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$Sn(OR_f)_2(H_2NMe_2)$

Table 1. Data Collection and Processing Parameters

Space group	$P2_1/n$ (monoclinic)
Cell constants	a = 9.957(3)Å
	b = 13.859(6)
	c = 11.808(5)
	β = 104.05(3)^{o}
	V = 1581Å^3
Molecular formula	$C_8H_9NO_2F_{12}Sn$
Formula weight	497.87
Formula units per cell	Z = 4
Density	ρ = 2.09 g-cm^{-3}
Absorption coefficient	μ = 17.47 cm^{-1}
Temperature	T = -50°C
Radiation (Mo Kα)	λ = 0.71073Å
Collection range	$4^{o} \leq 2\theta \leq 50^{o}$
Scan width	$\Delta\theta = 1.35+(K\alpha_2-K\alpha_1)^{o}$
Scan speed range	1.5 to 15.0^{o}-min^{-1}
Total data collected	2779
Independent data, $I>3\sigma(I)$	1952
Total variables	221
$R=\Sigma\|\|F_o\|-\|F_c\|\|/\Sigma\|F_o\|$	0.041
$R_w=[\Sigma w(\|F_o\|-\|F_c\|)^2/\Sigma w\|F_o\|^2]^{1/2}$	0.038
Weights	$w = \sigma(F)^{-2}$

Table 2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$)

	x	y	z	U(eq)
Sn	6166(1)	1455(1)	5472(1)	38(1)
F(1)	8214(5)	3539(5)	3661(5)	85(3)
F(2)	8606(5)	3091(4)	5469(5)	76(2)
F(3)	8277(5)	4593(4)	5013(6)	96(3)
F(4)	5472(6)	3912(4)	2575(4)	73(2)
F(5)	5749(6)	5106(3)	3747(5)	75(2)
F(6)	4106(5)	4107(4)	3707(5)	70(2)
F(7)	3654(6)	2701(4)	6041(5)	90(3)
F(8)	1933(6)	1729(5)	5856(5)	89(3)
F(9)	1740(6)	3047(5)	4889(6)	106(3)
F(10)	1378(5)	589(4)	3867(5)	70(2)
F(11)	2379(6)	967(5)	2560(5)	104(3)
F(12)	889(5)	1929(4)	2982(5)	93(3)
O(1)	5966(5)	2603(3)	4335(4)	38(2)
O(2)	4063(4)	1106(3)	4800(4)	36(2)
N	6727(7)	630(5)	3997(7)	48(3)
C(1)	6327(7)	3546(6)	4574(6)	40(3)
C(2)	7856(9)	3719(6)	4658(9)	61(4)
C(3)	5422(9)	4178(6)	3642(8)	51(4)
C(4)	3102(7)	1809(6)	4341(7)	42(3)
C(5)	2580(9)	2320(7)	5265(10)	63(4)
C(6)	1940(8)	1319(8)	3422(9)	59(4)
C(7)	5771(9)	697(7)	2807(8)	66(4)
C(8)	8152(8)	889(7)	3935(9)	69(4)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 3. Bond lengths (Å)

Sn-O(1)	2.061 (5)	Sn-O(2)	2.107 (4)
Sn-N	2.264 (8)	F(1)-C(2)	1.334 (13)
F(2)-C(2)	1.372 (10)	F(3)-C(2)	1.317 (10)
F(4)-C(3)	1.325 (11)	F(5)-C(3)	1.325 (10)
F(6)-C(3)	1.334 (11)	F(7)-C(5)	1.337 (10)
F(8)-C(5)	1.338 (13)	F(9)-C(5)	1.316 (11)
F(10)-C(6)	1.325 (12)	F(11)-C(6)	1.297 (12)
F(12)-C(6)	1.347 (10)	O(1)-C(1)	1.367 (9)
O(2)-C(4)	1.381 (8)	N-C(7)	1.497 (11)
N-C(8)	1.482 (11)	C(1)-C(2)	1.521 (11)
C(1)-C(3)	1.520 (11)	C(4)-C(5)	1.495 (14)
C(4)-C(6)	1.539 (11)		

Table 4. Bond angles (°)

O(1)-Sn-O(2)	90.1(2)	O(1)-Sn-N	83.7(2)
O(2)-Sn-N	90.2(2)	Sn-O(1)-C(1)	128.7(4)
Sn-O(2)-C(4)	121.1(4)	Sn-N-C(7)	118.1(5)
Sn-N-C(8)	109.5(5)	C(7)-N-C(8)	109.7(8)
O(1)-C(1)-C(2)	111.8(6)	O(1)-C(1)-C(3)	108.8(6)
C(2)-C(1)-C(3)	111.4(7)	F(1)-C(2)-F(2)	106.3(7)
F(1)-C(2)-F(3)	108.7(8)	F(2)-C(2)-F(3)	106.5(7)
F(1)-C(2)-C(1)	113.0(7)	F(2)-C(2)-C(1)	108.2(7)
F(3)-C(2)-C(1)	113.7(8)	F(4)-C(3)-F(5)	107.1(8)
F(4)-C(3)-F(6)	107.4(6)	F(5)-C(3)-F(6)	106.8(7)
F(4)-C(3)-C(1)	112.1(7)	F(5)-C(3)-C(1)	113.7(7)
F(6)-C(3)-C(1)	109.5(7)	O(2)-C(4)-C(5)	112.2(6)
O(2)-C(4)-C(6)	107.2(6)	C(5)-C(4)-C(6)	112.9(7)
F(7)-C(5)-F(8)	106.9(8)	F(7)-C(5)-F(9)	105.5(8)
F(8)-C(5)-F(9)	107.3(8)	F(7)-C(5)-C(4)	109.0(7)
F(8)-C(5)-C(4)	112.8(8)	F(9)-C(5)-C(4)	114.9(9)
F(10)-C(6)-F(11)	106.2(8)	F(10)-C(6)-F(12)	105.6(7)
F(11)-C(6)-F(12)	108.1(8)	F(10)-C(6)-C(4)	112.0(7)
F(11)-C(6)-C(4)	112.4(7)	F(12)-C(6)-C(4)	112.1(8)

Table 5. Anisotropic displacement parameters ($Å^2 x10^3$)

