Supporting Information

Design, Synthesis and In Vivo SAR of a Novel Series of Pyrazolines as Potent Selective Androgen Receptor Modulators

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1) Preparation of anilines 3

The required starting material anilies **3** were obtained from either commercial source or prepared by the known method. Some novel anilines were prepared by the following procedure.

4-Amino-3-ethyl-2-trifluoromethyl-benzonitrile and 4-Amino-5-chloro-2-trifluoromethyl-benzonitrile

These two anilines were prepared according to PCT Int. Appl. 2004, WO 2004045518.

4-Amino-5-ethyl-2-trifluoromethyl-benzonitrile

4-Amino-5-iodo-2-trifluoromethyl-benzonitrile (936 mg, 3.0 mmol), CuI (I) (57 mg, 0.3 mmol), $PdCl_2(PPh)_3$ (105.3 mg, 0.15 mmol), triethyl amine (1.01 g, 10 mmol) and ethynyl-trimethyl-silane (450 mg, 4.5 mmol) were mixed in THF (30 mL). The reaction mixture was stirred at room temperature overnight. Tetrabutylammonium fluoride (1.0 M in THF, 3.0 mL, 3.0 mmol) was added to the reaction mixture and stirred at room temperature for 20 min. The reaction was quenched by addition of H_2O and extracted with ethyl acetate. The organic layer was combined and washed with brine, dried over Na_2SO_4 and concentrated to afford the crude product 4-amino-5-ethynyl-2-trifluoromethyl-benzonitrile.
The crude product (3.0 g, 90% pure) mixed with Pd/C (0.3 g) in methanol (50 ml) with the H_2 (40 psi). The reaction was shaked at room temperature for overnight. Upon separation on silica gel (100% CH_2Cl_2), the tile compound was obtained in pure form as a colorless liquid (3.0 g, 100%).
^{1}H NMR ($CDCl_3$) δ 7.50 (s, 1H), 7.00 (s, 1H), 4.50 (br, 2H), 2.50 (m, 2H), 1.30 (m, 3H). MS (m/z): 214, $(M+H)^+$.

4-Amino-5-methoxy-2-trifluoromethyl-benzonitrile

4-Amino-5-iodo-2-trifluoromethyl-benzonitrile (312 mg, 1.0 mmol), CuI (I) (20 mg, 0.1 mmol), Cs_2CO_3 (652 mg, 2.0 mmol) and 1,10-phenanthroline (36 mg, 0.2 mmol) were mixed in methanol (20 mL). The reaction was refluxed overnight and then solvent was removed under vacuum. Upon separation on silica gel (100% CH_2Cl_2), the tile compound was obtained in pure form as a colorless liquid (100 mg, 48%).
^{1}H NMR ($CDCl_3$) δ 7.05 (s, 1H), 6.90 (s, 1H), 4.50 (br, 2H), 3.90 (s, 3H). MS (m/z): 216, $(M+H)^+$.

4-Amino-5-chloro-2-trifluoromethyl-benzonitrile

4-Amino-2-trifluoromethyl-benzonitrile (1.95 g, 10.5 mmol), NCS (2.07 g, 15.5 mmol) in MeOH (50 mL) at 0 ^oC was stirred for 2 hrs. The solvent was removed and the residue was partitioned between ethyl acetate and water. The organic layer was washed with sodium thiosulfate, water, brine, dried over anhydrous Na_2SO_4, filtered and concentrated to give the crude material, which was then purified by column chromatography using hexanes and ethyl acetate to yield the title compound (700 mg, 31%) as a brown solid along with side product 4-amino-3,5-dichloro-2-trifluoromethyl-benzonitrile.
^{1}H NMR ($CDCl_3$) δ 7.65 (s, 1H), 7.02 (s, 1H), 4.90 (br, s, 2H). MS (m/z): 221, $(M+H)^+$.

4-Amino-5-cyano-2-trifluoromethyl-benzonitrile

4-Amino-5-iodo-2-trifluoromethyl-benzonitrile (467 mg, 1.5 mmol), CuCN (155 mg, 1.7 mmol) in NMP (10 mL) was heated at 150 ^oC for 4 hrs. The reaction mixture was passed through a pad of Celite. The solution was partitioned between ethyl acetate and water. The organic layer was washed with water, brine, dried over anhydrous Na_2SO_4, filtered and concentrated to yield the title compound as brown solid (152 mg, 45%).
^{1}H NMR ($CDCl_3$) δ 7.82 (s, 1H), 7.15 (s, 1H), 5.45 (br, s, 2H). MS (m/z): 212, $(M+H)^+$.

4-Amino-5-ethylsulfanyl-2-trifluoromethyl-benzonitrile

4-Amino-5-iodo-2-trifluoromethyl-benzonitrile (6.24 g, 20.0 mmol), CuI (I) (380 mg, 2.0 mmol), K_2CO_3 (6.52 g, 40.0 mmol) and ethyl thiol (1.25 g, 20.0 mmol) were mixed in ethanol (50 mL). The reaction was refluxed overnight and then solvent was removed under vacuum. Upon separation on silica gel (100% DCM), the tile compound was obtained in pure form as a colorless liquid (4.36 g, 90%).

^{1}H NMR ($CDCl_3$) δ 7.70 (s, 1H), 7.00 (s, 1H), 5.10 (br, 2H), 2.85 (m, 2H), 1.25 (m, 3H). MS (m/z): 264, $(M+H_2O)^+$.

2) Summary of Purity of Compounds[1]

Cmpds	Formula	CHN Calculated	CHN Found	HPLC Purity
6a	$C_{20}H_{18}F_3N_5O_4$	C, 53.45; H, 4.04; N, 15.58	C, 53.70; H, 4.18; N, 14.97	97%
6b	$C_{21}H_{18}F_3N_5O_2$	C, 58.74; H, 4.23; N, 16.31	C, 58.32; H, 4.04; N, 16.37	-
6c	$C_{20}H_{15}F_6N_5O_4$	C, 47.72; H, 3.00; N, 13.91	C, 47.21; H, 3.12; N, 14.35	98%
6d	$C_{21}H_{18}F_6N_6O_2$	C, 65.27; H, 4.70; N, 21.75	C, 64.96; H, 5.47; N, 21.05	98%
6e	$C_{20}H_{18}ClF_3N_4O_2$	C, 54.74; H, 4.13; N, 12.77	C, 54.81; H, 4.05; N, 12.61	-
6f	$C_{21}H_{18}F_3N_5O_2$	C, 58.74; H, 4.23; N, 16.31	C, 58.24; H, 4.06; N, 16.30	-
6g	$C_{22}H_{20}F_3N_5O_2$ ·0.35 EtOAc	C, 59.26; H, 4.85; N, 14.77	C, 59.54; H, 4.55; N, 15.01	-
6h	$C_{19}H_{14}F_4N_4O$· 0.7 MeOH	C, 57.32; H, 4.10; N, 14.57	C, 57.45; H, 3.88; N, 14.35	-
6i	$C_{18}H_{14}F_4N_4O_3$· 0.2 H_2O	C, 52.23; H, 3.51; N, 13.54	C, 52.10; H, 3.35; N, 13.78	-
7a	$C_{13}H_{11}F_3N_4O$	C, 52.71; H, 3.74; N, 18.91	C, 48.86; H, 3.95; N, 15.16	95%
7b	$C_{14}H_{13}F_3N_4O$	C, 54.19; H, 4.22; N, 18.06	C, 54.05; H, 4.10; N, 18.25	-
7c	$C_{14}H_{10}F_6N_4O$	C, 46.16; H, 2.77; N, 15.38	C, 46.29; H, 2.53; N, 15.28	-
7d	$C_{13}H_{10}F_6N_4O$· 1.2 H_2O	C, 40.64; H, 2.62; N, 14.58	C, 41.77; H, 3.34; N, 14.99	-
7e	$C_{13}H_{10}ClF_6N_3O$·0.2 CH_2Cl_2	C, 41.78; H, 2.70; N, 11.24	C, 41.55; H, 2.90; N, 11.65	-
7f	$C_{13}H_{10}BrF_6N_3O$	C, 37.34; H, 2.41; N, 10.05	C, 38.05; H, 2.75; N, 9.56	97%
7g	$C_{12}H_{10}Cl_2F_3N_3O$· 0.2 MeOH	C, 42.28; H, 3.14; N, 12.12	C, 42.40; H, 2.98; N, 11.75	-
7h	$C_{13}H_{11}F_3N_4O$	C, 52.71; H, 3.74; N, 18.91	C, 52.50; H, 3.65; N, 19.01	-
7i	$C_{15}H_{15}F_3N_4O$	C, 55.55; H, 4.66; N, 17.28	C, 55.62; H, 4.50; N, 17.15	-
7j	$C_{16}H_{17}F_3N_4O$· 0.5 H_2O	C, 55.33; H, 5.22; N, 16.13	C, 55.45; H, 5.60; N, 15.88	-
7k	$C_{15}H_{12}F_6N_4O$	C, 47.63; H, 3.26; N, 14.81	C, 47.61; H, 3.56; N, 15.12	-
7l	$C_{15}H_{10}F_8N_4O$	C, 43.49; H, 2.43; N, 13.52	C, 43.11; H, 2.11; N, 13.90	-
7m	$C_{14}H_7F_9N_4O$	C, 40.21; H, 1.69; N, 13.40	C, 40.27; H, 1.35; N, 13.18	-
7n	$C_{14}H_{10}F_6N_4O$	C, 46.16; H, 2.77; N, 15.38	C, 46.14; H, 2.36; N, 15.30	-
7o	$C_{16}H_{15}F_3N_4O_3$· 0.25 H_2O	C, 51.55; H, 4.19; N, 15.03	C, 51.76; H, 4.05; N, 14.88	-
7p	$C_{15}H_{14}F_6N_4O$	C, 47.63; H, 3.20; N, 14.81	C, 47.20; H, 2.97; N, 13.90	97%
7q	$C_{16}H_{12}F_6N_4O$	C, 48.99; H, 3.50; N, 14.28	C, 49.15; H, 3.11; N, 13.95	-
7r	$C_{16}H_{17}F_3N_4O$· 0.5 C_5H_5N	C, 58.80; H, 5.20; N, 16.68	C, 58.88; H, 5.17; N, 16.98	-
7s	$C_{17}H_{19}F_3N_4O$	C, 57.95; H, 5.44; N, 15.90	C, 57.77; H, 5.40; N, 15.75	-
8a	$C_{16}H_{14}F_6N_4O$	C, 48.99; H, 3.60; N, 14.28	C, 48.75; H, 3.46; N, 14.51	-
8b	$C_{16}H_{14}F_6N_4O$	C, 48.99; H, 3.60; N, 14.28	C, 48.71; H, 3.52; N, 14.55	-
8c	$C_{15}H_{12}F_6N_4O_2$· 0.2 EtOAc	C, 46.07; H, 3.33; N, 13.60	C, 45.88; H, 3.13; N, 13.51	-
8d	$C_{14}H_9ClF_6N_4O$	C, 42.18; H, 2.28; N, 14.05	C, 41.61; H, 1.88; N, 13.08	97%
8e	$C_{14}H_9IF_6N_4O$	C, 34.31; H, 1.85; N, 11.43	C, 34.25; H, 1.70; N, 11.64	-
8f	$C_{15}H_9F_6N_5O$	C, 46.28; H, 2.33; N, 17.99	C, 46.31; H, 3.10; N, 17.65	-
8g	$C_{16}H_{14}F_6N_4OS$	C, 45.28; H, 3.33; N, 13.20	C, 44.50; H, 3.45; N, 12.51	95%
9a	$C_{15}H_{12}F_6N_4O$	C, 47.63; H, 3.20; N, 14.81	C, 47.36; H, 3.38; N, 14.35	-
9b	$C_{16}H_{14}F_6N_4O$	C, 48.99; H, 3.60; N, 14.28	C, 48.75; H, 3.52; N, 14.15	-
9c	$C_{22}H_{20}F_3N_5O_2$.0.5 H_2O	C, 58.40; H, 4.68; N, 15.48	C, 58.38; H, 4.64; N, 15.38	-
9d	$C_{16}H_{17}F_3N_4O$	C, 56.80; H, 5.06; N, 16.56	C, 56.56; H, 4.91; N, 12.35	-
9e	$C_{14}H_{12}F_3N_3O_2$.1.4 H_2O	C, 49.97; H, 4.43; N, 12.49	C, 50.13; H, 4.18; N, 12.38	-

9f	$C_{19}H_{13}F_4N_3O_2 \cdot 0.5$ MeOH	C, 57.50; H, 3.71; N, 10.32	C, 57.75; H, 3.86; N, 9.98	-
9g	$C_{16}H_9F_9N_4O_2$	C, 41.75; H, 1.97; N, 12.17	C, 41.81; H, 2.23; N, 11.95	-
10a	$C_{15}H_{12}F_6N_4O$	C, 47.63; H, 3.20; N, 14.81	C, 47.46; H, 3.09; N, 13.89	-
10b	$C_{16}H_{14}F_6N_4O$	C, 48.99; H, 3.60; N, 14.28	C, 49.40; H, 3.13; N, 15.13	97%
10c	$C_{14}H_{10}F_6N_4S$	C, 44.21; H, 2.65; N, 14.73	C, 42.75; H, 1.89; N, 15.20	95%

[1] For those compounds without satisfied CHN analysis data, the purity was further checked by LC-MS condition.

