)	12(6)	-4(6)
C(9)	73(8)	40(5)	49(5)	-3(4)	11(6)	2(6)
C(10)	58(7)	37(5)	53(5)	5(4)	-2(6)	-8(6)
C(11)	53(7)	34(6)	47(6)	-2(5)	5(5)	-8(6)
N(12)	50(6)	34(5)	48(5)	-1(4)	0(4)	-12(4)
C(13)	55(7)	34(5)	55(6)	10(5)	-1(6)	-12(6)
C(14)	54(7)	27(6)	63(7)	2(5)	-3(6)	-5(5)
O(2)	71(6)	39(4)	89(6)	3(4)	19(5)	-8(5)
N(15)	42(5)	38(4)	54(5)	-12(4)	-3(4)	-1(4)
C(16)	54(8)	42(6)	87(8)	-14(5)	22(7)	-3(6)
C(17)	49(8)	48(7)	96(10)	-3(7)	-9(7)	-2(7)
S(18)	45(2)	58(2)	79(2)	-17(2)	10(2)	-13(2)
S(19)	68(2)	48(2)	65(2)	8(1)	16(2)	-15(2)
C(20)	69(8)	45(6)	47(6)	12(5)	0(6)	-17(6)
C(21)	51(7)	50(6)	47(5)	4(5)	-15(5)	-16(6)

C(22)	101(13)	62(8)	62(8)	21(7)	-6(9)	-13(9)
O(3)	127(10)	67(6)	86(6)	-9(5)	9(7)	5(8)
C(23)	125(18)	102(13)	147(16)	-6(12)	-15(15)	-37(14)
C(24)	220(30)	87(11)	175(18)	31(12)	-110(20)	-67(17)

Table 5S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Re compound.

	x	y	z	U(eq)
H(1A)	-4908	14985	8828	76
H(2A)	-4972	13604	9320	75
H(3A)	-1072	13156	9150	80
H(2'A)	-4004	12856	9745	137
H(3'A)	-3945	10798	10073	174
H(5'A)	672	9014	9711	138
H(6'A)	369	11049	9371	110
H(4A)	-29	15156	9443	107
H(4B)	-2031	15349	9579	107
H(5A)	-760	17352	9187	84
H(6A)	-3698	17602	9497	120
H(6B)	-3583	18697	9229	120
H(7A)	-6004	17280	9058	111
H(7B)	-6009	16098	9315	111
H(9A)	-1125	17686	8728	65
H(9B)	-3347	17817	8740	65
H(10A)	-3393	15329	8448	59
H(10B)	-2797	16978	8301	59
H(11A)	-12	14958	8533	54
H(11B)	287	16314	8309	54
H(13A)	-2863	12603	8198	58
H(13B)	-1552	12672	8458	58
H(16A)	1545	9479	7781	73
H(16B)	2040	8914	8080	73
H(17A)	4715	9337	7770	77
H(17B)	4927	10083	8066	77
H(20A)	-493	17060	7895	64
H(20B)	-1182	16481	7604	64
H(21A)	-1828	13863	7769	59
H(21B)	-2899	15151	7954	59

H(23A)	-7072	11416	9129	150
H(23B)	-7190	12818	8908	150
H(24A)	-8339	10409	8726	240
H(24B)	-6432	9496	8793	240
H(24C)	-6473	10891	8570	240