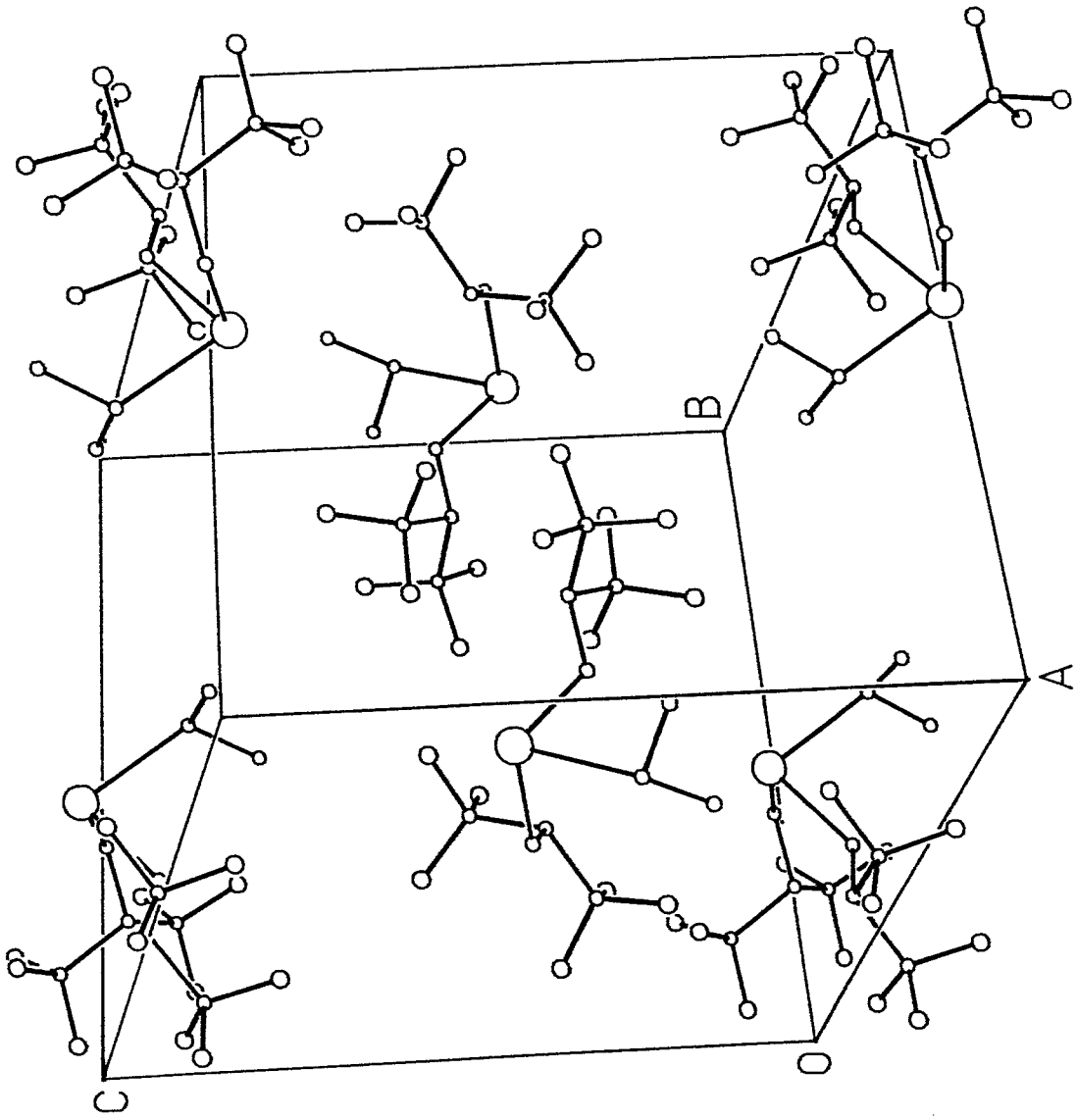
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sn	29(1)	48(1)	32(1)	8(1)	0(1)	-1(1)
F(1)	69(3)	112(5)	86(4)	5(4)	42(3)	-10(4)
F(2)	47(3)	84(4)	86(4)	8(3)	-2(3)	-9(3)
F(3)	79(4)	62(4)	139(6)	-11(4)	8(4)	-34(3)
F(4)	110(4)	72(4)	35(3)	12(3)	11(3)	19(3)
F(5)	111(5)	35(3)	74(4)	6(3)	13(3)	5(3)
F(6)	62(3)	80(4)	65(4)	16(3)	11(3)	20(3)
F(7)	70(4)	103(5)	84(4)	-48(4)	-5(3)	2(3)
F(8)	92(4)	119(5)	67(4)	-10(4)	43(3)	-12(4)
F(9)	70(4)	89(4)	151(7)	-7(5)	11(4)	37(3)
F(10)	49(3)	72(4)	77(4)	6(3)	-8(3)	-23(3)
F(11)	72(4)	195(7)	37(3)	-34(4)	0(3)	-24(4)
F(12)	51(3)	109(4)	95(5)	35(4)	-32(3)	2(3)
O(1)	45(3)	35(3)	32(3)	6(2)	5(2)	-2(2)
O(2)	25(3)	48(3)	33(3)	2(2)	-1(2)	-3(2)
N	47(4)	40(4)	61(5)	5(4)	19(4)	1(3)
C(1)	48(4)	39(4)	32(4)	4(4)	9(3)	3(4)
C(2)	55(5)	43(6)	79(7)	9(5)	7(5)	-9(5)
C(3)	65(6)	51(6)	39(5)	2(4)	16(4)	6(5)
C(4)	27(4)	55(5)	37(5)	8(4)	-3(3)	-2(4)
C(5)	44(5)	57(6)	86(8)	-5(6)	7(5)	7(5)
C(6)	41(5)	77(7)	55(6)	5(6)	2(4)	-16(5)
C(7)	79(7)	68(7)	50(6)	-14(5)	14(5)	7(5)
C(8)	53(6)	67(7)	98(9)	-5(6)	39(6)	-3(5)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 6. H-Atom coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$)

	x	y	z	U
H(N)	6640(79)	0(59)	4239(76)	65(8)
H(1)	6171	3717	5355	65(8)
H(4)	3532	2326	3955	65(8)
H(7A)	5795	1367	2499	65(8)
H(7B)	4807	539	2857	65(8)
H(7C)	6070	230	2270	65(8)
H(8A)	8174	1577	3687	65(8)
H(8B)	8449	462	3358	65(8)
H(8C)	8795	801	4722	65(8)


C
B
A
O

$[Pb(\mu\text{-}OR_f)(OR_f)(p\text{-}pyNMe_2)]_2$

Table 1. Data Collection and Processing Parameters

Space group	$P\bar{1}$ (triclinic)
Cell constants	a = 9.252(2)Å
	b = 9.742(2)
	c = 11.141(3)
	α = 75.92(2)^{o}
	β = 77.04(2)
	γ = 87.34(2)
	V = 949Å^3
Molecular formula	$C_{26}H_{24}N_4O_4F_{24}Pb_2$
Formula weight	1326.92
Formula units per cell	Z = 1
Density	ρ = 2.32 g-cm^{-3}
Absorption coefficient	μ = 90.8 cm^{-1}
Temperature	T = -50°C
Radiation (Mo Kα)	λ = 0.71073Å
Collection range	$4^{o} \leq 2\theta \leq 55^{o}$
Scan width	$\Delta\theta = 1.25+(K\alpha_2-K\alpha_1)^{o}$
Scan speed range	2.0 to 15.0^{o}-min^{-1}
Total data collected	4195
Independent data, I>3σ(I)	3689
Total variables	272
$R=\Sigma\|\|F_o\|-\|F_c\|\|/\Sigma\|F_o\|$	0.037
$R_w=[\Sigma w(\|F_o\|-\|F_c\|)^2/\Sigma w\|F_o\|^2]^{1/2}$	0.039
Weights	$w = \sigma(F)^{-2}$