3) X-ray Single Crystallographic Data of (R)-13·0.5 CH_2Cl_2

Description of Single-Crystal Sample and Mounting Used for Data Collection:

1) Color: Colorless
2) Shape: Block
3) Dimensions: 0.03 mm. x 0.09 mm. x 0.09 mm.
4) Indices of Faces:
5) Crystal Mount: Crystal was frozen in Paratone N oil and suspended inside a nylon cryoloop.
6) Crystal Orientation: Crystal had a random orientation.

Space Group and Cell Data:

1) Crystal System: Triclinic Space Group and Number: P1 - C (No. 1)
2) Number of Computer-Centered Reflections Used in the Least-Squares Refinement of the Cell Dimensions: 1384 having 7.64° < 2Θ(MoK) < 36.94° and measured at -80±2 °C
3) Lattice Constants with esd's:

a = 8.604(3) Å	α = 87.075(6)°	V = 2631(2) $Å^3$
b = 14.493(5) Å	β = 84.034(6)°	Z = 4 formula units
c = 21.258(7) Å	γ = 85.755(6)°	λ = 0.71073 Å

4) Formula Weight: 675.77 amu Calculated Density:1.706 $g \cdot cm^{-3}$
5) Linear Absorption Coefficient: 1.392 mm^{-1} F(000) = 1324.
6) Comments: The sample was recrystallized from a saturated dichloromethane solution.

Description of Data Collection:

1) Instrument: Bruker SMART APEX CCD Single Crystal Diffraction System
2) X-ray Source: Sealed fine-focus X-ray tube
3) Radiation: MoK Power: 50 kV 35 mA
4) Monochromator: Graphite
5) Incident Beam Collimator Diameter: 0.5 mm Temperature: -80±2°C
6) Scan Axis: Omega
7) Scan Width: 0.30° 2Θ Range of Data : 7.64° - 46.51°
8) Sample to Detector Distance: 6.000 cm
9) Portion of Ewald Sphere Collected: Hemisphere
10) Number of frames collected: 1868 Seconds/frame: 20
11) Total Number of Reflections Collected: 16403
12) Number of Independent Reflections Collected: 13647
13) Data Collected: $-9 \le h \le 9$; $-16 \le k \le 16$; $-23 \le l \le 23$ $R_{in} = 0.080$

Data Reduction:

Lorentz, polarization and absorption correction; Range of relative transmission factors: 0.925 -1.000

Empirical Correction using Measurements for Equivalent Reflections (143 Reflections used)

Structure Solution:

1) Method(s) Used in Structure Solution: Direct Methods: SHELXTL/PC
2) Hydrogen Atom Positions Located After Refinement Cycle #3 by Difference Fourier and Calculated

Structure Refinement:

1) Final Scale Factor: 0.1651(2)
2) Extinction Parameter[6] Refined? No
   Form: $k[1+0.001(x)(F_c^2)(\lambda^3)/\sin(2\theta)]^{-1/4}$
3) Anomalous Dispersion Corrections for Which Atoms: I, Cl, F, O, N, C
4) Variable Occupancies for Which Atoms? None
5) Refinement Constraints/Restraints: The eight hydrogens bonded to nitrogen were initially located from a difference Fourier synthesis. They were then included in the structure factor calculations as idealized atoms (assuming sp^2-hybridization of the nitrogen atoms and a N-H bond length of 0.88 Å) "riding" on their respective nitrogen atoms. The four methyl groups (C_{15}, C_{45}, C_{75}, C_{105} and their hydrogens) were refined as rigid rotors (using idealized sp^3-hybridized geometry and a C-H bond length of 0.98 Å) which were allowed to rotate around their respective C-C bonds in least-squares cycles. The remaining hydrogen atoms were included in the structure factor calculations as idealized atoms (assuming sp^2- or sp^3-hybridization of the carbon atoms and C-H bond lengths of 0.95-0.99 Å) "riding" on their respective carbon atoms. The isotropic thermal parameters of all hydrogen atoms were fixed at values 1.2 (nonmethyl) or 1.5 (methyl) times the equivalent isotropic thermal parameter of the carbon or nitrogen atom to which they are covalently bonded. Moderate restraints had to be applied to the anisotropic thermal parameters of eighteen nonhydrogen atoms.
6) Shift/Error Analysis for Final Least-Squares Cycle[7]:
   Maximum Shift for all Parameters: 0.000 σ_p Mean Shift for all Parameters: 0.000 σ_p
7) Peaks found in Final Difference Fourier Map: There were no peaks present in the final difference Fourier map above the background level (0.71 $e^-/Å^3$). The minimum and mean electron density in the final difference Fourier were -0.98 and 0.00 $e^-/Å^3$, respectively. The rms deviation from the mean electron density was 0.10 $e^-/Å^3$.

Table 1. Atomic Coordinates for Nonhydrogen Atoms in Crystalline **R**-$C_{22}H_{14}F_6IN_7O$ · 0.5 CH_2Cl_2 [a]

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z	Equivalent Isotropic Thermal Parameter, U, $Å^2 \times 10^3$ [c]
		Molecule 1		
I_1	5747(2)	1389(1)	-5863(1)	54(1)
F_1	654(15)	2345(9)	460(5)	72(4)
F_2	2455(19)	1679(10)	-98(6)	86(5)
F_3	2656(19)	3039(10)	126(7)	82(5)
F_4	1793(18)	-370(10)	-3966(7)	75(5)
F_5	448(19)	-1382(9)	-3431(10)	103(7)
F_6	1933(17)	-600(10)	-2968(7)	74(5)
O_1	4664(18)	3883(10)	-2996(7)	47(4)
N_1	2508(18)	3683(9)	-2328(7)	29(4)
N_2	363(16)	2756(9)	-2432(7)	21(4)
N_3	494(18)	3535(10)	-1525(7)	32(4)
N_4	1457(17)	3352(11)	-1012(7)	39(4)
N_5	-1767(19)	1869(11)	-2089(7)	30(4)
N_6	-1590(30)	-580(14)	-4728(9)	61(7)
C_1	1130(20)	3297(15)	-2111(9)	36(6)
C_2	871(19)	2793(11)	-604(9)	29(4)
C_3	-600(20)	2388(14)	-786(8)	44(6)
C_4	-890(30)	2967(14)	-1421(11)	50(7)
C_5	-800(20)	2481(13)	-1996(9)	26(5)
C_6	3430(20)	3533(13)	-2907(10)	33(5)
N_7	2790(20)	3003(10)	-3308(8)	39(5)
C_8	3530(20)	2678(13)	-3892(9)	27(5)
C_9	4660(20)	3135(13)	-4258(9)	31(5)
C_{10}	5270(20)	2745(14)	-4805(9)	34(6)
C_{11}	4770(20)	1978(13)	-5031(9)	34(5)
C_{12}	3650(30)	1487(14)	-4637(10)	37(6)
C_{13}	2990(20)	1888(14)	-4081(10)	37(6)
C_{14}	1630(30)	2474(13)	-36(10)	42(6)
C_{15}	-2480(20)	3640(16)	-1297(13)	64(8)
C_{16}	-1650(30)	1425(14)	-2650(10)	36(6)

Table 1.(continued)

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z	Equivalent Isotropic Thermal Parameter, U, $Å^2 \times 10^3$ [c]
C_{17}	-460(30)	708(14)	-2764(10)	36(6)
C_{18}	-400(30)	188(13)	-3317(9)	32(5)
C_{19}	-1540(30)	392(13)	-3733(11)	42(7)
C_{20}	-2670(30)	1039(14)	-3664(10)	30(6)
C_{21}	-2750(20)	1578(14)	-3117(9)	35(6)
C_{22}	950(30)	-513(16)	-3399(10)	46(7)
C_{23}	-1530(30)	-149(15)	-4318(13)	53(7)
		Molecule 2		
I_{31}	-6657(2)	-3319(1)	1488(1)	54(1)
F_{31}	880(20)	-4221(11)	-4485(8)	122(6)
F_{32}	1279(16)	-3360(10)	-3766(9)	121(6)
F_{33}	892(15)	-4817(9)	-3559(7)	82(4)
F_{34}	-6775(16)	1265(9)	-2419(7)	69(4)
F_{35}	-7198(17)	1036(9)	-1438(6)	69(4)
F_{36}	-5499(16)	1941(8)	-1811(7)	65(4)
O_{31}	-5820(20)	-5258(10)	-1578(8)	61(5)
N_{31}	-4763(18)	-4431(11)	-2437(7)	30(4)
N_{32}	-4262(19)	-2892(11)	-2563(7)	26(4)
N_{33}	-3740(20)	-3818(11)	-3394(8)	39(5)
N_{34}	-2220(20)	-4272(10)	-3413(8)	52(5)
N_{35}	-3414(19)	-1440(10)	-3030(8)	35(5)
N_{36}	-3930(20)	1177(12)	-464(9)	60(5)
C_{31}	-4300(20)	-3665(13)	-2736(9)	27(5)
C_{32}	-1250(20)	-3747(14)	-3778(9)	41(5)
C_{33}	-1970(30)	-2883(15)	-4038(10)	45(6)
C_{34}	-3560(30)	-2819(12)	-3670(10)	33(6)
C_{35}	-3670(20)	-2299(14)	-3036(9)	26(5)
C_{36}	-5370(20)	-4520(14)	-1801(12)	37(6)
N_{37}	-5201(19)	-3806(11)	-1423(8)	37(5)
C_{38}	-5650(20)	-3715(13)	-770(9)	28(5)
C_{39}	-6180(20)	-4439(14)	-400(10)	39(5)

Table 1.(continued)

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z	Equivalent Isotropic Thermal Parameter, U, $Å^2 \times 10^3$ [c]
C_{40}	-6540(30)	-4295(16)	258(14)	75(9)
C_{41}	-6160(20)	-3499(13)	523(9)	27(5)
C_{42}	-5480(30)	-2787(15)	165(10)	45(6)
C_{43}	-5220(20)	-2926(14)	-532(10)	40(6)
C_{44}	540(30)	-4041(18)	-3869(12)	62(7)
C_{45}	-4920(30)	-2498(16)	-4069(11)	61(7)
C_{46}	-3700(30)	-980(14)	-2474(10)	38(6)
C_{47}	-4740(20)	-235(14)	-2438(11)	37(6)
C_{48}	-4870(20)	348(13)	-1899(8)	24(5)
C_{49}	-3930(20)	128(14)	-1405(9)	31(5)
C_{50}	-2830(20)	-641(14)	-1435(10)	38(6)
C_{51}	-2730(30)	-1199(14)	-1960(15)	60(8)
C_{52}	-5950(30)	1093(19)	-1881(13)	51(7)
C_{53}	-3960(20)	724(14)	-869(10)	37(5)
		Molecule 3		
I_{61}	-907(2)	3450(1)	5865(1)	54(1)
F_{61}	7676(16)	-189(9)	415(6)	85(4)
F_{62}	7090(16)	-750(8)	1333(6)	75(4)
F_{63}	5425(17)	-629(9)	616(7)	107(6)
F_{64}	3516(19)	5577(11)	3990(9)	91(6)
F_{65}	4755(18)	6460(9)	3440(9)	94(6)
F_{66}	3178(18)	5683(11)	3041(9)	97(6)
O_{61}	294(17)	1316(10)	2926(7)	39(4)
N_{61}	2382(17)	1607(9)	2207(7)	28(4)
N_{62}	4454(18)	2548(10)	2321(7)	31(4)
N_{63}	4351(17)	1867(10)	1383(7)	24(4)
N_{64}	4498(17)	939(10)	1214(6)	29(4)
N_{65}	6910(20)	3198(13)	2092(9)	52(6)
N_{66}	6780(30)	5618(14)	4745(12)	83(8)
C_{61}	3740(20)	1982(13)	1990(12)	37(6)
C_{62}	6010(20)	757(13)	1065(8)	34(5)