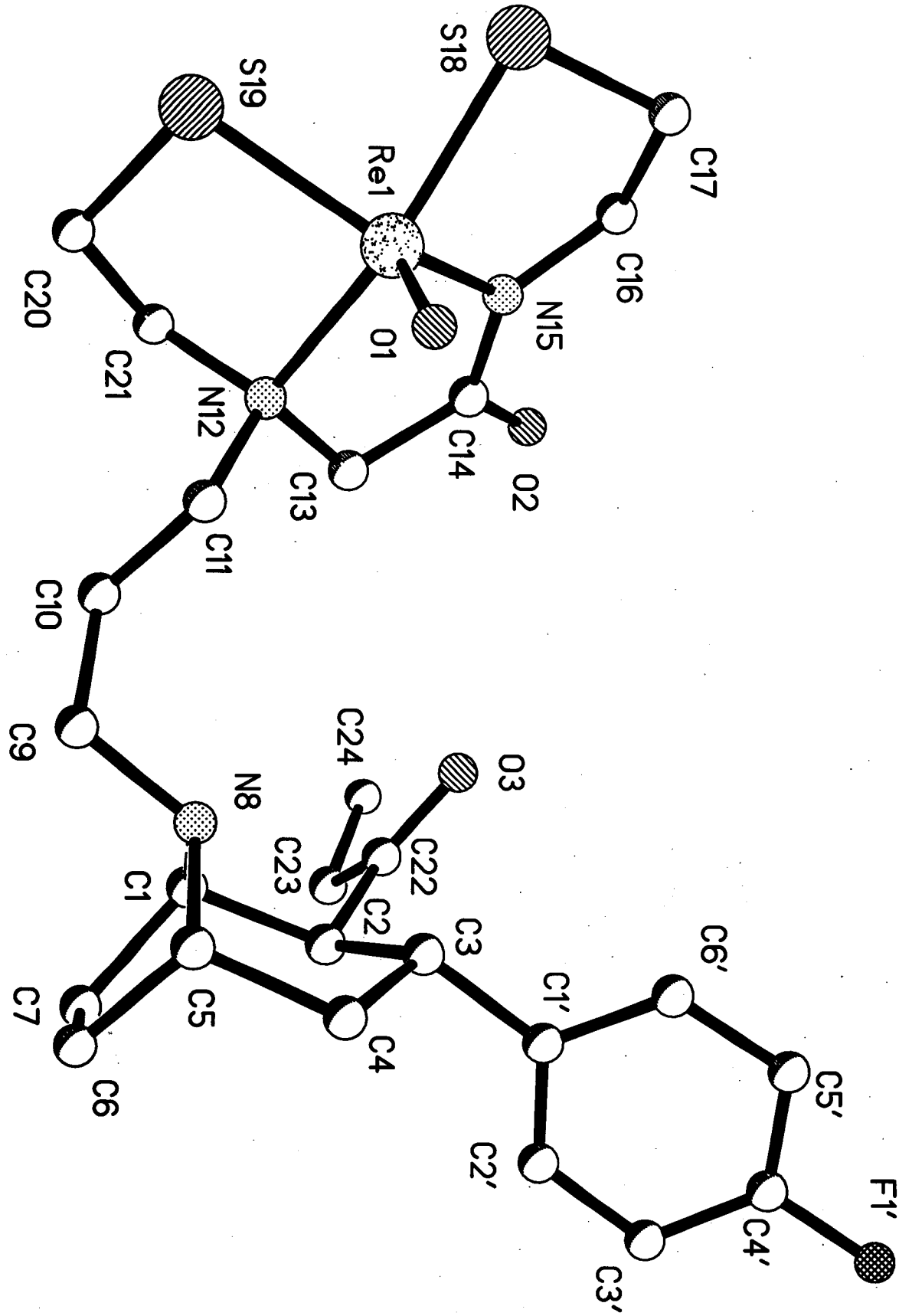
Table 6S. Torsion angles [°] for Re compound.