Table 2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$)

	x	y	z	U(eq)
Pb	5078(1)	6410(1)	6109(1)	31(1)
F(1)	3095(7)	1679(5)	6859(6)	60(2)
F(2)	1443(6)	2034(6)	8461(6)	67(2)
F(3)	3768(7)	2489(6)	8278(6)	67(3)
F(4)	1363(6)	3376(6)	5435(6)	61(3)
F(5)	1166(6)	5528(6)	5574(6)	66(3)
F(6)	-68(6)	3917(7)	7068(6)	73(3)
F(7)	2940(8)	5815(7)	11145(6)	85(3)
F(8)	2589(10)	4478(7)	9978(7)	104(4)
F(9)	1214(7)	6277(8)	10126(7)	88(3)
F(10)	4252(9)	8288(8)	10027(7)	97(4)
F(11)	4791(8)	8887(7)	7973(7)	86(3)
F(12)	2554(8)	8906(6)	8969(8)	86(4)
O(1)	3834(5)	4521(5)	6025(5)	33(2)
O(2)	3290(6)	6628(6)	7804(6)	41(2)
N(1)	3564(8)	7955(7)	4943(7)	39(3)
N(2)	1199(8)	10887(7)	2725(7)	43(3)
C(1)	2508(9)	4097(8)	6935(7)	32(3)
C(2)	2682(10)	2575(9)	7634(9)	43(3)
C(3)	1200(9)	4231(9)	6270(9)	41(3)
C(4)	3701(10)	6659(9)	8907(9)	42(3)
C(5)	2585(12)	5842(11)	10030(10)	56(4)
C(6)	3806(13)	8211(12)	8970(10)	58(4)
C(7)	3282(10)	7757(9)	3858(9)	42(3)
C(8)	2492(9)	8681(8)	3105(9)	41(3)
C(9)	1938(9)	9947(8)	3448(8)	36(3)
C(10)	2207(10)	10148(8)	4613(9)	40(3)
C(11)	3017(10)	9149(9)	5290(8)	42(3)
C(12)	648(11)	12226(9)	3073(11)	61(5)
C(13)	1029(12)	10713(11)	1514(10)	68(5)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 3. Bond lengths (Å)

Pb-O(1)	2.247	(6)	Pb-O(2)	2.260	(6)
Pb-N(1)	2.363	(7)	Pb-O(1')	2.716	(6)
F(1)-C(2)	1.357	(12)	F(2)-C(2)	1.337	(10)
F(3)-C(2)	1.349	(13)	F(4)-C(3)	1.373	(13)
F(5)-C(3)	1.315	(9)	F(6)-C(3)	1.302	(9)
F(7)-C(5)	1.348	(14)	F(8)-C(5)	1.343	(13)
F(9)-C(5)	1.308	(13)	F(10)-C(6)	1.351	(15)
F(11)-C(6)	1.320	(11)	F(12)-C(6)	1.315	(13)
O(1)-C(1)	1.410	(8)	O(2)-C(4)	1.372	(12)
N(1)-C(7)	1.352	(14)	N(1)-C(11)	1.355	(11)
N(2)-C(9)	1.336	(11)	N(2)-C(12)	1.486	(12)
N(2)-C(13)	1.444	(15)	C(1)-C(2)	1.518	(11)
C(1)-C(3)	1.539	(13)	C(4)-C(5)	1.509	(12)
C(4)-C(6)	1.540	(15)	C(7)-C(8)	1.377	(13)
C(8)-C(9)	1.419	(12)	C(9)-C(10)	1.434	(14)
C(10)-C(11)	1.380	(12)			

Table 4. Bond angles (°)

O(1)-Pb-O(2)	88.2(2)	O(1)-Pb-N(1)	90.9(2)
O(2)-Pb-N(1)	83.9(2)	O(1)-Pb-O(1')	67.1(2)
O(2)-Pb-O(1')	153.6(2)	N(1)-Pb-O(1')	87.2(2)
Pb-O(1)-C(1)	118.7(5)	Pb-O(1)-Pb'	112.9(2)
C(1)-O(1)-Pb'	127.7(5)	Pb-O(2)-C(4)	118.5(5)
Pb-N(1)-C(7)	122.4(5)	Pb-N(1)-C(11)	121.0(7)
C(7)-N(1)-C(11)	116.4(7)	C(9)-N(2)-C(12)	121.3(9)
C(9)-N(2)-C(13)	121.4(8)	C(12)-N(2)-C(13)	117.0(8)
O(1)-C(1)-C(2)	108.1(6)	O(1)-C(1)-C(3)	109.7(6)
C(2)-C(1)-C(3)	110.7(7)	F(1)-C(2)-F(2)	106.7(8)
F(1)-C(2)-F(3)	104.9(7)	F(2)-C(2)-F(3)	107.9(7)
F(1)-C(2)-C(1)	113.8(7)	F(2)-C(2)-C(1)	112.9(7)
F(3)-C(2)-C(1)	110.1(8)	F(4)-C(3)-F(5)	105.2(8)
F(4)-C(3)-F(6)	107.7(8)	F(5)-C(3)-F(6)	109.7(7)
F(4)-C(3)-C(1)	112.0(7)	F(5)-C(3)-C(1)	109.3(7)
F(6)-C(3)-C(1)	112.6(8)	O(2)-C(4)-C(5)	109.7(8)
O(2)-C(4)-C(6)	108.8(7)	C(5)-C(4)-C(6)	111.0(8)
F(7)-C(5)-F(8)	104.7(8)	F(7)-C(5)-F(9)	106.6(9)
F(8)-C(5)-F(9)	107.2(10)	F(7)-C(5)-C(4)	112.6(9)
F(8)-C(5)-C(4)	109.2(9)	F(9)-C(5)-C(4)	115.8(8)
F(10)-C(6)-F(11)	108.3(10)	F(10)-C(6)-F(12)	107.4(9)
F(11)-C(6)-F(12)	107.1(8)	F(10)-C(6)-C(4)	110.6(8)
F(11)-C(6)-C(4)	109.1(9)	F(12)-C(6)-C(4)	114.0(10)
N(1)-C(7)-C(8)	124.3(8)	C(7)-C(8)-C(9)	119.7(9)
N(2)-C(9)-C(8)	121.4(9)	N(2)-C(9)-C(10)	122.4(8)
C(8)-C(9)-C(10)	116.2(8)	C(9)-C(10)-C(11)	119.0(8)
N(1)-C(11)-C(10)	124.4(9)		

Table 5. Anisotropic displacement parameters ($Å^2 x10^3$)