Table 1.(continued)

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z	Equivalent Isotropic Thermal Parameter, U, Å^2 x 10^3 [c]
C_{63}	7020(20)	1469(14)	1196(11)	49(6)
C_{64}	5880(20)	2299(13)	1319(9)	28(5)
C_{65}	5890(30)	2730(15)	1930(12)	46(6)
C_{66}	1510(30)	1700(12)	2834(9)	26(5)
N_{67}	2197(18)	2181(10)	3229(7)	27(4)
C_{68}	1450(20)	2440(14)	3802(9)	28(5)
C_{69}	440(30)	1872(15)	4158(11)	47(6)
C_{70}	-230(20)	2175(14)	4788(10)	38(6)
C_{71}	130(30)	2984(16)	5001(10)	43(6)
C_{72}	1230(30)	3499(15)	4673(11)	49(7)
C_{73}	1900(20)	3231(13)	4066(10)	35(6)
C_{74}	6460(30)	-179(16)	844(10)	54(6)
C_{75}	5890(30)	3017(16)	775(12)	67(8)
C_{76}	6720(30)	3685(13)	2693(10)	30(5)
C_{77}	5560(30)	4375(16)	2779(11)	44(7)
C_{78}	5520(30)	4901(14)	3303(13)	51(8)
C_{79}	6660(30)	4696(15)	3775(13)	52(7)
C_{80}	7830(30)	3917(17)	3590(14)	62(8)
C_{81}	7890(30)	3436(15)	3101(11)	49(7)
C_{82}	4300(30)	5633(19)	3406(15)	60(8)
C_{83}	6710(30)	5217(16)	4279(12)	54(8)
		Molecule 4		
I_{91}	1822(2)	-1526(1)	-1481(1)	52(1)
F_{91}	1914(14)	-1726(9)	5130(6)	77(4)
F_{92}	3518(17)	-1984(14)	4334(7)	118(7)
F_{93}	2700(20)	-594(12)	4543(9)	140(8)
F_{94}	1500(20)	-6198(11)	2357(11)	127(8)
F_{95}	323(17)	-6646(9)	1600(8)	79(5)
F_{96}	2213(17)	-5818(10)	1372(9)	91(6)
O_{91}	822(18)	433(9)	1545(7)	35(4)

Table 1.(continued)

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z	Equivalent Isotropic Thermal Parameter, U, Å^2 x 10^3 [c]
N_{91}	70(20)	-405(11)	2406(8)	42(5)
N_{92}	-590(20)	-1949(11)	2512(9)	42(5)
N_{93}	-708(19)	-1078(10)	3422(8)	33(4)
N_{94}	609(18)	-801(11)	3708(7)	42(4)
N_{95}	-1338(19)	-3363(10)	3054(9)	35(5)
N_{96}	-790(20)	-5508(13)	242(9)	62(6)
C_{91}	-420(20)	-1131(14)	2780(12)	39(6)
C_{92}	960(20)	-1478(15)	4120(8)	43(5)
C_{93}	60(30)	-2355(16)	4132(12)	54(7)
C_{94}	-1180(20)	-1993(13)	3662(9)	28(5)
C_{95}	-1070(20)	-2521(14)	3042(11)	39(6)
C_{96}	490(30)	-289(15)	1733(11)	36(6)
N_{97}	558(19)	-1105(11)	1446(9)	38(5)
C_{98}	860(30)	-1155(14)	768(11)	48(7)
C_{99}	1730(20)	-554(14)	416(9)	38(5)
C_{100}	1940(20)	-657(12)	-229(8)	30(5)
C_{101}	1410(30)	-1378(15)	-520(10)	43(6)
C_{102}	590(20)	-2027(14)	-109(13)	47(7)
C_{103}	270(30)	-1893(14)	523(9)	43(6)
C_{104}	2300(30)	-1428(18)	4523(12)	57(6)
C_{105}	-2890(20)	-1936(13)	3954(9)	35(5)
C_{106}	-1310(20)	-3809(13)	2512(13)	40(7)
C_{107}	-350(30)	-4613(14)	2401(10)	39(6)
C_{108}	-150(30)	-5061(13)	1821(12)	48(7)
C_{109}	-1050(20)	-4706(13)	1327(11)	41(6)
C_{110}	-2050(30)	-3966(15)	1391(11)	48(7)
C_{111}	-2160(20)	-3485(13)	1997(9)	31(5)
C_{112}	1160(40)	-5960(20)	1781(14)	76(11)
C_{113}	-900(20)	-5181(15)	759(13)	53(7)
		Solvent Molecule of Crystallization 1		
Cl_{1S}	5938(7)	130(4)	2704(3)	70(2)

Table 1.(continued)

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z	Equivalent Isotropic Thermal Parameter, U, $Å^2 \times 10^3$ [c]
Cl_{2S}	4126(9)	-1501(6)	2638(4)	108(3)
C_{1S}	4150(30)	-423(17)	2776(17)	126(14)
		Solvent Molecule of Crystallization 2		
Cl_{3S}	456(14)	5986(7)	-2141(4)	163(4)
Cl_{4S}	-1541(8)	6297(5)	-986(4)	95(2)
C_{2S}	260(20)	5887(12)	-1286(9)	46(6)

[a]The numbers in parentheses are the estimated standard deviations in the last significant digit.
[b]Atoms are labeled in agreement with Figure 1.
[c]This is one-third of the trace of the orthogonalized U_{ij} tensor.

Table 2.Anisotropic Thermal Parameters for Nonhydrogen Atoms in Crystalline **R**-$C_{22}H_{14}F_6IN_7O \cdot 0.5\ CH_2Cl_2$ [a,b]

Atom Type[c]	Anisotropic Thermal Parameters ($Å^2 \times 10^3$) U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
			Molecule 1			
I_1	51(1)	70(1)	40(1)	-19(1)	7(1)	-8(1)
F_1	92(10)	98(10)	25(7)	1(6)	1(6)	-14(8)
F_2	115(13)	100(11)	37(9)	-12(8)	-13(8)	53(9)
F_3	91(12)	82(11)	79(11)	-3(9)	-32(9)	-31(10)
F_4	86(11)	82(10)	55(10)	-15(8)	20(8)	0(9)
F_5	75(12)	37(9)	210(20)	-22(10)	-61(12)	-5(8)
F_6	62(10)	101(12)	63(10)	-30(9)	-18(8)	4(9)
O_1	43(10)	56(10)	47(10)	-11(8)	-12(8)	-29(8)
N_1	48(11)	25(9)	15(9)	-13(7)	7(8)	-13(8)
N_2	21(7)	17(7)	28(7)	-6(6)	-10(6)	-11(6)
N_3	35(10)	45(11)	22(10)	-10(8)	-16(8)	-11(8)
N_4	38(10)	51(11)	31(10)	-26(8)	-3(8)	-7(9)
N_5	41(11)	38(10)	13(10)	-8(8)	-9(8)	-2(9)
N_6	83(17)	76(15)	25(12)	-30(11)	-3(11)	9(13)
C_1	33(13)	55(14)	16(11)	9(10)	6(9)	12(11)
C_2	25(11)	20(10)	45(12)	15(9)	-22(9)	-10(8)
C_3	48(15)	64(15)	13(12)	0(10)	20(10)	19(12)
C_4	48(15)	42(13)	67(17)	-28(12)	5(12)	-36(12)
C_5	29(9)	33(8)	17(8)	-12(7)	2(7)	0(7)
C_6	30(13)	38(12)	34(13)	-17(10)	-11(11)	-6(11)
N_7	36(11)	26(9)	56(13)	-3(9)	10(9)	-20(8)
C_8	35(9)	28(8)	18(8)	-10(7)	3(7)	-2(7)
C_9	51(14)	28(11)	16(11)	-5(9)	-1(10)	-8(10)
C_{10}	42(14)	57(14)	4(11)	3(10)	-8(10)	-10(11)
C_{11}	38(9)	35(8)	28(9)	-16(7)	6(7)	-3(8)
C_{12}	43(15)	34(12)	38(15)	-14(11)	-14(12)	-4(11)
C_{13}	40(14)	50(14)	22(13)	10(11)	-10(11)	-15(12)
C_{14}	71(16)	17(11)	39(13)	-1(10)	-7(12)	0(11)
C_{15}	24(13)	66(16)	100(20)	-43(15)	6(13)	0(12)
C_{16}	45(15)	32(12)	33(14)	-15(10)	15(11)	-24(11)
C_{17}	36(14)	39(13)	32(14)	-2(11)	2(11)	-9(12)
C_{18}	45(15)	30(12)	19(12)	6(10)	9(11)	-7(11)

Table 2.(continued)

Atom Type[c]	Anisotropic Thermal Parameters (Å^2 x 10^3) U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C_{19}	55(16)	15(11)	52(16)	-14(11)	36(13)	-11(12)
C_{20}	37(14)	34(13)	18(11)	13(10)	-2(10)	-11(12)
C_{21}	39(13)	43(12)	17(12)	7(10)	20(10)	-3(10)
C_{22}	58(15)	58(15)	19(11)	-8(11)	27(11)	-21(13)
C_{23}	90(20)	27(13)	46(19)	9(13)	-18(16)	-2(13)
			Molecule 2			
I_{31}	64(1)	64(1)	35(1)	-9(1)	2(1)	-2(1)
F_{31}	163(17)	91(12)	97(13)	-19(9)	58(12)	25(11)
F_{32}	56(10)	89(11)	225(19)	-55(12)	17(11)	-43(9)
F_{33}	78(10)	63(9)	106(12)	-26(8)	5(8)	-18(8)
F_{34}	55(9)	84(10)	65(11)	-19(8)	-16(8)	32(7)
F_{35}	86(11)	64(9)	47(9)	-2(7)	48(8)	7(8)
F_{36}	68(10)	29(7)	97(11)	4(7)	-6(8)	-1(7)
O_{31}	82(14)	33(10)	70(13)	-24(9)	3(11)	-28(10)
N_{31}	32(10)	36(10)	18(10)	-7(8)	14(8)	1(8)
N_{32}	41(11)	23(9)	13(9)	10(7)	4(8)	-8(8)
N_{33}	41(12)	34(11)	39(12)	3(9)	8(9)	-4(9)
N_{34}	79(14)	22(9)	56(12)	-15(8)	-8(10)	-8(10)
N_{35}	48(12)	23(10)	32(11)	-9(8)	19(9)	-10(8)
N_{36}	66(13)	59(13)	58(13)	-34(11)	7(10)	-7(10)
C_{31}	44(14)	18(11)	16(11)	6(9)	10(10)	-12(10)
C_{32}	50(14)	42(13)	32(12)	-22(10)	8(10)	-10(11)
C_{33}	64(17)	51(14)	22(12)	-1(11)	3(11)	-26(13)
C_{34}	50(15)	18(11)	33(14)	-10(10)	-14(11)	-3(10)
C_{35}	20(11)	41(13)	18(12)	-11(10)	-1(9)	3(10)
C_{36}	6(11)	25(12)	80(19)	5(12)	-6(11)	-7(9)
N_{37}	39(11)	27(10)	44(12)	12(9)	2(9)	-18(8)
C_{38}	42(12)	33(11)	8(11)	-11(9)	8(9)	7(10)
C_{39}	45(9)	43(9)	28(9)	15(7)	-2(7)	-4(8)
C_{40}	80(20)	41(15)	100(20)	2(15)	29(17)	-18(14)
C_{41}	32(6)	29(6)	22(6)	-8(5)	-6(5)	-6(5)
C_{42}	67(16)	54(15)	18(12)	-7(11)	-19(11)	-12(13)