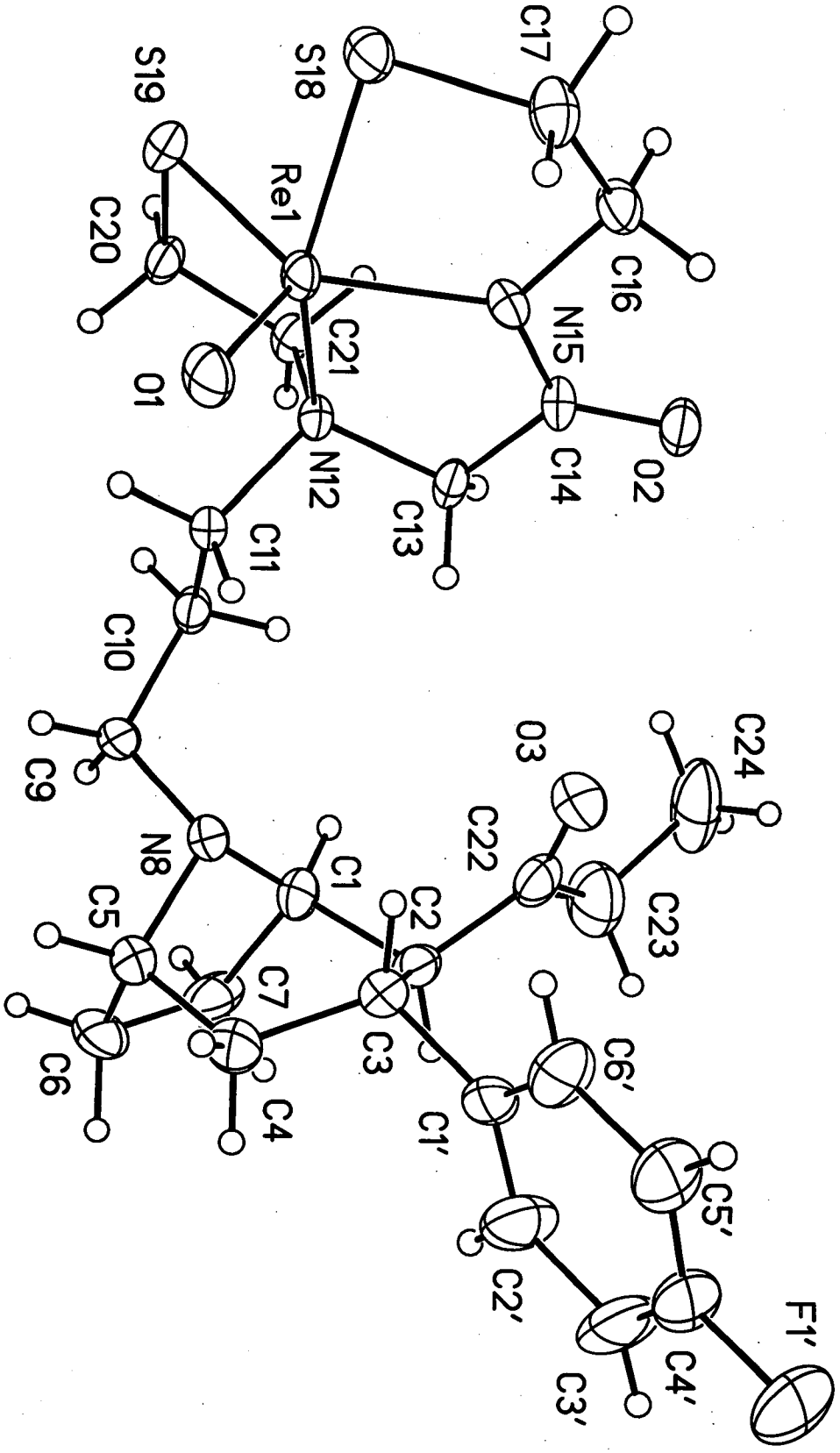
N(8)-C(1)-C(2)-C(22)	-105.2(14)
C(7)-C(1)-C(2)-C(22)	140.6(15)
N(8)-C(1)-C(2)-C(3)	15.6(14)
C(7)-C(1)-C(2)-C(3)	-98.7(15)
C(22)-C(2)-C(3)-C(4)	163.5(11)
C(1)-C(2)-C(3)-C(4)	43.9(13)
C(22)-C(2)-C(3)-C(1')	-74.5(12)
C(1)-C(2)-C(3)-C(1')	165.9(9)
C(4)-C(3)-C(1')-C(2')	67(3)
C(2)-C(3)-C(1')-C(2')	-54(2)
C(4)-C(3)-C(1')-C(6')	-107.0(17)
C(2)-C(3)-C(1')-C(6')	132.1(15)
C(6')-C(1')-C(2')-C(3')	-4(3)
C(3)-C(1')-C(2')-C(3')	-179(2)
C(1')-C(2')-C(3')-C(4')	6(4)
C(2')-C(3')-C(4')-C(5')	-4(4)
C(2')-C(3')-C(4')-F(1')	178.7(19)
C(3')-C(4')-C(5')-C(6')	2(4)
F(1')-C(4')-C(5')-C(6')	179.3(17)
C(2')-C(1')-C(6')-C(5')	2(3)
C(3)-C(1')-C(6')-C(5')	176.8(16)
C(4')-C(5')-C(6')-C(1')	-1(3)
C(1')-C(3)-C(4)-C(5)	-165.8(14)
C(2)-C(3)-C(4)-C(5)	-45.7(18)
C(3)-C(4)-C(5)-N(8)	-13(2)
C(3)-C(4)-C(5)-C(6)	103.6(17)
N(8)-C(5)-C(6)-C(7)	30.0(13)
C(4)-C(5)-C(6)-C(7)	-85.9(14)
C(5)-C(6)-C(7)-C(1)	-4.2(13)
N(8)-C(1)-C(7)-C(6)	-22.6(14)
C(2)-C(1)-C(7)-C(6)	94.9(15)
C(2)-C(1)-N(8)-C(9)	163.1(9)
C(7)-C(1)-N(8)-C(9)	-79.3(12)
C(2)-C(1)-N(8)-C(5)	-77.1(12)