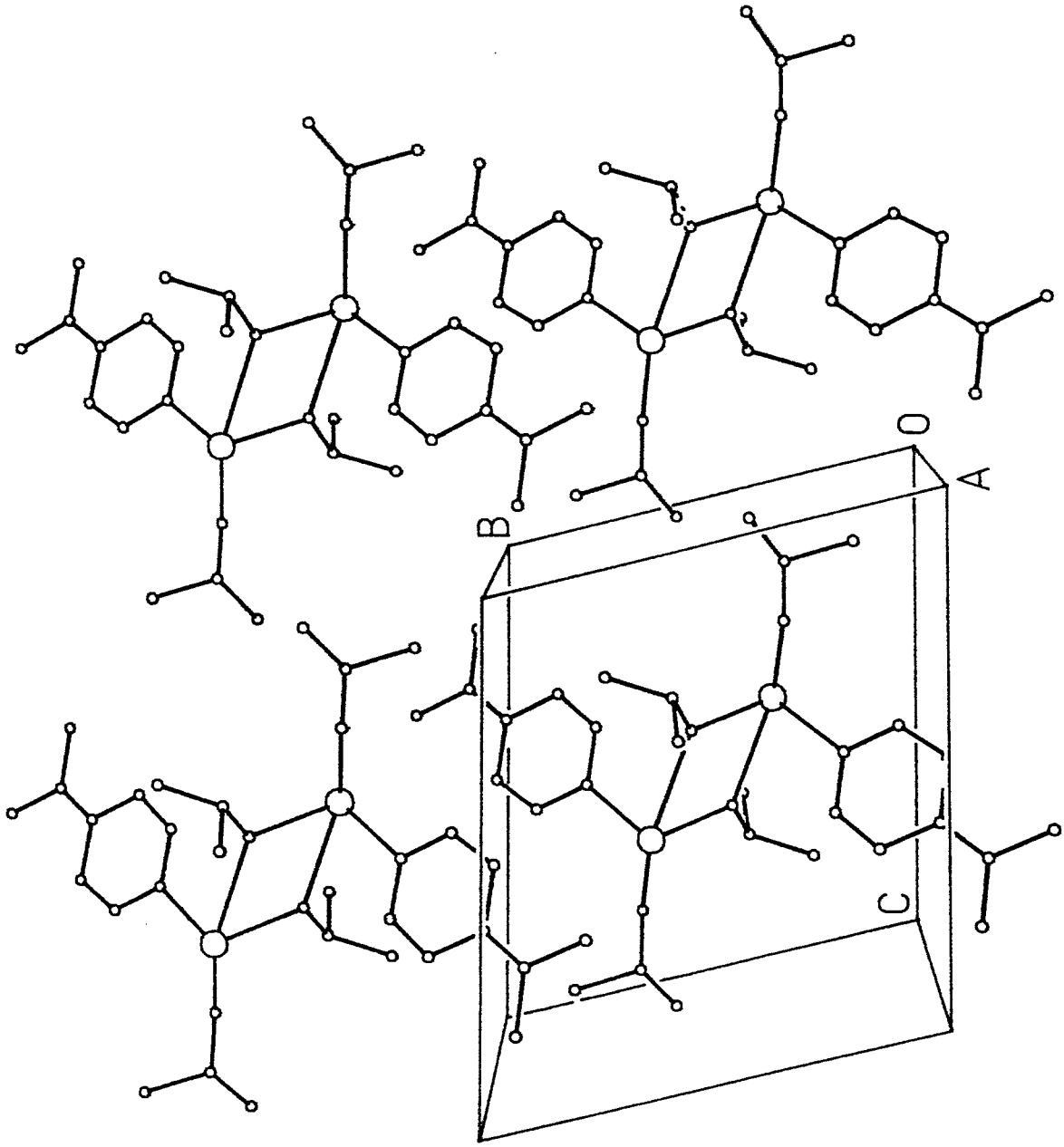
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pb	35(1)	31(1)	30(1)	-11(1)	-8(1)	2(1)
F(1)	85(4)	34(3)	62(4)	-12(3)	-19(3)	10(3)
F(2)	65(4)	59(4)	55(4)	11(3)	8(3)	-9(3)
F(3)	77(4)	69(4)	56(4)	-2(3)	-34(3)	9(3)
F(4)	62(4)	76(4)	70(4)	-46(4)	-37(3)	22(3)
F(5)	62(4)	49(3)	91(5)	-1(3)	-39(4)	7(3)
F(6)	36(3)	123(5)	56(4)	-22(4)	1(3)	-11(3)
F(7)	107(6)	112(6)	31(4)	-14(4)	-14(4)	10(4)
F(8)	178(8)	53(4)	66(5)	-3(4)	-3(5)	-23(5)
F(9)	50(4)	129(6)	66(5)	-9(4)	8(3)	-1(4)
F(10)	137(7)	103(5)	77(5)	-40(5)	-49(5)	-19(5)
F(11)	104(6)	75(4)	79(5)	-23(4)	-7(4)	-38(4)
F(12)	100(5)	55(4)	109(7)	-32(4)	-27(5)	31(4)
O(1)	27(3)	31(3)	42(4)	-20(3)	0(2)	5(2)
O(2)	50(4)	47(3)	29(3)	-15(3)	-10(3)	-2(3)
N(1)	51(4)	27(3)	40(4)	-5(3)	-17(4)	5(3)
N(2)	53(5)	42(4)	34(4)	-8(3)	-15(4)	14(4)
C(1)	41(5)	37(4)	14(4)	0(3)	-8(3)	0(4)
C(2)	50(5)	43(5)	34(5)	-10(4)	-7(4)	6(4)
C(3)	36(5)	38(5)	53(6)	-23(4)	-10(4)	14(4)
C(4)	44(5)	45(5)	36(5)	-9(4)	-10(4)	4(4)
C(5)	70(7)	51(6)	43(6)	-13(5)	-6(5)	10(5)
C(6)	74(8)	68(7)	37(6)	-20(5)	-9(6)	-18(6)
C(7)	57(6)	35(4)	36(5)	-15(4)	-10(4)	7(4)
C(8)	49(5)	39(5)	41(5)	-20(4)	-11(4)	9(4)
C(9)	38(5)	34(4)	35(5)	-7(4)	-7(4)	3(4)
C(10)	55(5)	27(4)	41(5)	-13(4)	-11(4)	10(4)
C(11)	61(6)	40(5)	32(5)	-16(4)	-15(4)	2(4)
C(12)	73(7)	39(5)	78(9)	-15(5)	-35(6)	19(5)
C(13)	92(9)	73(7)	56(7)	-23(6)	-48(7)	30(6)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 6. H-Atom coordinates ($x10^4$) and isotropic displacement parameters (A^2x10^3)

	x	y	z	U
H(1)	2303	4714	7551	72(10)
H(4)	4690	6206	8925	72(10)
H(7)	3672	6881	3584	72(10)
H(8)	2310	8461	2320	72(10)
H(10)	1814	10998	4930	72(10)
H(11)	3212	9318	6090	72(10)
H(12A)	126	12787	2420	72(10)
H(12B)	1504	12790	3114	72(10)
H(12C)	-57	12004	3920	72(10)
H(13A)	446	11519	1119	72(10)
H(13B)	494	9803	1638	72(10)
H(13C)	2029	10695	944	72(10)


O
A
B
C

$\{[Me_2NH_2][Pb(\mu\text{-}OR_f)(OR_f)_2]\}_2$

Table 1. Data Collection and Processing Parameters

Space group	$P2_1/c$ (monoclinic)
Cell constants	a = 11.498(3)Å
	b = 10.976(4)
	c = 17.196(4)
	β = 105.09(2)^{o}
	V = 2095Å^3
Molecular formula	$2C_2H_8N^+ \cdot C_{18}H_6O_6F_{36}Pb_2^{2-}$
Formula weight	1508.84
Formula units per cell	Z = 2
Density	ρ = 2.39 g-cm^{-3}
Absorption coefficient	μ = 82.8 cm^{-1}
Temperature	T = -50°C
Radiation (Mo Kα)	λ = 0.71073Å
Collection range	$4^{o} \leq 2\theta \leq 50^{o}$
Scan width	$\Delta\theta = 1.30+(K\alpha_2-K\alpha_1)^{o}$
Scan speed range	1.5 to 15.0^{o}-min^{-1}
Total data collected	4074
Independent data, $I>3\sigma(I)$	2795
Total variables	309
$R=\Sigma\|\|F_o\|-\|F_c\|\|/\Sigma\|F_o\|$	0.032
$R_w=[\Sigma w(\|F_o\|-\|F_c\|)^2/\Sigma w\|F_o\|^2]^{1/2}$	0.031
Weights	$w = \sigma(F)^{-2}$