Table 2.(continued)

Atom Type[c]	Anisotropic Thermal Parameters (Å^2 x 10^3) U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C_{43}	42(14)	33(12)	40(15)	-2(11)	20(11)	6(10)
C_{44}	65(8)	60(8)	61(8)	-9(5)	-6(5)	-6(5)
C_{45}	80(20)	64(16)	43(16)	-1(13)	-15(14)	-11(15)
C_{46}	50(16)	26(12)	35(14)	-5(10)	25(12)	-7(11)
C_{47}	18(12)	38(13)	52(16)	11(11)	7(10)	-6(10)
C_{48}	22(11)	39(12)	7(10)	6(9)	4(8)	12(10)
C_{49}	23(11)	38(12)	27(12)	13(9)	4(9)	7(10)
C_{50}	38(14)	37(13)	40(14)	21(11)	-22(11)	-4(11)
C_{51}	26(14)	26(13)	130(30)	14(15)	-7(16)	0(11)
C_{52}	20(14)	70(20)	57(19)	-16(15)	20(12)	-9(14)
C_{53}	33(13)	34(13)	43(14)	-18(11)	2(10)	4(10)
			Molecule 3			
I_{61}	53(1)	73(1)	37(1)	-15(1)	9(1)	-17(1)
F_{61}	97(11)	85(10)	65(9)	-25(8)	10(8)	40(8)
F_{62}	108(12)	52(8)	57(9)	-11(7)	17(8)	32(8)
F_{63}	98(12)	84(11)	150(15)	-90(11)	-46(11)	9(9)
F_{64}	75(12)	93(12)	95(14)	-2(10)	15(10)	45(10)
F_{65}	82(12)	31(8)	165(17)	-20(9)	7(11)	6(8)
F_{66}	66(12)	106(13)	123(16)	-44(11)	-53(11)	44(10)
O_{61}	37(10)	52(10)	29(9)	-19(7)	6(8)	-12(8)
N_{61}	31(10)	21(8)	33(10)	0(7)	-7(8)	-7(7)
N_{62}	33(9)	32(9)	24(9)	19(7)	13(7)	-3(8)
N_{63}	26(9)	32(9)	13(9)	3(7)	-2(7)	-1(7)
N_{64}	34(10)	32(9)	24(9)	-21(7)	-2(7)	-8(7)
N_{65}	54(13)	64(13)	47(14)	-1(10)	-19(11)	-39(11)
N_{66}	120(20)	47(14)	90(20)	10(14)	-31(17)	-32(14)
C_{61}	19(12)	11(10)	81(19)	-6(11)	7(11)	4(9)
C_{62}	30(12)	48(13)	24(11)	-3(9)	1(9)	7(10)
C_{63}	34(14)	48(14)	65(16)	-19(12)	5(12)	5(11)
C_{64}	18(11)	43(12)	22(12)	-19(10)	11(9)	-1(9)
C_{65}	34(14)	46(14)	58(17)	-15(12)	1(12)	6(12)
C_{66}	42(14)	20(11)	19(12)	-8(9)	-8(10)	-5(10)

Table 2.(continued)

Atom Type[c]	Anisotropic Thermal Parameters (Å^2 x 10^3) U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N_{67}	26(10)	40(10)	13(9)	-3(8)	8(7)	-7(8)
C_{68}	12(10)	49(12)	24(11)	-8(9)	-4(8)	8(9)
C_{69}	45(15)	46(14)	48(16)	-4(12)	6(12)	-3(12)
C_{70}	28(13)	43(13)	43(16)	22(11)	-16(12)	0(11)
C_{71}	65(17)	45(14)	24(13)	-3(11)	-19(12)	-12(12)
C_{72}	69(19)	43(14)	37(16)	0(12)	-14(14)	-7(14)
C_{73}	36(13)	30(12)	38(15)	-19(10)	12(11)	-6(10)
C_{74}	69(18)	58(16)	36(14)	-16(13)	-5(13)	7(14)
C_{75}	51(16)	71(17)	74(19)	37(14)	1(13)	-14(13)
C_{76}	41(13)	29(11)	21(12)	-19(9)	7(10)	-7(10)
C_{77}	38(15)	56(16)	40(16)	-20(13)	7(12)	-16(13)
C_{78}	32(15)	23(13)	100(20)	22(14)	-9(15)	-16(12)
C_{79}	42(14)	45(14)	70(17)	27(13)	0(13)	-33(12)
C_{80}	52(15)	55(15)	67(18)	28(14)	4(13)	43(12)
C_{81}	76(19)	30(13)	44(16)	-29(12)	14(14)	-21(13)
C_{82}	13(12)	67(16)	100(20)	-42(15)	-5(13)	6(12)
C_{83}	90(20)	43(15)	28(16)	-19(13)	3(14)	1(14)
			Molecule 4			
I_{91}	69(1)	57(1)	29(1)	-4(1)	2(1)	-11(1)
F_{91}	60(9)	121(12)	49(8)	-6(8)	-7(7)	1(8)
F_{92}	43(9)	230(20)	80(11)	-45(12)	14(8)	7(11)
F_{93}	150(17)	117(15)	177(18)	-11(13)	-99(14)	-70(13)
F_{94}	180(20)	58(11)	140(20)	7(12)	-12(16)	49(12)
F_{95}	70(10)	36(8)	130(14)	-8(8)	-4(9)	1(7)
F_{96}	61(11)	69(10)	125(15)	21(10)	52(10)	20(8)
O_{91}	58(11)	19(8)	26(9)	9(7)	6(8)	-14(7)
N_{91}	52(12)	31(10)	43(13)	-6(9)	16(10)	-18(9)
N_{92}	67(14)	16(9)	45(13)	1(9)	10(10)	-30(9)
N_{93}	44(11)	31(10)	26(10)	-9(8)	7(8)	-20(8)
N_{94}	55(12)	54(11)	20(9)	-14(8)	-5(8)	-8(9)
N_{95}	32(11)	14(9)	59(13)	-5(9)	4(9)	-4(8)

Table 2.(continued)

Atom Type[c]	Anisotropic Thermal Parameters (Å^2 x 10^3) U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N_{96}	69(14)	69(14)	48(12)	-13(11)	15(10)	-14(11)
C_{91}	25(11)	27(13)	62(17)	21(12)	-7(11)	7(10)
C_{92}	53(14)	66(15)	14(10)	-24(10)	-3(10)	-10(12)
C_{93}	55(17)	60(16)	53(17)	-14(13)	-14(13)	-20(14)
C_{94}	42(13)	33(12)	12(11)	-9(9)	7(10)	-14(10)
C_{95}	40(14)	35(13)	48(16)	-9(11)	-35(12)	-10(11)
C_{96}	37(14)	33(14)	38(15)	-2(12)	2(11)	-6(11)
N_{97}	35(11)	29(10)	52(13)	-12(9)	1(9)	-5(8)
C_{98}	73(18)	28(12)	40(16)	13(11)	13(13)	-11(12)
C_{99}	29(13)	52(13)	28(12)	-18(10)	20(10)	4(10)
C_{100}	67(14)	19(10)	5(9)	-5(8)	-6(9)	-3(10)
C_{101}	55(10)	50(9)	26(9)	-11(7)	-4(7)	-10(8)
C_{102}	33(13)	20(11)	90(18)	-35(11)	-3(12)	8(10)
C_{103}	88(19)	30(13)	13(13)	10(10)	-12(12)	-9(13)
C_{104}	49(16)	57(17)	64(18)	20(14)	-16(14)	-11(14)
C_{105}	35(13)	34(12)	34(13)	-17(10)	12(10)	7(10)
C_{106}	3(11)	11(10)	100(20)	-13(12)	8(12)	3(8)
C_{107}	58(16)	37(13)	23(13)	-11(10)	-1(11)	-8(12)
C_{108}	41(14)	13(11)	90(20)	-5(12)	5(13)	1(10)
C_{109}	42(14)	32(13)	49(15)	-15(12)	-21(12)	24(11)
C_{110}	59(16)	41(14)	46(15)	-26(11)	10(12)	-15(12)
C_{111}	21(11)	38(11)	33(12)	8(9)	-16(9)	14(9)
C_{112}	130(30)	60(20)	29(16)	5(14)	41(18)	0(20)
C_{113}	34(14)	37(14)	90(20)	2(14)	6(13)	-1(11)
Solvent Molecule of Crystallization 1						
Cl_{1S}	85(5)	74(4)	51(4)	-15(3)	-1(3)	6(4)
Cl_{2S}	102(6)	106(6)	120(7)	-56(5)	-5(5)	-13(5)
C_{1S}	39(16)	60(19)	260(40)	50(20)	40(20)	3(14)
Solvent Molecule of Crystallization 2						
Cl_{3S}	276(13)	124(8)	87(7)	-33(6)	-36(7)	37(8)
Cl_{4S}	57(4)	90(5)	143(7)	-26(5)	-27(4)	0(4)
C_{2S}	70(16)	23(11)	51(14)	4(10)	-48(12)	0(10)

Table 2.(continued)

Atom Type[c]	Anisotropic Thermal Parameters ($Å^2 \times 10^3$)					
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

[a]The numbers in parentheses are the estimated standard deviations in the last significant digit.
[b]The form of the anisotropic thermal parameter is: $\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)]$.
[c]Atoms are labeled in agreement with Figure 1.

Table 3.Atomic Coordinates for Hydrogen Atoms in Crystalline **R**-$C_{22}H_{14}F_6IN_7O \cdot 0.5\ CH_2Cl_2$ [a]

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z
		Molecule 1	
H_{1N}	2859	4070	-2077
H_{3a}	-1482	2489	-461
H_{3b}	-419	1718	-858
H_{7N}	1834	2844	-3200
H_9	5009	3700	-4133
H_{10}	6109	3033	-5042
H_{12}	3359	901	-4750
H_{13}	2168	1605	-3835
H_{15a}	-2428	4188	-1586
H_{15b}	-2572	3832	-860
H_{15c}	-3388	3305	-1372
H_{17}	306	574	-2469
H_{20}	-3422	1147	-3968
H_{21}	-3569	2053	-3060
		Molecule 2	
H_{31N}	-4685	-4934	-2656
H_{33a}	-2063	-2913	-4498
H_{33b}	-1361	-2350	-3964
H_{37N}	-4742	-3332	-1613
H_{39}	-6302	-5018	-572
H_{40}	-7046	-4754	518
H_{42}	-5205	-2244	348
H_{43}	-4761	-2466	-806
H_{45a}	-5141	-3003	-4330
H_{45b}	-4625	-1963	-4343
H_{45c}	-5846	-2322	-3791
H_{47}	-5402	-92	-2772
H_{50}	-2160	-781	-1104
H_{51}	-2011	-1729	-1976
		Molecule 3	
H_{61N}	1971	1267	1942
H_{63a}	7778	1595	829

Table 3.(continued)

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z
H_{63b}	7602	1289	1570
H_{67N}	3155	2341	3124
H_{69}	185	1304	4003
H_{70}	-914	1796	5041
H_{72}	1545	4037	4850
H_{73}	2651	3595	3839
H_{75a}	5094	3521	876
H_{75b}	5648	2729	391
H_{75c}	6919	3266	707
H_{77}	4796	4490	2483
H_{80}	8616	3763	3871
H_{81}	8668	2947	3021
		Molecule 4	
H_{91N}	133	99	2613
H_{93a}	-436	-2512	4558
H_{93b}	721	-2894	3972
H_{97N}	413	-1617	1677
H_{99}	2184	-72	606
H_{100}	2475	-203	-483
H_{102}	247	-2563	-280
H_{103}	-335	-2306	784
H_{10e}	-3570	-1636	3647
H_{10f}	-2970	-1574	4334
H_{10g}	-3210	-2562	4067
H_{107}	215	-4877	2740
H_{110}	-2681	-3752	1060
H_{111}	-2830	-2937	2039
		Solvent Molecule of Crystallization 1	
H_{1Sa}	3677	-341	3212
H_{1Sb}	3444	-76	2490
		Solvent Molecule of Crystallization 2	
H_{2Sa}	435	5229	-1146

Table 3.(continued)

Atom Type[b]	Fractional Coordinates 10^4x	10^4y	10^4z
H_{2Sb}	1062	6238	-1118

[a]The eight hydrogens bonded to nitrogen were initially located from a difference Fourier synthesis. They were then included in the structure factor calculations as idealized atoms (assuming sp^2-hybridization of the nitrogen atoms and a N-H bond length of 0.88 Å) "riding" on their respective nitrogen atoms. The four methyl groups (C_{15}, C_{45}, C_{75}, C_{105} and their hydrogens) were refined as rigid rotors (using idealized sp^3-hybridized geometry and a C-H bond length of 0.98 Å) which were allowed to rotate around their respective C-C bonds in least-squares cycles. The remaining hydrogen atoms were included in the structure factor calculations as idealized atoms (assuming sp^2- or sp^3-hybridization of the carbon atoms and C-H bond lengths of 0.95-0.99 Å) "riding" on their respective carbon atoms. The isotropic thermal parameters of all hydrogen atoms were fixed at values 1.2 (nonmethyl) or 1.5 (methyl) times the equivalent isotropic thermal parameter of the carbon or nitrogen atom to which they are covalently bonded.