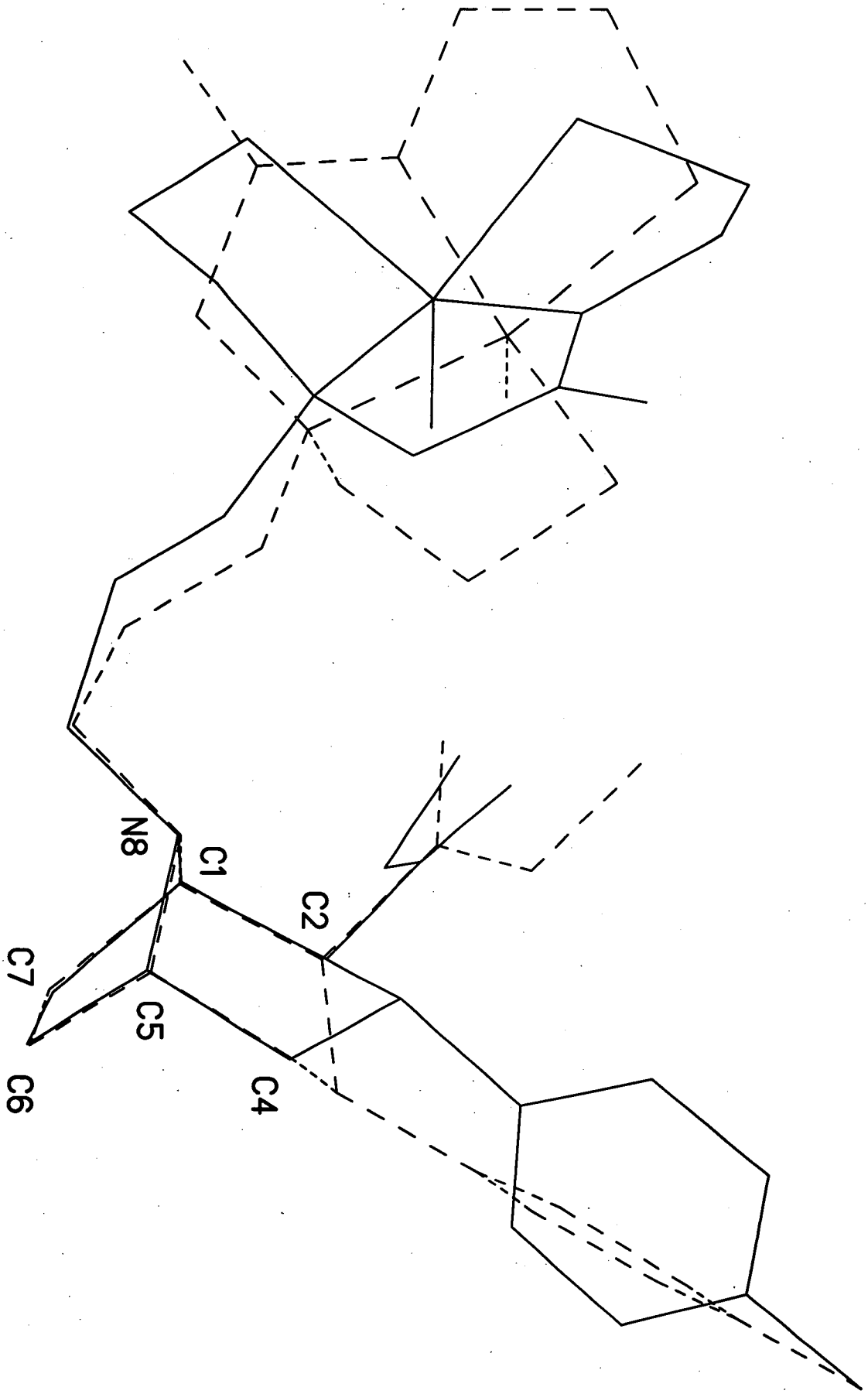
C(7)-C(1)-N(8)-C(5)	40.5(12)
C(6)-C(5)-N(8)-C(1)	-45.0(12)
C(4)-C(5)-N(8)-C(1)	74.4(14)
C(6)-C(5)-N(8)-C(9)	76.2(14)
C(4)-C(5)-N(8)-C(9)	-164.4(14)
C(1)-N(8)-C(9)-C(10)	-76.6(13)
C(5)-N(8)-C(9)-C(10)	169.6(12)
N(8)-C(9)-C(10)-C(11)	-76.9(13)
C(9)-C(10)-C(11)-N(12)	161.9(8)
C(10)-C(11)-N(12)-C(13)	-69.7(12)
C(10)-C(11)-N(12)-C(21)	51.4(12)
C(10)-C(11)-N(12)-Re(1)	170.4(7)
O(1)-Re(1)-N(12)-C(13)	-99.3(7)
N(15)-Re(1)-N(12)-C(13)	16.6(7)
S(18)-Re(1)-N(12)-C(13)	69.2(8)
S(19)-Re(1)-N(12)-C(13)	145.9(7)
O(1)-Re(1)-N(12)-C(21)	139.3(7)
N(15)-Re(1)-N(12)-C(21)	-104.8(7)
S(18)-Re(1)-N(12)-C(21)	-52.2(9)
S(19)-Re(1)-N(12)-C(21)	24.5(6)
O(1)-Re(1)-N(12)-C(11)	19.8(7)
N(15)-Re(1)-N(12)-C(11)	135.7(7)
S(18)-Re(1)-N(12)-C(11)	-171.7(5)
S(19)-Re(1)-N(12)-C(11)	-95.1(6)
C(21)-N(12)-C(13)-C(14)	99.5(10)
C(11)-N(12)-C(13)-C(14)	-139.7(9)
Re(1)-N(12)-C(13)-C(14)	-21.1(10)
N(12)-C(13)-C(14)-O(2)	-166.5(12)
N(12)-C(13)-C(14)-N(15)	15.0(13)
O(2)-C(14)-N(15)-C(16)	5.6(17)
C(13)-C(14)-N(15)-C(16)	-176.0(10)
O(2)-C(14)-N(15)-Re(1)	-178.8(10)
C(13)-C(14)-N(15)-Re(1)	-0.3(13)
O(1)-Re(1)-N(15)-C(14)	90.0(9)
N(12)-Re(1)-N(15)-C(14)	-9.3(8)
S(18)-Re(1)-N(15)-C(14)	-165.3(8)