Table 2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$)

	x	y	z	U(eq)
Pb	5566(1)	6354(1)	5794(1)	35(1)
F(1)	8983(6)	8051(6)	5036(5)	98(4)
F(2)	8745(6)	9970(6)	5201(4)	92(3)
F(3)	9430(5)	8839(6)	6218(4)	82(3)
F(4)	6865(7)	10672(5)	5686(5)	116(4)
F(5)	7537(7)	9674(7)	6772(5)	109(4)
F(6)	5798(6)	9309(6)	6045(5)	101(4)
F(7)	5666(7)	2427(6)	7382(4)	105(4)
F(8)	7436(6)	2759(6)	7182(4)	89(3)
F(9)	5827(6)	3075(5)	6230(4)	83(3)
F(10)	6636(6)	5782(6)	8430(4)	88(3)
F(11)	6504(6)	3875(6)	8664(4)	94(3)
F(12)	8066(5)	4573(6)	8331(3)	81(3)
F(13)	7349(5)	3019(5)	4729(4)	83(3)
F(14)	8171(6)	3812(6)	5880(3)	84(3)
F(15)	9072(5)	3910(6)	4933(4)	81(3)
F(16)	6729(5)	4664(6)	3448(3)	73(3)
F(17)	8435(5)	5607(5)	3862(3)	73(3)
F(18)	6748(5)	6550(6)	3764(3)	73(3)
O(1)	7351(5)	7477(5)	5922(3)	39(2)
O(2)	6721(5)	5294(5)	6838(3)	45(2)
O(3)	6185(5)	5172(5)	4916(3)	36(2)
C(1)	7358(8)	8590(8)	5566(5)	45(3)
C(2)	8631(9)	8888(10)	5509(7)	64(4)
C(3)	6903(10)	9575(10)	6019(8)	68(5)
C(4)	6231(8)	4503(8)	7299(6)	51(4)
C(5)	6321(12)	3154(10)	7022(7)	70(5)
C(6)	6849(11)	4693(11)	8196(6)	66(5)
C(7)	7343(8)	5186(7)	4831(5)	38(3)
C(8)	7984(8)	3974(9)	5084(6)	56(4)
C(9)	7337(9)	5487(9)	3985(6)	52(4)
N(1)	8899(6)	6458(7)	7180(4)	48(3)
C(10)	9188(10)	7115(10)	7967(6)	81(5)
C(11)	9995(9)	5920(10)	6988(7)	75(5)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 3. Bond lengths (Å)

Pb-O(1)	2.354	(5)	Pb-O(2)	2.258	(5)
Pb-O(3)	2.243	(6)	Pb-O(3')	2.659	(5)
F(1)-C(2)	1.355	(14)	F(2)-C(2)	1.321	(13)
F(3)-C(2)	1.324	(11)	F(4)-C(3)	1.329	(13)
F(5)-C(3)	1.314	(14)	F(6)-C(3)	1.316	(14)
F(7)-C(5)	1.352	(15)	F(8)-C(5)	1.313	(15)
F(9)-C(5)	1.335	(13)	F(10)-C(6)	1.305	(14)
F(11)-C(6)	1.333	(14)	F(12)-C(6)	1.363	(14)
F(13)-C(8)	1.331	(11)	F(14)-C(8)	1.340	(12)
F(15)-C(8)	1.344	(12)	F(16)-C(9)	1.350	(11)
F(17)-C(9)	1.339	(12)	F(18)-C(9)	1.353	(11)
O(1)-C(1)	1.368	(10)	O(2)-C(4)	1.391	(12)
O(3)-C(7)	1.376	(11)	C(1)-C(2)	1.528	(15)
C(1)-C(3)	1.503	(16)	C(4)-C(5)	1.567	(14)
C(4)-C(6)	1.534	(13)	C(7)-C(8)	1.529	(12)
C(7)-C(9)	1.490	(14)	N(1)-C(10)	1.492	(12)
N(1)-C(11)	1.505	(14)			

Table 4. Bond angles (°)

O(1)-Pb-O(2)	83.0(2)	O(1)-Pb-O(3)	86.8(2)
O(2)-Pb-O(3)	90.7(2)	O(1)-Pb-O(3')	155.5(2)
O(2)-Pb-O(3')	105.0(2)	O(3)-Pb-O(3')	70.2(2)
Pb-O(1)-C(1)	122.1(4)	Pb-O(2)-C(4)	122.3(5)
Pb-O(3)-C(7)	123.3(4)	Pb-O(3)-Pb'	109.8(2)
C(7)-O(3)-Pb'	126.6(5)	O(1)-C(1)-C(2)	109.7(7)
O(1)-C(1)-C(3)	111.5(8)	C(2)-C(1)-C(3)	110.4(8)
F(1)-C(2)-F(2)	107.1(10)	F(1)-C(2)-F(3)	106.4(8)
F(2)-C(2)-F(3)	106.7(8)	F(1)-C(2)-C(1)	109.6(8)
F(2)-C(2)-C(1)	114.5(8)	F(3)-C(2)-C(1)	112.2(9)
F(4)-C(3)-F(5)	107.3(9)	F(4)-C(3)-F(6)	107.0(9)
F(5)-C(3)-F(6)	106.2(11)	F(4)-C(3)-C(1)	113.9(11)
F(5)-C(3)-C(1)	113.0(9)	F(6)-C(3)-C(1)	109.1(8)
O(2)-C(4)-C(5)	110.3(9)	O(2)-C(4)-C(6)	109.8(8)
C(5)-C(4)-C(6)	112.6(8)	F(7)-C(5)-F(8)	109.8(9)
F(7)-C(5)-F(9)	106.8(9)	F(8)-C(5)-F(9)	109.0(11)
F(7)-C(5)-C(4)	109.2(10)	F(8)-C(5)-C(4)	112.7(9)
F(9)-C(5)-C(4)	109.2(8)	F(10)-C(6)-F(11)	108.7(10)
F(10)-C(6)-F(12)	107.6(9)	F(11)-C(6)-F(12)	106.6(8)
F(10)-C(6)-C(4)	111.1(8)	F(11)-C(6)-C(4)	112.5(9)
F(12)-C(6)-C(4)	110.2(9)	O(3)-C(7)-C(8)	111.6(7)
O(3)-C(7)-C(9)	110.3(6)	C(8)-C(7)-C(9)	110.5(8)
F(13)-C(8)-F(14)	106.7(8)	F(13)-C(8)-F(15)	107.3(8)
F(14)-C(8)-F(15)	106.3(7)	F(13)-C(8)-C(7)	112.9(7)
F(14)-C(8)-C(7)	110.1(8)	F(15)-C(8)-C(7)	113.2(8)
F(16)-C(9)-F(17)	107.4(8)	F(16)-C(9)-F(18)	104.6(7)
F(17)-C(9)-F(18)	107.1(8)	F(16)-C(9)-C(7)	112.9(8)
F(17)-C(9)-C(7)	114.3(7)	F(18)-C(9)-C(7)	109.9(8)
C(10)-N(1)-C(11)	112.8(7)		