[b]Hydrogen atoms bonded to carbon are labeled with the same numerical subscript(s) as their carbon atoms and carry an additional literal subscript (a, b, c, e, f or g) where necessary to distinguish between hydrogens bonded to the same carbon. Hydrogen atoms bonded to nitrogen are labeled with the same numerical subscript(s) as their nitrogen and carry an additional literal subscripted N. The three hydrogen atoms bonded to methyl carbon C_{105} are labeled H_{10e}, H_{10f} and H_{10g}.

Table 4. Bond Lengths in Crystalline **R**-$C_{22}H_{14}F_6IN_7O \cdot 0.5\ CH_2Cl_2$ [a]

Type[b]	Length, Å	Type[b]	Length, Å
Molecule 1		Molecule 2	
I_1-C_{11}	2.08(2)	I_{31}-C_{41}	2.09(2)
F_1-C_{14}	1.31(2)	F_{31}-C_{44}	1.35(3)
F_2-C_{14}	1.31(2)	F_{32}-C_{44}	1.25(2)
F_3-C_{14}	1.32(2)	F_{33}-C_{44}	1.30(2)
F_4-C_{22}	1.37(2)	F_{34}-C_{52}	1.40(3)
F_5-C_{22}	1.37(2)	F_{35}-C_{52}	1.37(2)
F_6-C_{22}	1.29(3)	F_{36}-C_{52}	1.34(3)
O_1-C_6	1.21(2)	O_{31}-C_{36}	1.22(2)
N_3-N_4	1.43(2)	N_{33}-N_{34}	1.42(2)
N_1-C_1	1.38(2)	N_{31}-C_{31}	1.32(2)
N_1-C_6	1.42(2)	N_{31}-C_{36}	1.41(3)
N_2-C_1	1.32(2)	N_{32}-C_{31}	1.20(2)
N_2-C_5	1.37(2)	N_{32}-C_{35}	1.38(2)
N_3-C_1	1.37(2)	N_{33}-C_{31}	1.46(2)
N_3-C_4	1.49(2)	N_{33}-C_{34}	1.55(2)
N_4-C_2	1.26(2)	N_{34}-C_{32}	1.34(2)
N_5-C_5	1.29(2)	N_{35}-C_{35}	1.28(2)
N_5-C_{16}	1.38(2)	N_{35}-C_{46}	1.38(2)
C_6-N_7	1.35(2)	C_{36}-N_{37}	1.36(3)
N_7-C_8	1.43(2)	N_{37}-C_{38}	1.42(2)
N_6-C_{23}	1.10(3)	N_{36}-C_{53}	1.11(2)
C_2-C_3	1.52(2)	C_{32}-C_{33}	1.46(3)
C_2-C_{14}	1.46(2)	C_{32}-C_{44}	1.57(3)

Table 4. (continued)

Type[b]	Length, Å	Type[b]	Length, Å
C_3-C_4	1.58(3)	C_{33}-C_{34}	1.52(3)
C_4-C_5	1.44(3)	C_{34}-C_{35}	1.57(3)
C_4-C_{15}	1.63(3)	C_{34}-C_{45}	1.53(3)
C_8-C_9	1.38(2)	C_{38}-C_{39}	1.36(3)
C_8-C_{13}	1.36(2)	C_{38}-C_{43}	1.36(2)
C_9-C_{10}	1.37(3)	C_{39}-C_{40}	1.43(3)
C_{10}-C_{11}	1.35(2)	C_{40}-C_{41}	1.38(3)
C_{11}-C_{12}	1.43(3)	C_{41}-C_{42}	1.38(3)
C_{12}-C_{13}	1.40(3)	C_{42}-C_{43}	1.50(3)
C_{16}-C_{17}	1.42(3)	C_{46}-C_{47}	1.35(3)
C_{16}-C_{21}	1.43(3)	C_{46}-C_{51}	1.44(3)
C_{17}-C_{18}	1.42(3)	C_{47}-C_{48}	1.45(3)
C_{18}-C_{19}	1.38(3)	C_{48}-C_{49}	1.39(3)
C_{18}-C_{22}	1.49(3)	C_{48}-C_{52}	1.37(3)
C_{19}-C_{20}	1.31(3)	C_{49}-C_{50}	1.41(3)
C_{19}-C_{23}	1.50(3)	C_{49}-C_{53}	1.46(3)
C_{20}-C_{21}	1.43(3)	C_{50}-C_{51}	1.40(3)
Molecule 3		Molecule 4	
I_{61}-C_{71}	2.09(2)	I_{91}-C_{101}	2.06(2)
F_{61}-C_{74}	1.32(2)	F_{91}-C_{104}	1.36(2)
F_{62}-C_{74}	1.41(2)	F_{92}-C_{104}	1.32(3)
F_{63}-C_{74}	1.28(2)	F_{93}-C_{104}	1.28(2)
F_{64}-C_{82}	1.36(3)	F_{94}-C_{112}	1.31(3)
F_{65}-C_{82}	1.30(3)	F_{95}-C_{112}	1.36(3)
F_{66}-C_{82}	1.28(3)	F_{96}-C_{112}	1.22(3)
O_{61}-C_{66}	1.22(2)	O_{91}-C_{96}	1.15(2)

Table 4. (continued)

Type[b]	Length, Å	Type[b]	Length, Å
N_{63}-N_{64}	1.40(2)	N_{93}-N_{94}	1.42(2)
N_{61}-C_{61}	1.36(2)	N_{91}-C_{91}	1.35(3)
N_{61}-C_{66}	1.48(2)	N_{91}-C_{96}	1.45(3)
N_{62}-C_{61}	1.32(2)	N_{92}-C_{91}	1.36(3)
N_{62}-C_{65}	1.46(3)	N_{92}-C_{95}	1.42(3)
N_{63}-C_{61}	1.36(3)	N_{93}-C_{91}	1.37(3)
N_{63}-C_{64}	1.49(2)	N_{93}-C_{94}	1.47(2)
N_{64}-C_{62}	1.32(2)	N_{94}-C_{92}	1.32(2)
N_{65}-C_{65}	1.23(2)	N_{95}-C_{95}	1.26(2)
N_{65}-C_{76}	1.48(3)	N_{95}-C_{106}	1.35(3)
C_{66}-N_{67}	1.32(2)	C_{96}-N_{97}	1.35(2)
N_{67}-C_{68}	1.38(2)	N_{97}-C_{98}	1.45(3)
N_{66}-C_{83}	1.18(3)	N_{96}-C_{113}	1.21(3)
C_{62}-C_{63}	1.45(2)	C_{92}-C_{93}	1.54(3)
C_{62}-C_{74}	1.47(3)	C_{92}-C_{104}	1.50(3)
C_{63}-C_{64}	1.51(3)	C_{93}-C_{94}	1.56(3)
C_{64}-C_{65}	1.47(3)	C_{94}-C_{95}	1.55(3)
C_{64}-C_{75}	1.52(3)	C_{94}-C_{105}	1.54(3)
C_{68}-C_{69}	1.39(3)	C_{98}-C_{99}	1.35(3)
C_{68}-C_{73}	1.39(2)	C_{98}-C_{103}	1.36(3)
C_{69}-C_{70}	1.48(3)	C_{99}-C_{100}	1.38(2)
C_{70}-C_{71}	1.34(3)	C_{100}-C_{101}	1.37(2)

Table 4. (continued)

Type[b]	Length, Å	Type[b]	Length, Å
C_{71}-C_{72}	1.37(3)	C_{101}-C_{102}	1.44(3)
C_{72}-C_{73}	1.43(3)	C_{102}-C_{103}	1.37(3)
C_{76}-C_{77}	1.37(3)	C_{106}-C_{107}	1.40(3)
C_{76}-C_{81}	1.40(3)	C_{106}-C_{111}	1.41(3)
C_{77}-C_{78}	1.38(3)	C_{107}-C_{108}	1.41(3)
C_{78}-C_{79}	1.46(3)	C_{108}-C_{109}	1.41(3)
C_{78}-C_{82}	1.45(3)	C_{108}-C_{112}	1.65(4)
C_{79}-C_{80}	1.50(3)	C_{109}-C_{110}	1.33(3)
C_{79}-C_{83}	1.35(3)	C_{109}-C_{113}	1.41(3)
C_{80}-C_{81}	1.28(3)	C_{110}-C_{111}	1.49(3)
Solvent Molecules of Crystallization			
Molecule 1		Molecule 2	
Cl_{1S}-C_{1S}	1.78(2)	Cl_{3S}-C_{2S}	1.81(2)
Cl_{2S}-C_{1S}	1.61(3)	Cl_{4S}-C_{2S}	1.70(2)

[a]The numbers in parentheses are the estimated standard deviations in the last significant digit.
[b]Atoms are labeled in agreement with Figure 1.

Table 5. Bond Angles in Crystalline **R**-$C_{22}H_{14}F_6IN_7O \cdot 0.5\ CH_2Cl_2$ [a]

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
Molecule 1		Molecule 2	
$C_1N_1C_6$	128(2)	$C_{31}N_{31}C_{36}$	126(2)
$C_1N_2C_5$	103(2)	$C_{31}N_{32}C_{35}$	112(2)
$C_1N_3N_4$	117(2)	$N_{34}N_{33}C_{31}$	109(2)
$N_4N_3C_4$	109(2)	$N_{34}N_{33}C_{34}$	107(1)
$C_1N_3C_4$	103(2)	$C_{31}N_{33}C_{34}$	102(1)
$C_2N_4N_3$	112(2)	$C_{32}N_{34}N_{33}$	108(2)
$C_2C_3C_4$	101(1)	$C_{32}C_{33}C_{34}$	102(2)
$N_3C_4C_3$	103(2)	$C_{33}C_{34}N_{33}$	103(2)
$C_5C_4N_3$	102(2)	$N_{33}C_{34}C_{35}$	99(2)
$N_3C_4C_{15}$	110(2)	$C_{45}C_{34}N_{33}$	111(2)
$C_5C_4C_3$	118(2)	$C_{33}C_{34}C_{35}$	116(2)
$C_3C_4C_{15}$	108(2)	$C_{33}C_{34}C_{45}$	114(2)
$C_5C_4C_{15}$	114(2)	$C_{45}C_{34}C_{35}$	112(2)
$F_1C_{14}F_2$	105(2)	$F_{32}C_{44}F_{31}$	107(2)
$F_1C_{14}F_3$	107(2)	$F_{33}C_{44}F_{31}$	105(2)
$F_1C_{14}C_2$	114(2)	$F_{31}C_{44}C_{32}$	107(2)
$F_2C_{14}F_3$	104(2)	$F_{32}C_{44}F_{33}$	117(2)
$F_2C_{14}C_2$	113(2)	$F_{32}C_{44}C_{32}$	108(2)
$F_3C_{14}C_2$	114(2)	$F_{33}C_{44}C_{32}$	112(2)
$F_5C_{22}F_4$	104(2)	$F_{35}C_{52}F_{34}$	99(2)
$F_6C_{22}F_4$	107(2)	$F_{36}C_{52}F_{34}$	100(2)
$F_4C_{22}C_{18}$	111(2)	$C_{48}C_{52}F_{34}$	116(2)
$F_6C_{22}F_5$	104(2)	$F_{36}C_{52}F_{35}$	103(2)
$F_5C_{22}C_{18}$	111(2)	$F_{35}C_{52}C_{48}$	116(2)
$F_6C_{22}C_{18}$	118(2)	$F_{36}C_{52}C_{48}$	120(2)
$C_5N_5C_{16}$	120(2)	$C_{35}N_{35}C_{46}$	120(2)
$N_2C_1N_1$	125(2)	$N_{32}C_{31}N_{31}$	132(2)
$N_3C_1N_1$	117(2)	$N_{31}C_{31}N_{33}$	112(2)
$N_2C_1N_3$	118(2)	$N_{32}C_{31}N_{33}$	117(2)