S(19)-Re(1)-N(15)-C(14)	-83.3(8)
O(1)-Re(1)-N(15)-C(16)	-94.6(10)
N(12)-Re(1)-N(15)-C(16)	166.1(10)
S(18)-Re(1)-N(15)-C(16)	10.0(9)
S(19)-Re(1)-N(15)-C(16)	92.0(9)
C(14)-N(15)-C(16)-C(17)	-167.7(11)
Re(1)-N(15)-C(16)-C(17)	16.8(16)
N(15)-C(16)-C(17)-S(18)	-40.1(14)
C(16)-C(17)-S(18)-Re(1)	43.1(10)
O(1)-Re(1)-S(18)-C(17)	89.6(6)
N(15)-Re(1)-S(18)-C(17)	-26.9(5)
N(12)-Re(1)-S(18)-C(17)	-78.8(7)
S(19)-Re(1)-S(18)-C(17)	-154.4(5)
O(1)-Re(1)-S(19)-C(20)	-98.9(5)
N(15)-Re(1)-S(19)-C(20)	74.6(5)
N(12)-Re(1)-S(19)-C(20)	3.2(4)
S(18)-Re(1)-S(19)-C(20)	153.6(4)
Re(1)-S(19)-C(20)-C(21)	-31.3(8)
S(19)-C(20)-C(21)-N(12)	55.4(10)
C(13)-N(12)-C(21)-C(20)	-173.1(9)
C(11)-N(12)-C(21)-C(20)	66.7(11)
Re(1)-N(12)-C(21)-C(20)	-51.8(10)
C(1)-C(2)-C(22)-O(3)	95.1(16)
C(3)-C(2)-C(22)-O(3)	-24.4(17)
C(1)-C(2)-C(22)-C(23)	-82.7(16)
C(3)-C(2)-C(22)-C(23)	157.8(13)
O(3)-C(22)-C(23)-C(24)	-7(3)
C(2)-C(22)-C(23)-C(24)	170.6(13)

Symmetry transformations used to generate equivalent atoms:


S18
S19
Re1
C17
C16
C20
O1
N15
C21
N12
C14
O2
C13
C11
C10
C9
C24
O3
N8
C23
C22
C1
C2
C3
C6'
C7
C5
C1'
C5'
C4
C6
C2'
F1'
C4'
C3'


C17
S18
S19
Re1
C20
C16
C21
N15
O1
C14
O2
N12
C13
C11
C10
C9
O3
C24
C22
N8
C1
C23
C5
C2
C7
C6'
C6
C3
C4
C1'
C5'
C2'
C4'
F1'
C3'


N8
C1
C2
C7
C5
C6
C4