Table 5. Anisotropic displacement parameters ($Å^2 x10^3$)

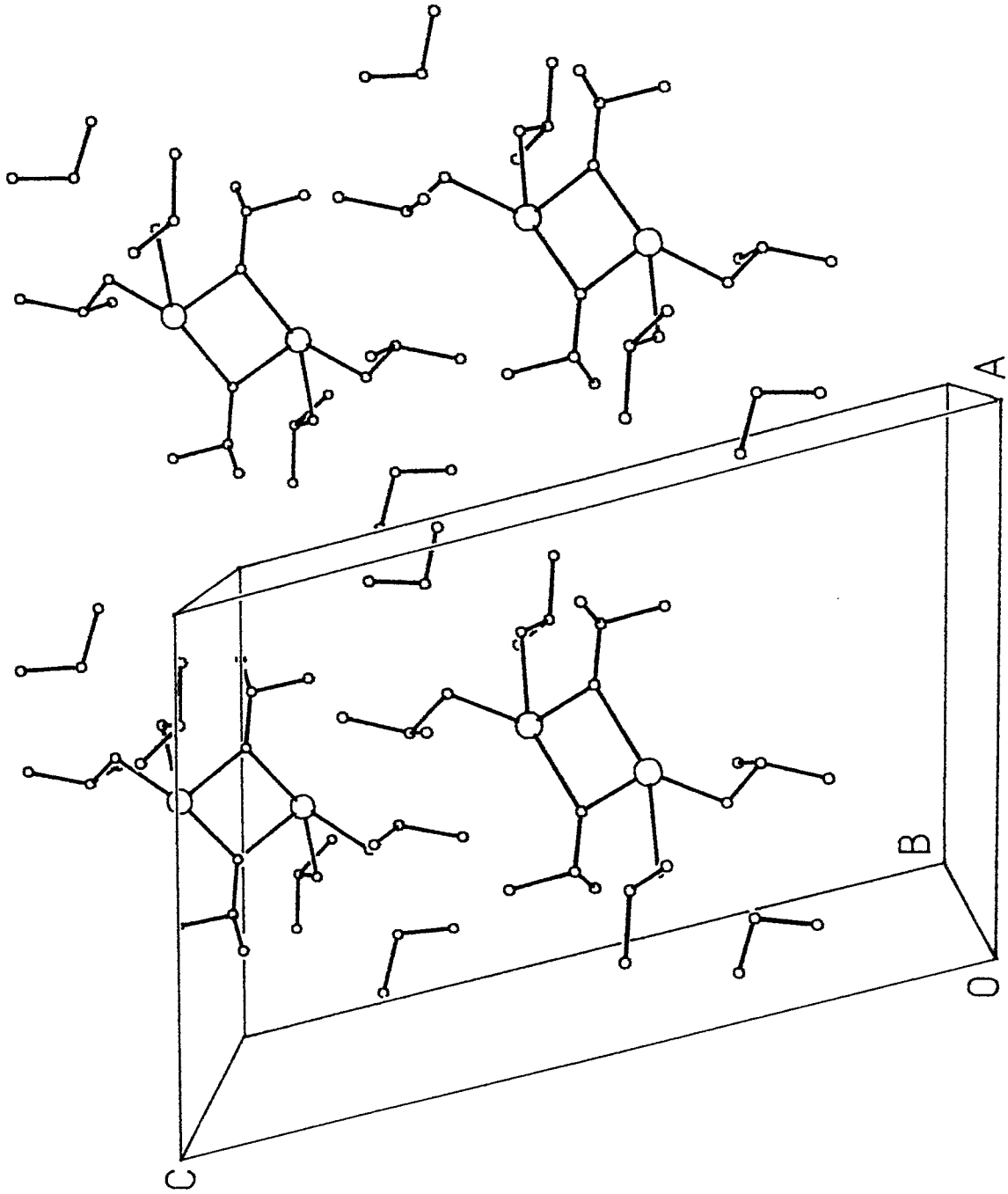
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pb	34(1)	31(1)	38(1)	-4(1)	9(1)	-2(1)
F(1)	99(6)	93(5)	128(6)	-30(5)	75(5)	-22(4)
F(2)	92(5)	68(4)	126(6)	28(4)	47(5)	-24(4)
F(3)	50(3)	91(5)	95(5)	8(4)	3(3)	-23(4)
F(4)	133(7)	42(4)	193(9)	7(5)	76(6)	7(4)
F(5)	115(6)	125(6)	93(5)	-64(5)	38(5)	-16(5)
F(6)	92(5)	60(4)	167(7)	-24(4)	63(5)	-1(4)
F(7)	130(6)	68(4)	111(6)	36(4)	23(5)	-33(4)
F(8)	88(5)	69(4)	97(5)	9(4)	3(4)	41(4)
F(9)	104(5)	56(4)	76(5)	-3(3)	2(4)	-8(4)
F(10)	116(6)	82(5)	67(4)	-8(4)	24(4)	19(4)
F(11)	108(5)	112(6)	70(4)	42(4)	35(4)	13(5)
F(12)	61(4)	114(5)	60(4)	12(4)	0(3)	6(4)
F(13)	72(4)	38(3)	121(6)	-19(4)	-5(4)	3(3)
F(14)	93(5)	93(5)	62(4)	20(4)	15(3)	31(4)
F(15)	52(3)	85(5)	115(5)	10(4)	36(3)	20(3)
F(16)	82(4)	91(4)	45(3)	-16(3)	17(3)	-13(4)
F(17)	56(4)	93(5)	83(4)	15(4)	42(3)	4(3)
F(18)	67(4)	73(4)	84(4)	21(4)	31(3)	5(4)
O(1)	35(3)	34(3)	44(4)	1(3)	5(3)	-6(3)
O(2)	41(4)	41(3)	52(4)	9(3)	12(3)	-4(3)
O(3)	33(3)	40(3)	39(3)	-9(3)	18(3)	-3(3)
C(1)	42(5)	42(5)	50(5)	-5(5)	10(4)	-5(5)
C(2)	61(7)	58(7)	74(7)	4(6)	19(6)	-15(6)
C(3)	60(7)	48(7)	105(10)	-4(7)	39(7)	-9(6)
C(4)	38(5)	53(6)	60(6)	15(5)	7(5)	15(5)
C(5)	89(10)	42(6)	72(8)	-4(6)	9(7)	-7(6)
C(6)	77(8)	73(8)	49(6)	18(6)	19(6)	13(7)
C(7)	39(5)	34(5)	44(5)	-7(4)	12(4)	-2(4)
C(8)	36(5)	64(7)	67(7)	0(6)	11(5)	6(5)
C(9)	44(6)	53(6)	62(7)	0(5)	19(5)	2(5)
N(1)	44(4)	51(4)	48(4)	-4(4)	10(3)	0(4)
C(10)	95(9)	78(8)	71(8)	-28(7)	23(7)	0(7)
C(11)	49(7)	88(8)	85(8)	-14(7)	15(6)	12(6)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 6. H-Atom coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$)

	x	y	z	U
H(1)	6803	8554	5013	54(15)
H(4)	5355	4684	7219	54(15)
H(7)	7799	5831	5197	54(15)
H(1A)	8527	7011	6761	108(15)
H(1B)	8339	5825	7187	108(15)
H(10A)	9578	6539	8409	108(15)
H(10B)	8429	7442	8069	108(15)
H(10C)	9750	7804	7951	108(15)
H(11A)	10589	6581	6980	108(15)
H(11B)	9755	5516	6448	108(15)
H(11C)	10368	5305	7408	108(15)