Table 5. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
$N_4C_2C_3$	114(2)	$N_{34}C_{32}C_{33}$	116(2)
$N_4C_2C_{14}$	123(2)	$N_{34}C_{32}C_{44}$	120(2)
$C_{14}C_2C_3$	122(2)	$C_{33}C_{32}C_{44}$	124(2)
$N_5C_5N_2$	125(2)	$N_{35}C_{35}N_{32}$	131(2)
$N_2C_5C_4$	113(2)	$N_{32}C_{35}C_{34}$	108(2)
$N_5C_5C_4$	122(2)	$N_{35}C_{35}C_{34}$	121(2)
$O_1C_6N_1$	119(2)	$O_{31}C_{36}N_{31}$	121(2)
$O_1C_6N_7$	127(2)	$O_{31}C_{36}N_{37}$	121(2)
$N_7C_6N_1$	115(2)	$N_{37}C_{36}N_{31}$	117(2)
$C_6N_7C_8$	126(2)	$C_{36}N_{37}C_{38}$	130(2)
$C_9C_8N_7$	124(2)	$C_{39}C_{38}N_{37}$	121(2)
$C_{13}C_8N_7$	115(2)	$C_{43}C_{38}N_{37}$	114(2)
$C_{13}C_8C_9$	121(2)	$C_{39}C_{38}C_{43}$	123(2)
$C_{10}C_9C_8$	118(2)	$C_{38}C_{39}C_{40}$	118(2)
$C_{11}C_{10}C_9$	124(2)	$C_{41}C_{40}C_{39}$	121(2)
$C_{10}C_{11}I_1$	123(2)	$C_{40}C_{41}I_{31}$	120(2)
$C_{12}C_{11}I_1$	119(1)	$C_{42}C_{41}I_{31}$	118(1)
$C_{10}C_{11}C_{12}$	117(2)	$C_{42}C_{41}C_{40}$	122(2)
$C_{13}C_{12}C_{11}$	119(2)	$C_{41}C_{42}C_{43}$	116(2)
$C_8C_{13}C_{12}$	120(2)	$C_{38}C_{43}C_{42}$	120(2)
$N_5C_{16}C_{17}$	120(2)	$C_{47}C_{46}N_{35}$	120(2)
$N_5C_{16}C_{21}$	124(2)	$N_{35}C_{46}C_{51}$	120(2)
$C_{17}C_{16}C_{21}$	116(2)	$C_{47}C_{46}C_{51}$	119(2)
$C_{16}C_{17}C_{18}$	120(2)	$C_{46}C_{47}C_{48}$	121(2)
$C_{19}C_{18}C_{17}$	118(2)	$C_{49}C_{48}C_{47}$	120(2)
$C_{17}C_{18}C_{22}$	115(2)	$C_{52}C_{48}C_{47}$	119(2)
$C_{19}C_{18}C_{22}$	126(2)	$C_{52}C_{48}C_{49}$	121(2)
$C_{20}C_{19}C_{18}$	125(2)	$C_{48}C_{49}C_{50}$	120(2)
$C_{18}C_{19}C_{23}$	120(2)	$C_{48}C_{49}C_{53}$	121(2)
$C_{20}C_{19}C_{23}$	115(3)	$C_{50}C_{49}C_{53}$	118(2)
$C_{19}C_{20}C_{21}$	118(2)	$C_{51}C_{50}C_{49}$	119(2)

Table 5. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
$C_{20}C_{21}C_{16}$	122(2)	$C_{50}C_{51}C_{46}$	121(2)
$N_{6}C_{23}C_{19}$	176(3)	$N_{36}C_{53}C_{49}$	178(2)
Molecule 3		Molecule 4	
$C_{61}N_{61}C_{66}$	128(2)	$C_{91}N_{91}C_{96}$	133(2)
$C_{61}N_{62}C_{65}$	104(2)	$C_{91}N_{92}C_{95}$	102(2)
$C_{61}N_{63}N_{64}$	113(1)	$C_{91}N_{93}N_{94}$	112(2)
$N_{64}N_{63}C_{64}$	112(1)	$N_{94}N_{93}C_{94}$	113(2)
$C_{61}N_{63}C_{64}$	106(1)	$C_{91}N_{93}C_{94}$	106(1)
$C_{62}N_{64}N_{63}$	105(1)	$C_{92}N_{94}N_{93}$	105(2)
$C_{62}C_{63}C_{64}$	103(2)	$C_{92}C_{93}C_{94}$	98(2)
$N_{63}C_{64}C_{63}$	102(1)	$N_{93}C_{94}C_{93}$	106(2)
$C_{65}C_{64}N_{63}$	102(2)	$N_{93}C_{94}C_{95}$	101(2)
$N_{63}C_{64}C_{75}$	109(2)	$N_{93}C_{94}C_{105}$	111(2)
$C_{65}C_{64}C_{63}$	117(2)	$C_{95}C_{94}C_{93}$	114(2)
$C_{63}C_{64}C_{75}$	114(2)	$C_{105}C_{94}C_{93}$	115(2)
$C_{65}C_{64}C_{75}$	112(2)	$C_{105}C_{94}C_{95}$	109(2)
$F_{61}C_{74}F_{62}$	101(2)	$F_{92}C_{104}F_{91}$	105(2)
$F_{63}C_{74}F_{61}$	106(2)	$F_{93}C_{104}F_{91}$	107(2)
$F_{61}C_{74}C_{62}$	112(2)	$F_{91}C_{104}C_{92}$	111(2)
$F_{63}C_{74}F_{62}$	107(2)	$F_{93}C_{104}F_{92}$	111(2)
$F_{62}C_{74}C_{62}$	110(2)	$F_{92}C_{104}C_{92}$	112(2)
$F_{63}C_{74}C_{62}$	118(2)	$F_{93}C_{104}C_{92}$	111(2)
$F_{65}C_{82}F_{64}$	97(2)	$F_{94}C_{112}F_{95}$	105(2)
$F_{66}C_{82}F_{64}$	102(2)	$F_{96}C_{112}F_{94}$	120(4)
$F_{64}C_{82}C_{78}$	114(3)	$F_{94}C_{112}C_{108}$	108(2)
$F_{66}C_{82}F_{65}$	108(3)	$F_{96}C_{112}F_{95}$	109(2)
$F_{65}C_{82}C_{78}$	116(2)	$F_{95}C_{112}C_{108}$	103(3)

Table 5. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
$F_{66}C_{82}C_{78}$	117(2)	$F_{96}C_{112}C_{108}$	111(2)
$C_{65}N_{65}C_{76}$	122(2)	$C_{95}N_{95}C_{106}$	120(2)
$N_{62}C_{61}N_{61}$	123(2)	$N_{91}C_{91}N_{92}$	119(2)
$N_{63}C_{61}N_{61}$	120(2)	$N_{91}C_{91}N_{93}$	122(2)
$N_{62}C_{61}N_{63}$	116(2)	$N_{92}C_{91}N_{93}$	119(2)
$N_{64}C_{62}C_{63}$	116(2)	$N_{94}C_{92}C_{93}$	118(2)
$N_{64}C_{62}C_{74}$	116(2)	$N_{94}C_{92}C_{104}$	121(2)
$C_{63}C_{62}C_{74}$	128(2)	$C_{104}C_{92}C_{93}$	121(2)
$N_{65}C_{65}N_{62}$	124(2)	$N_{95}C_{95}N_{92}$	128(2)
$N_{62}C_{65}C_{64}$	110(2)	$N_{92}C_{95}C_{94}$	112(2)
$N_{65}C_{65}C_{64}$	126(2)	$N_{95}C_{95}C_{94}$	121(2)
$O_{61}C_{66}N_{61}$	117(2)	$O_{91}C_{96}N_{91}$	117(2)
$O_{61}C_{66}N_{67}$	129(2)	$O_{91}C_{96}N_{97}$	131(2)
$N_{67}C_{66}N_{61}$	114(2)	$N_{97}C_{96}N_{91}$	111(2)
$C_{66}N_{67}C_{68}$	122(2)	$C_{96}N_{97}C_{98}$	122(2)
$N_{67}C_{68}C_{69}$	122(2)	$C_{99}C_{98}N_{97}$	123(2)
$N_{67}C_{68}C_{73}$	118(2)	$C_{103}C_{98}N_{97}$	114(2)
$C_{69}C_{68}C_{73}$	119(2)	$C_{99}C_{98}C_{103}$	123(2)
$C_{68}C_{69}C_{70}$	118(2)	$C_{98}C_{99}C_{100}$	118(2)
$C_{71}C_{70}C_{69}$	120(2)	$C_{101}C_{100}C_{99}$	123(2)
$C_{70}C_{71}I_{61}$	120(2)	$C_{100}C_{101}I_{91}$	122(2)
$C_{72}C_{71}I_{61}$	119(2)	$C_{102}C_{101}I_{91}$	123(2)
$C_{70}C_{71}C_{72}$	121(2)	$C_{100}C_{101}C_{102}$	115(2)
$C_{71}C_{72}C_{73}$	120(2)	$C_{103}C_{102}C_{101}$	122(2)
$C_{68}C_{73}C_{72}$	121(2)	$C_{98}C_{103}C_{102}$	118(2)
$C_{77}C_{76}N_{65}$	119(2)	$N_{95}C_{106}C_{107}$	122(2)
$C_{81}C_{76}N_{65}$	114(2)	$N_{95}C_{106}C_{111}$	124(2)
$C_{77}C_{76}C_{81}$	126(2)	$C_{107}C_{106}C_{111}$	114(2)
$C_{76}C_{77}C_{78}$	119(2)	$C_{106}C_{107}C_{108}$	125(2)
$C_{77}C_{78}C_{79}$	121(2)	$C_{109}C_{108}C_{107}$	118(2)

Table 5. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
$C_{77}C_{78}C_{82}$	120(2)	$C_{107}C_{108}C_{112}$	116(2)
$C_{82}C_{78}C_{79}$	120(3)	$C_{109}C_{108}C_{112}$	126(2)
$C_{78}C_{79}C_{80}$	112(2)	$C_{110}C_{109}C_{108}$	122(2)
$C_{83}C_{79}C_{78}$	123(3)	$C_{113}C_{109}C_{108}$	118(2)
$C_{83}C_{79}C_{80}$	125(3)	$C_{110}C_{109}C_{113}$	120(2)
$C_{81}C_{80}C_{79}$	128(3)	$C_{109}C_{110}C_{111}$	118(2)
$C_{80}C_{81}C_{76}$	115(2)	$C_{106}C_{111}C_{110}$	123(2)
$N_{66}C_{83}C_{79}$	175(3)	$N_{96}C_{113}C_{109}$	174(3)
Solvent Molecules of Crystallization			
Molecule 1		Molecule 2	
$Cl_{2S}C_{1S}Cl_{1S}$	121(2)	$Cl_{4S}C_{2S}Cl_{3S}$	112(1)

[a]The numbers in parentheses are the estimated standard deviations in the last significant digit.
[b]Atoms are labeled in agreement with Figure 1.