A
B
C
O

$Ge(OR_f)_2(H_2NPh)$

Table 1. Data Collection and Processing Parameters

Space group	$P\bar{1}$ (triclinic)
Cell constants	a = 9.093(2)Å
	b = 10.629(4)
	c = 11.183(2)
	α = 115.13(2)^{o}
	β = 94.52(2)
	γ = 109.60(2)
	V = 890Å^{3}
Molecular formula	$C_{12}H_9NO_2F_{12}Ge$
Formula weight	499.81
Formula units per cell	Z = 2
Density	ρ = 1.86 g-cm^{-3}
Absorption coefficient	μ = 18.2 cm^{-1}
Temperature	T = -50°C
Radiation (Mo Kα)	λ = 0.71073Å
Collection range	$4^{o} \leq 2\theta \leq 50^{o}$
Scan width	$\Delta\theta = 1.30+(K\alpha_2-K\alpha_1)^{o}$
Scan speed range	1.5 to 15.0^{o}-min^{-1}
Total data collected	3121
Independent data, I>3σ(I)	2355
Total variables	260
$R=\Sigma\|\|F_o\|-\|F_c\|\|/\Sigma\|F_o\|$	0.041
$R_w=[\Sigma w(\|F_o\|-\|F_c\|)^2/\Sigma w\|F_o\|^2]^{1/2}$	0.032
Weights	$w = \sigma(F)^{-2}$

Table 2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$)

	x	y	z	U(eq)
Ge	1976(1)	4272(1)	4762(1)	47(1)
F(1)	1309(5)	3353(4)	-49(3)	127(3)
F(2)	2102(7)	2280(5)	921(4)	156(4)
F(3)	3756(6)	4335(6)	1100(4)	123(3)
F(4)	3019(5)	6803(4)	2350(4)	104(3)
F(5)	1514(5)	6685(4)	3686(3)	116(3)
F(6)	501(4)	5640(4)	1534(3)	102(2)
F(7)	2173(4)	100(4)	5655(3)	94(2)
F(8)	3384(4)	2521(4)	6832(3)	94(2)
F(9)	4360(4)	1305(4)	5279(3)	79(2)
F(10)	2632(4)	35(4)	2627(3)	90(2)
F(11)	557(4)	470(4)	2328(3)	93(2)
F(12)	493(4)	-1070(3)	3103(3)	92(2)
O(1)	2873(4)	4746(3)	3481(3)	53(2)
O(2)	2931(3)	2905(3)	4579(3)	48(2)
N	4082(5)	6021(4)	6251(4)	42(2)
C(1)	1779(6)	4444(5)	2340(5)	57(3)
C(2)	2238(10)	3588(8)	1059(6)	88(5)
C(3)	1708(8)	5898(7)	2466(6)	73(4)
C(4)	2002(6)	1570(5)	4596(5)	46(3)
C(5)	3002(7)	1370(6)	5584(6)	61(3)
C(6)	1436(7)	232(6)	3144(5)	60(3)
C(7)	3632(6)	7068(5)	7367(5)	54(3)
C(8)	3462(6)	8295(6)	7263(5)	66(3)
C(9)	2994(6)	9266(6)	8252(6)	69(3)
C(10)	2695(7)	9009(6)	9322(5)	71(3)
C(11)	2834(6)	7759(6)	9415(5)	71(4)
C(12)	3271(6)	6837(7)	8474(5)	67(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 3. Bond lengths (Å)

Ge-O(1)	1.870 (4)	Ge-O(2)	1.878 (4)
Ge-N	2.092 (3)	F(1)-C(2)	1.320 (9)
F(2)-C(2)	1.293 (11)	F(3)-C(2)	1.328 (9)
F(4)-C(3)	1.313 (8)	F(5)-C(3)	1.327 (7)
F(6)-C(3)	1.320 (8)	F(7)-C(5)	1.347 (8)
F(8)-C(5)	1.325 (5)	F(9)-C(5)	1.322 (8)
F(10)-C(6)	1.307 (7)	F(11)-C(6)	1.324 (8)
F(12)-C(6)	1.340 (7)	O(1)-C(1)	1.399 (7)
O(2)-C(4)	1.396 (6)	N-C(7)	1.473 (7)
C(1)-C(2)	1.515 (9)	C(1)-C(3)	1.516 (10)
C(4)-C(5)	1.505 (9)	C(4)-C(6)	1.530 (6)
C(7)-C(8)	1.413 (10)	C(7)-C(12)	1.403 (9)
C(8)-C(9)	1.367 (8)	C(9)-C(10)	1.364 (10)
C(10)-C(11)	1.421 (11)	C(11)-C(12)	1.295 (8)

Table 4. Bond angles (°)

O(1)-Ge-O(2)	93.4(2)	O(1)-Ge-N	87.6(1)
O(2)-Ge-N	88.3(2)	Ge-O(1)-C(1)	116.3(3)
Ge-O(2)-C(4)	117.2(3)	Ge-N-C(7)	108.9(3)
O(1)-C(1)-C(2)	108.9(6)	O(1)-C(1)-C(3)	110.9(3)
C(2)-C(1)-C(3)	112.8(6)	F(1)-C(2)-F(2)	108.2(5)
F(1)-C(2)-F(3)	107.2(7)	F(2)-C(2)-F(3)	107.2(8)
F(1)-C(2)-C(1)	111.8(7)	F(2)-C(2)-C(1)	110.2(7)
F(3)-C(2)-C(1)	112.0(4)	F(4)-C(3)-F(5)	106.8(4)
F(4)-C(3)-F(6)	105.9(6)	F(5)-C(3)-F(6)	107.7(6)
F(4)-C(3)-C(1)	113.9(6)	F(5)-C(3)-C(1)	109.5(6)
F(6)-C(3)-C(1)	112.7(4)	O(2)-C(4)-C(5)	108.5(4)
O(2)-C(4)-C(6)	109.2(5)	C(5)-C(4)-C(6)	112.4(5)
F(7)-C(5)-F(8)	106.1(5)	F(7)-C(5)-F(9)	107.9(6)
F(8)-C(5)-F(9)	107.9(4)	F(7)-C(5)-C(4)	111.6(4)
F(8)-C(5)-C(4)	109.7(5)	F(9)-C(5)-C(4)	113.3(5)
F(10)-C(6)-F(11)	107.5(5)	F(10)-C(6)-F(12)	108.3(5)
F(11)-C(6)-F(12)	106.9(4)	F(10)-C(6)-C(4)	113.0(4)
F(11)-C(6)-C(4)	109.6(5)	F(12)-C(6)-C(4)	111.3(5)
N-C(7)-C(8)	118.1(5)	N-C(7)-C(12)	122.6(6)
C(8)-C(7)-C(12)	119.2(5)	C(7)-C(8)-C(9)	120.2(6)
C(8)-C(9)-C(10)	118.1(7)	C(9)-C(10)-C(11)	121.8(6)
C(10)-C(11)-C(12)	119.9(7)	C(7)-C(12)-C(11)	120.8(7)