Table 6. Torsion Angles in Crystalline **R**-$C_{22}H_{14}F_6IN_7O \cdot 0.5\ CH_2Cl_2$ [a]

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
Molecule 1		Molecule 2	
C_1-N_3-N_4-C_2	-119(2)	C_{31}-N_{33}-N_{34}-C_{32}	-123(2)
C_4-N_3-N_4-C_2	-2(2)	C_{34}-N_{33}-N_{34}-C_{32}	-13(2)
C_5-N_2-C_1-N_3	-9(2)	C_{35}-N_{32}-C_{31}-N_{33}	0(3)
C_5-N_2-C_1-N_1	174(2)	C_{35}-N_{32}-C_{31}-N_{31}	180(2)
N_4-N_3-C_1-N_2	126(2)	N_{34}-N_{33}-C_{31}-N_{32}	103(2)
C_4-N_3-C_1-N_2	6(2)	C_{34}-N_{33}-C_{31}-N_{32}	-10(2)
N_4-N_3-C_1-N_1	-57(2)	N_{34}-N_{33}-C_{31}-N_{31}	-77(2)
C_4-N_3-C_1-N_1	-177(2)	C_{34}-N_{33}-C_{31}-N_{31}	170(2)
C_6-N_1-C_1-N_2	-5(3)	C_{36}-N_{31}-C_{31}-N_{32}	0(4)
C_6-N_1-C_1-N_3	178(2)	C_{36}-N_{31}-C_{31}-N_{33}	-180(2)
N_3-N_4-C_2-C_{14}	179(2)	N_{33}-N_{34}-C_{32}-C_{44}	177(2)
N_3-N_4-C_2-C_3	6(2)	N_{33}-N_{34}-C_{32}-C_{33}	1(2)
N_4-C_2-C_3-C_4	-6(2)	N_{34}-C_{32}-C_{33}-C_{34}	11(2)
C_{14}-C_2-C_3-C_4	-180(2)	C_{44}-C_{32}-C_{33}-C_{34}	-165(2)
C_1-N_3-C_4-C_5	0(2)	C_{31}-N_{33}-C_{34}-C_{35}	14(2)
N_4-N_3-C_4-C_5	-125(2)	N_{34}-N_{33}-C_{34}-C_{35}	-101(2)
C_1-N_3-C_4-C_3	123(2)	C_{31}-N_{33}-C_{34}-C_{33}	134(2)
N_4-N_3-C_4-C_3	-2(2)	N_{34}-N_{33}-C_{34}-C_{33}	19(2)
C_1-N_3-C_4-C_{15}	-122(2)	C_{31}-N_{33}-C_{34}-C_{45}	-103(2)
N_4-N_3-C_4-C_{15}	113(2)	N_{34}-N_{33}-C_{34}-C_{45}	142(2)
C_2-C_3-C_4-C_5	116(2)	C_{32}-C_{33}-C_{34}-C_{35}	90(2)
C_2-C_3-C_4-N_3	5(2)	C_{32}-C_{33}-C_{34}-N_{33}	-17(2)
C_2-C_3-C_4-C_{15}	-112(2)	C_{32}-C_{33}-C_{34}-C_{45}	-138(2)
C_{16}-N_5-C_5-N_2	2(3)	C_{46}-N_{35}-C_{35}-N_{32}	2(3)
C_{16}-N_5-C_5-C_4	179(2)	C_{46}-N_{35}-C_{35}-C_{34}	173(2)
C_1-N_2-C_5-N_5	-173(2)	C_{31}-N_{32}-C_{35}-N_{35}	-178(2)
C_1-N_2-C_5-C_4	9(2)	C_{31}-N_{32}-C_{35}-C_{34}	10(2)
N_3-C_4-C_5-N_5	177(2)	N_{33}-C_{34}-C_{35}-N_{35}	172(2)
C_3-C_4-C_5-N_5	64(3)	C_{33}-C_{34}-C_{35}-N_{35}	62(3)
C_{15}-C_4-C_5-N_5	-65(3)	C_{45}-C_{34}-C_{35}-N_{35}	-71(2)
N_3-C_4-C_5-N_2	-5(2)	N_{33}-C_{34}-C_{35}-N_{32}	-15(2)
C_3-C_4-C_5-N_2	-118(2)	C_{33}-C_{34}-C_{35}-N_{32}	-125(2)

Table 6. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
C_{15}-C_4-C_5-N_2	113(2)	C_{45}-C_{34}-C_{35}-N_{32}	102(2)
C_1-N_1-C_6-O_1	-175(2)	C_{31}-N_{31}-C_{36}-O_{31}	177(2)
C_1-N_1-C_6-N_7	6(3)	C_{31}-N_{31}-C_{36}-N_{37}	-13(3)
O_1-C_6-N_7-C_8	7(4)	O_{31}-C_{36}-N_{37}-C_{38}	-9(3)
N_1-C_6-N_7-C_8	-174(2)	N_{31}-C_{36}-N_{37}-C_{38}	-178(2)
C_6-N_7-C_8-C_{13}	154(2)	C_{36}-N_{37}-C_{38}-C_{43}	176(2)
C_6-N_7-C_8-C_9	-28(3)	C_{36}-N_{37}-C_{38}-C_{39}	9(3)
C_{13}-C_8-C_9-C_{10}	-2(3)	C_{43}-C_{38}-C_{39}-C_{40}	11(3)
N_7-C_8-C_9-C_{10}	180(2)	N_{37}-C_{38}-C_{39}-C_{40}	177(2)
C_8-C_9-C_{10}-C_{11}	4(3)	C_{38}-C_{39}-C_{40}-C_{41}	-9(4)
C_9-C_{10}-C_{11}-C_{12}	-7(3)	C_{39}-C_{40}-C_{41}-C_{42}	3(4)
C_9-C_{10}-C_{11}-I_1	-179(2)	C_{39}-C_{40}-C_{41}-I_{31}	-179(2)
C_{10}-C_{11}-C_{12}-C_{13}	8(3)	C_{40}-C_{41}-C_{42}-C_{43}	1(3)
I_1-C_{11}-C_{12}-C_{13}	-180(2)	I_{31}-C_{41}-C_{42}-C_{43}	-177(2)
C_9-C_8-C_{13}-C_{12}	4(3)	C_{39}-C_{38}-C_{43}-C_{42}	-7(3)
N_7-C_8-C_{13}-C_{12}	-178(2)	N_{37}-C_{38}-C_{43}-C_{42}	-174(2)
C_{11}-C_{12}-C_{13}-C_8	-7(3)	C_{41}-C_{42}-C_{43}-C_{38}	0(3)
N_4-C_2-C_{14}-F_1	145(2)	N_{34}-C_{32}-C_{44}-F_{31}	115(2)
C_3-C_2-C_{14}-F_1	-43(2)	C_{33}-C_{32}-C_{44}-F_{31}	-69(3)
N_4-C_2-C_{14}-F_2	-96(2)	N_{34}-C_{32}-C_{44}-F_{32}	-130(2)
C_3-C_2-C_{14}-F_2	77(2)	C_{33}-C_{32}-C_{44}-F_{32}	46(3)
N_4-C_2-C_{14}-F_3	22(3)	N_{34}-C_{32}-C_{44}-F_{33}	0(3)
C_3-C_2-C_{14}-F_3	-165(2)	C_{33}-C_{32}-C_{44}-F_{33}	176(2)
C_5-N_5-C_{16}-C_{17}	76(2)	C_{35}-N_{35}-C_{46}-C_{47}	-120(2)
C_5-N_5-C_{16}-C_{21}	-110(2)	C_{35}-N_{35}-C_{46}-C_{51}	69(3)
N_5-C_{16}-C_{17}-C_{18}	175(2)	N_{35}-C_{46}-C_{47}-C_{48}	-170(2)
C_{21}-C_{16}-C_{17}-C_{18}	0(3)	C_{51}-C_{46}-C_{47}-C_{48}	1(3)
C_{16}-C_{17}-C_{18}-C_{19}	-1(3)	C_{46}-C_{47}-C_{48}-C_{49}	-1(3)
C_{16}-C_{17}-C_{18}-C_{22}	177(2)	C_{46}-C_{47}-C_{48}-C_{52}	-180(2)
C_{17}-C_{18}-C_{19}-C_{20}	1(3)	C_{47}-C_{48}-C_{49}-C_{50}	2(3)
C_{22}-C_{18}-C_{19}-C_{20}	-177(2)	C_{52}-C_{48}-C_{49}-C_{50}	180(2)

Table 6. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
C_{17}-C_{18}-C_{19}-C_{23}	-179(2)	C_{47}-C_{48}-C_{49}-C_{53}	177(2)
C_{22}-C_{18}-C_{19}-C_{23}	3(3)	C_{52}-C_{48}-C_{49}-C_{53}	-5(3)
C_{18}-C_{19}-C_{20}-C_{21}	0(3)	C_{48}-C_{49}-C_{50}-C_{51}	-2(3)
C_{23}-C_{19}-C_{20}-C_{21}	180(2)	C_{53}-C_{49}-C_{50}-C_{51}	-177(2)
C_{19}-C_{20}-C_{21}-C_{16}	0(3)	C_{49}-C_{50}-C_{51}-C_{46}	2(3)
N_{5}-C_{16}-C_{21}-C_{20}	-174(2)	N_{35}-C_{46}-C_{51}-C_{50}	169(2)
C_{17}-C_{16}-C_{21}-C_{20}	0(3)	C_{47}-C_{46}-C_{51}-C_{50}	-2(3)
C_{19}-C_{18}-C_{22}-F_{6}	178(2)	C_{49}-C_{48}-C_{52}-F_{36}	57(3)
C_{17}-C_{18}-C_{22}-F_{6}	1(3)	C_{47}-C_{48}-C_{52}-F_{36}	-124(2)
C_{19}-C_{18}-C_{22}-F_{5}	-61(3)	C_{49}-C_{48}-C_{52}-F_{35}	-67(3)
C_{17}-C_{18}-C_{22}-F_{5}	121(2)	C_{47}-C_{48}-C_{52}-F_{35}	111(2)
C_{19}-C_{18}-C_{22}-F_{4}	54(3)	C_{49}-C_{48}-C_{52}-F_{34}	177(2)
C_{17}-C_{18}-C_{22}-F_{4}	-124(2)	C_{47}-C_{48}-C_{52}-F_{34}	-5(3)
C_{20}-C_{19}-C_{23}-N_{6}	-83(40)	C_{50}-C_{49}-C_{53}-N_{36}	45(57)
C_{18}-C_{19}-C_{23}-N_{6}	97(39)	C_{48}-C_{49}-C_{53}-N_{36}	-130(56)
	Molecule 3		Molecule 4
C_{61}-N_{63}-N_{64}-C_{62}	-119(2)	C_{91}-N_{93}-N_{94}-C_{92}	-121(2)
C_{64}-N_{63}-N_{64}-C_{62}	2(2)	C_{94}-N_{93}-N_{94}-C_{92}	-1(2)
C_{65}-N_{62}-C_{61}-N_{63}	-10(2)	C_{95}-N_{92}-C_{91}-N_{93}	1(3)
C_{65}-N_{62}-C_{61}-N_{61}	177(2)	C_{95}-N_{92}-C_{91}-N_{91}	179(2)
N_{64}-N_{63}-C_{61}-N_{62}	135(2)	N_{94}-N_{93}-C_{91}-N_{92}	123(2)
C_{64}-N_{63}-C_{61}-N_{62}	11(2)	C_{94}-N_{93}-C_{91}-N_{92}	-1(3)
N_{64}-N_{63}-C_{61}-N_{61}	-52(2)	N_{94}-N_{93}-C_{91}-N_{91}	-56(3)
C_{64}-N_{63}-C_{61}-N_{61}	-176(2)	C_{94}-N_{93}-C_{91}-N_{91}	-179(2)
C_{66}-N_{61}-C_{61}-N_{62}	-4(3)	C_{96}-N_{91}-C_{91}-N_{92}	-1(4)
C_{66}-N_{61}-C_{61}-N_{63}	-176(2)	C_{96}-N_{91}-C_{91}-N_{93}	178(2)
N_{63}-N_{64}-C_{62}-C_{74}	-178(2)	N_{93}-N_{94}-C_{92}-C_{104}	-179(2)
N_{63}-N_{64}-C_{62}-C_{63}	8(2)	N_{93}-N_{94}-C_{92}-C_{93}	6(2)
N_{64}-C_{62}-C_{63}-C_{64}	-14(2)	N_{94}-C_{92}-C_{93}-C_{94}	-8(2)
C_{74}-C_{62}-C_{63}-C_{64}	173(2)	C_{104}-C_{92}-C_{93}-C_{94}	178(2)
C_{61}-N_{63}-C_{64}-C_{65}	-6(2)	C_{91}-N_{93}-C_{94}-C_{95}	0(2)

Table 6. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
N_{64}-N_{63}-C_{64}-C_{65}	-131(2)	N_{94}-N_{93}-C_{94}-C_{95}	-123(2)
C_{61}-N_{63}-C_{64}-C_{63}	116(2)	C_{91}-N_{93}-C_{94}-C_{93}	120(2)
N_{64}-N_{63}-C_{64}-C_{63}	-9(2)	N_{94}-N_{93}-C_{94}-C_{93}	-3(2)
C_{61}-N_{63}-C_{64}-C_{75}	-124(2)	C_{91}-N_{93}-C_{94}-C_{105}	-116(2)
N_{64}-N_{63}-C_{64}-C_{75}	111(2)	N_{94}-N_{93}-C_{94}-C_{105}	122(2)
C_{62}-C_{63}-C_{64}-C_{65}	123(2)	C_{92}-C_{93}-C_{94}-C_{95}	116(2)
C_{62}-C_{63}-C_{64}-N_{63}	12(2)	C_{92}-C_{93}-C_{94}-N_{93}	6(2)
C_{62}-C_{63}-C_{64}-C_{75}	-105(2)	C_{92}-C_{93}-C_{94}-C_{105}	-117(2)
C_{76}-N_{65}-C_{65}-N_{62}	-5(4)	C_{106}-N_{95}-C_{95}-N_{92}	-6(3)
C_{76}-N_{65}-C_{65}-C_{64}	173(2)	C_{106}-N_{95}-C_{95}-C_{94}	177(2)
C_{61}-N_{62}-C_{65}-N_{65}	-176(2)	C_{91}-N_{92}-C_{95}-N_{95}	-177(2)
C_{61}-N_{62}-C_{65}-C_{64}	6(2)	C_{91}-N_{92}-C_{95}-C_{94}	0(2)
N_{63}-C_{64}-C_{65}-N_{65}	-178(2)	N_{93}-C_{94}-C_{95}-N_{95}	177(2)
C_{63}-C_{64}-C_{65}-N_{65}	72(3)	C_{93}-C_{94}-C_{95}-N_{95}	65(2)
C_{75}-C_{64}-C_{65}-N_{65}	-61(3)	C_{105}-C_{94}-C_{95}-N_{95}	-65(3)
N_{63}-C_{64}-C_{65}-N_{62}	0(2)	N_{93}-C_{94}-C_{95}-N_{92}	0(2)
C_{63}-C_{64}-C_{65}-N_{62}	-110(2)	C_{93}-C_{94}-C_{95}-N_{92}	-113(2)
C_{75}-C_{64}-C_{65}-N_{62}	117(2)	C_{105}-C_{94}-C_{95}-N_{92}	117(2)
C_{61}-N_{61}-C_{66}-O_{61}	179(2)	C_{91}-N_{91}-C_{96}-O_{91}	178(2)
C_{61}-N_{61}-C_{66}-N_{67}	-3(3)	C_{91}-N_{91}-C_{96}-N_{97}	-7(3)
O_{61}-C_{66}-N_{67}-C_{68}	-11(3)	O_{91}-C_{96}-N_{97}-C_{98}	-10(4)
N_{61}-C_{66}-N_{67}-C_{68}	171(2)	N_{91}-C_{96}-N_{97}-C_{98}	176(2)
C_{66}-N_{67}-C_{68}-C_{73}	-153(2)	C_{96}-N_{97}-C_{98}-C_{103}	-154(2)
C_{66}-N_{67}-C_{68}-C_{69}	36(3)	C_{96}-N_{97}-C_{98}-C_{99}	30(3)
C_{73}-C_{68}-C_{69}-C_{70}	5(3)	C_{103}-C_{98}-C_{99}-C_{100}	5(4)
N_{67}-C_{68}-C_{69}-C_{70}	176(2)	N_{97}-C_{98}-C_{99}-C_{100}	-180(2)
C_{68}-C_{69}-C_{70}-C_{71}	0(3)	C_{98}-C_{99}-C_{100}-C_{101}	-5(3)
C_{69}-C_{70}-C_{71}-C_{72}	-6(3)	C_{99}-C_{100}-C_{101}-C_{102}	1(3)
C_{69}-C_{70}-C_{71}-I_{61}	177(2)	C_{99}-C_{100}-C_{101}-I_{91}	-178(2)
C_{70}-C_{71}-C_{72}-C_{73}	6(4)	C_{100}-C_{101}-C_{102}-C_{103}	4(3)
I_{61}-C_{71}-C_{72}-C_{73}	-176(2)	I_{91}-C_{101}-C_{102}-C_{103}	-177(2)

Table 6. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
C_{69}-C_{68}-C_{73}-C_{72}	-5(3)	C_{99}-C_{98}-C_{103}-C_{102}	0(4)
N_{67}-C_{68}-C_{73}-C_{72}	-176(2)	N_{97}-C_{98}-C_{103}-C_{102}	-176(2)
C_{71}-C_{72}-C_{73}-C_{68}	0(3)	C_{101}-C_{102}-C_{103}-C_{98}	-4(4)
N_{64}-C_{62}-C_{74}-F_{61}	147(2)	N_{94}-C_{92}-C_{104}-F_{91}	138(2)
C_{63}-C_{62}-C_{74}-F_{61}	-40(3)	C_{93}-C_{92}-C_{104}-F_{91}	-48(3)
N_{64}-C_{62}-C_{74}-F_{62}	-102(2)	N_{94}-C_{92}-C_{104}-F_{92}	-106(2)
C_{63}-C_{62}-C_{74}-F_{62}	72(3)	C_{93}-C_{92}-C_{104}-F_{92}	68(3)
N_{64}-C_{62}-C_{74}-F_{63}	22(3)	N_{94}-C_{92}-C_{104}-F_{93}	19(3)
C_{63}-C_{62}-C_{74}-F_{63}	-164(2)	C_{93}-C_{92}-C_{104}-F_{93}	-167(2)
C_{65}-N_{65}-C_{76}-C_{77}	-64(3)	C_{95}-N_{95}-C_{106}-C_{107}	124(2)
C_{65}-N_{65}-C_{76}-C_{81}	122(2)	C_{95}-N_{95}-C_{106}-C_{111}	-52(3)
N_{65}-C_{76}-C_{77}-C_{78}	-172(2)	N_{95}-C_{106}-C_{107}-C_{108}	-173(2)
C_{81}-C_{76}-C_{77}-C_{78}	2(3)	C_{111}-C_{106}-C_{107}-C_{108}	3(3)
C_{76}-C_{77}-C_{78}-C_{79}	-3(3)	C_{106}-C_{107}-C_{108}-C_{109}	-4(3)
C_{76}-C_{77}-C_{78}-C_{82}	-180(2)	C_{106}-C_{107}-C_{108}-C_{112}	175(2)
C_{77}-C_{78}-C_{79}-C_{80}	3(3)	C_{107}-C_{108}-C_{109}-C_{110}	1(3)
C_{82}-C_{78}-C_{79}-C_{80}	180(2)	C_{112}-C_{108}-C_{109}-C_{110}	-178(2)
C_{77}-C_{78}-C_{79}-C_{83}	177(2)	C_{107}-C_{108}-C_{109}-C_{113}	-177(2)
C_{82}-C_{78}-C_{79}-C_{83}	-7(3)	C_{112}-C_{108}-C_{109}-C_{113}	4(3)
C_{78}-C_{79}-C_{80}-C_{81}	-2(3)	C_{108}-C_{109}-C_{110}-C_{111}	3(3)
C_{83}-C_{79}-C_{80}-C_{81}	-176(3)	C_{113}-C_{109}-C_{110}-C_{111}	-180(2)
C_{79}-C_{80}-C_{81}-C_{76}	1(4)	C_{109}-C_{110}-C_{111}-C_{106}	-3(3)
N_{65}-C_{76}-C_{81}-C_{80}	173(2)	N_{95}-C_{106}-C_{111}-C_{110}	177(2)
C_{77}-C_{76}-C_{81}-C_{80}	0(3)	C_{107}-C_{106}-C_{111}-C_{110}	1(3)
C_{79}-C_{78}-C_{82}-F_{66}	-168(2)	C_{109}-C_{108}-C_{112}-F_{96}	61(4)
C_{77}-C_{78}-C_{82}-F_{66}	9(4)	C_{107}-C_{108}-C_{112}-F_{96}	-119(3)
C_{79}-C_{78}-C_{82}-F_{65}	62(3)	C_{109}-C_{108}-C_{112}-F_{95}	-56(3)
C_{77}-C_{78}-C_{82}-F_{65}	-121(3)	C_{107}-C_{108}-C_{112}-F_{95}	125(2)
C_{79}-C_{78}-C_{82}-F_{64}	-49(3)	C_{109}-C_{108}-C_{112}-F_{94}	-167(2)
C_{77}-C_{78}-C_{82}-F_{64}	128(2)	C_{107}-C_{108}-C_{112}-F_{94}	14(3)
C_{80}-C_{79}-C_{83}-N_{66}	-44(41)	C_{110}-C_{109}-C_{113}-N_{96}	37(22)

Table 6. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)
C_{78}-C_{79}-C_{83}-N_{66}	143(39)	C_{108}-C_{109}-C_{113}-N_{96}	-145(21)

[a]The numbers in parentheses are the estimated standard deviations in the last significant digit.
[b]Atoms are labeled in agreement with Figure 1.

Table 6. (continued)

Type[b]	Angle, (deg)	Type[b]	Angle, (deg)

Table 7.Hydrogen-Bonding Interactions in Crystalline **R**-$C_{22}H_{14}F_6IN_7O \cdot 0.5\ CH_2Cl_2$

Donor Atom (D)[a]	Acceptor Atom (A)	Distance Å D···A	Distance Å H···A	Angle deg. D-H···A	Angle deg. H-D···A	Angle deg. H···A-X[b]	Asymmetric Unit of A[c]
N_1-H_{1N}	O_{31}	2.820	1.96	164	11	118(C_{36})	x+1, y+1, z
N_7-H_{7N}	N_2	2.708	1.98	139	29	94(C_1)	x, y, z
						163(C_5)	x, y, z
N_7-H_{7N}	I_{61}	3.765	3.26	119	49	101(C_{71})	x, y, z-1
N_{31}-H_{31N}	O_1	2.864	2.03	158	15	129(C_6)	x-1, y-1, z
N_{37}-H_{37N}	N_{32}	2.787	2.10	134	33	92(C_{31})	x, y, z
						154(C_{35})	x, y, z
N_{61}-H_{61N}	O_{91}	2.754	1.89	167	9	127(C_{96})	x, y, z
N_{67}-H_{67N}	N_{62}	2.679	1.98	135	31	96(C_{61})	x, y, z
						155(C_{65})	x, y, z
N_{91}-H_{91N}	O_{61}	2.805	1.94	170	7	121(C_{66})	x, y, z
N_{97}-H_{97N}	N_{92}	2.667	1.96	137	30	97(C_{91})	x, y, z
						158(C_{95})	x, y, z

[a] The hydrogen atom involved in the interaction is also indicated.
[b] The symbol X is used to denote other atoms which are bonded to the acceptor atom.
[c] All donor atoms belong to the asymmetric unit for which fractional atomic coordinates are given in Tables 1 and 3.