Table 5. Anisotropic displacement parameters ($Å^2 x10^3$)

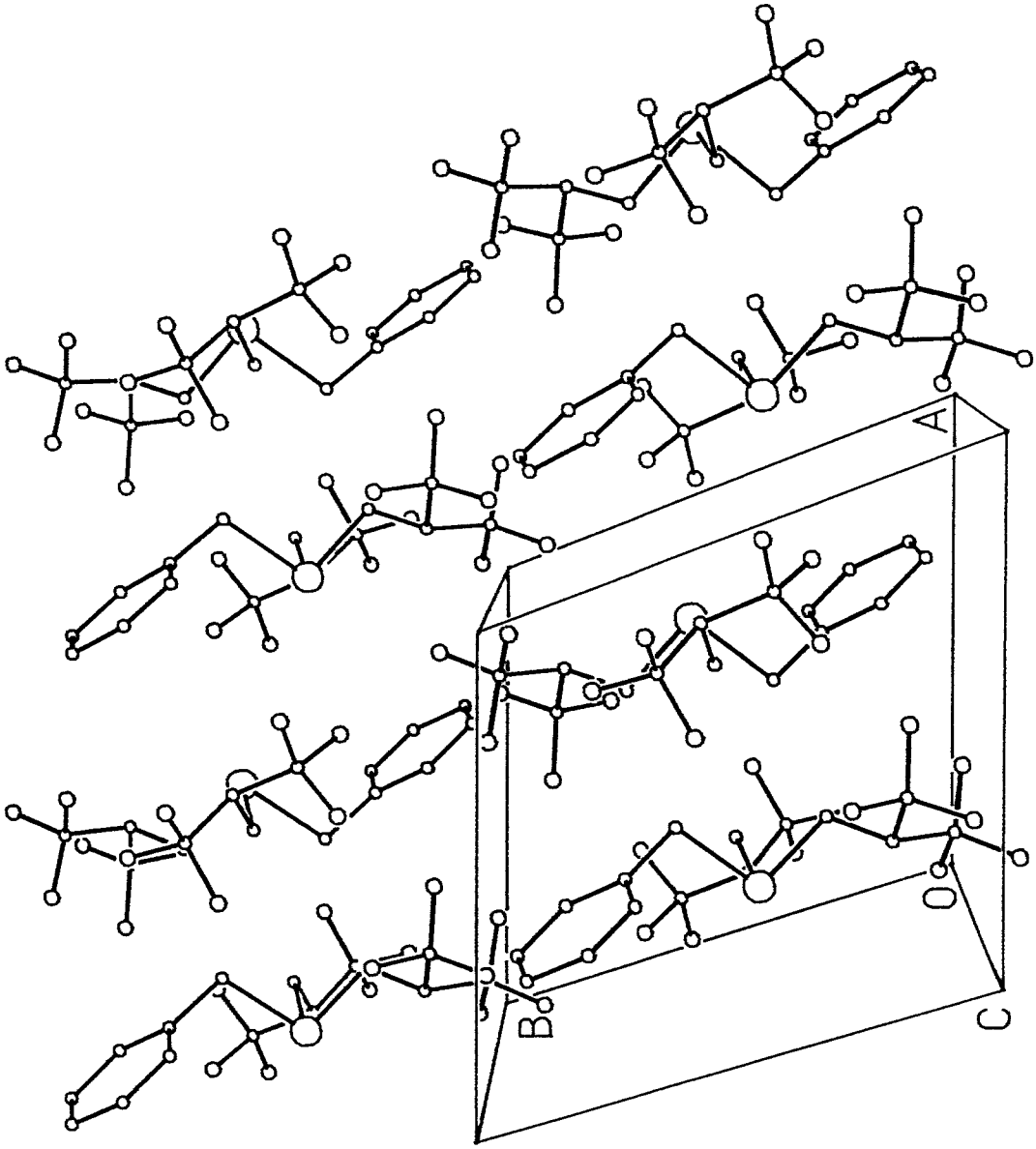
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ge	48(1)	44(1)	50(1)	18(1)	12(1)	28(1)
F(1)	177(4)	138(4)	44(2)	10(2)	-20(2)	94(3)
F(2)	295(6)	105(3)	92(3)	24(3)	31(3)	143(4)
F(3)	136(4)	180(5)	74(3)	53(3)	36(3)	98(4)
F(4)	106(3)	78(3)	120(3)	59(2)	-10(3)	21(2)
F(5)	217(5)	94(3)	75(3)	38(2)	36(3)	109(3)
F(6)	116(3)	88(3)	95(3)	38(2)	-30(2)	53(2)
F(7)	116(3)	79(2)	99(3)	65(2)	14(2)	29(2)
F(8)	115(3)	89(3)	49(2)	19(2)	6(2)	32(2)
F(9)	75(2)	93(3)	84(2)	46(2)	12(2)	47(2)
F(10)	101(3)	97(3)	58(2)	14(2)	27(2)	55(2)
F(11)	101(3)	94(3)	65(2)	28(2)	-13(2)	41(2)
F(12)	114(3)	43(2)	83(2)	15(2)	10(2)	15(2)
O(1)	61(2)	60(2)	41(2)	24(2)	-2(2)	29(2)
O(2)	49(2)	39(2)	67(2)	29(2)	22(2)	23(2)
N	50(3)	45(3)	34(2)	12(2)	14(2)	29(2)
C(1)	71(4)	47(3)	46(3)	18(3)	-8(3)	26(3)
C(2)	127(6)	88(5)	47(4)	19(4)	-4(4)	67(5)
C(3)	98(5)	53(4)	53(4)	14(3)	-12(4)	38(4)
C(4)	51(3)	42(3)	51(3)	24(3)	17(3)	23(3)
C(5)	78(4)	46(3)	54(4)	24(3)	13(3)	19(3)
C(6)	66(4)	52(4)	56(4)	21(3)	11(3)	25(3)
C(7)	51(3)	48(3)	55(3)	17(3)	4(3)	23(3)
C(8)	87(4)	62(4)	55(4)	28(3)	15(3)	39(3)
C(9)	88(4)	59(4)	61(4)	10(3)	21(3)	53(3)
C(10)	91(5)	64(4)	45(4)	4(3)	13(3)	47(4)
C(11)	75(4)	72(4)	52(4)	13(3)	22(3)	35(4)
C(12)	72(4)	87(4)	38(3)	28(3)	19(3)	28(4)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 6. H-Atom coordinates ($x10^4$) and isotropic displacement parameters ($Å^2 x10^3$)

	x	y	z	U
H(1N)	4889(58)	6502(53)	5889(49)	81(6)
H(2N)	4706(57)	5627(55)	6494(47)	81(6)
H(1)	662	3786	2282	81(6)
H(4)	1014	1624	4909	81(6)
H(8)	3685	8452	6464	81(6)
H(9)	2873	10140	8192	81(6)
H(10)	2370	9720	10062	81(6)
H(11)	2594	7591	10206	81(6)
H(12)	3352	5951	8536	81(6)


A
B
C