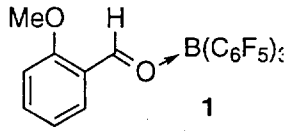
General. General procedures were as described previously.[1] Allyltributylstannane was purchased from Aldrich and used without further purification. Both *o*-anisaldehyde and *p*-anisaldehyde were purified before use by distillation.

1. Spectral data for $B(C_6F_5)_3$ adduct of *o*-anisaldehyde, 1:

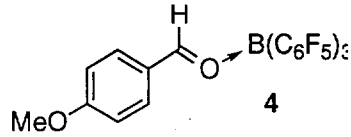


1

To 51 mg (0.10 mmol) of $B(C_6F_5)_3$ in an NMR tube was added 14 mg (0.10 mmol) of *o*-anisaldehyde dissolved in C_6D_6. NMR spectra of the fluorescent green solution were collected at room temperature. ^{1}H NMR(300 MHz): 9.73 (s, 1H, -C*H*O), 7.98 (d, 1H, J = 8.0 Hz, H_a), 6.86 (m, 1H, H_b), 6.32 (apparent t, 1H, J = 8.0 Hz, H_c), 5.79 (d, 1H, J = 8.7 Hz, H_d), 2.70 (s, 3H, -OCH_3); ^{13}C NMR (100 MHz): 194.6, 167.5, 150.3 (m), 147.9 (m), 145.3, 139.5 (m), 137.1 (m), 132.9, 122.7, 120.5, 113.1; ^{19}F NMR (282.4 MHz): 134.2 (d, 6F, *o-F's*), 154.4 (t, 3F, *p-F's*), 162.6 (apparent t, 6F, *m-F's*); ^{11}B NMR (64.2 MHz): 3.3.

X-ray quality yellow crystals were grown by dissolving 51 mg of $B(C_6F_5)_3$ and 20 mg of *o*-anisaldehyde in toluene/hexane mixture and cooling to -35 °C.

2. Spectral data for $B(C_6F_5)_3$ adduct of *p*-anisaldehyde, 4:



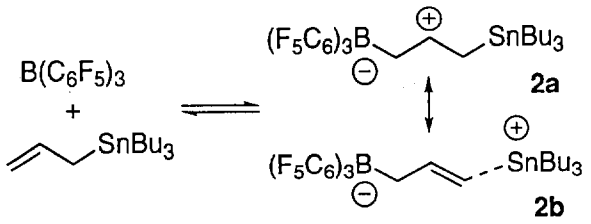
4

To 51 mg (0.10 mmol) of $B(C_6F_5)_3$ in an NMR tube was added 12 μL (0.10 mmol) of *p*-anisaldehyde dissolved in deuterated solvent. NMR spectra of the colorless solution were collected at room temperature in C_6D_6 unless indicated otherwise. ^{1}H NMR (300 MHz): 8.64 (s, 1H), 8.20-7.80 (br. s, 1H), 6.90-6.50 (br. s, 1H), 6.12 (d, 2H, J = 8.7 Hz), 2.92 (s, 3H); ^{13}C NMR (100 MHz): 194.0, 171.7 (br. s), 150.3 (m), 147.9 (m), 142.6 (m), 140.2 (m), 139.5 (m), 137.0 (m), 135.0 (br. s), 124.3, 117.2 (br. s), 115.6 (br. s), 56.2; ^{19}F NMR (282.4 MHz, d^8-tol): -133.6 (dd, 6 F, *o-F's*), -155.5 (t, 3F, *p-F's*), -163.0 (m, 6F, *m-F's*); ^{11}B NMR (64.2 MHz): 3.2 ppm.

3. Competition study of *o*-anisaldehyde and *p*-anisaldehyde for $B(C_6F_5)_3$:

An NMR tube was loaded with 0.1 mmol of each of *o*- and *p*-anisaldehyde, 0.02 mmol of $B(C_6F_5)_3$ and d^8-toluene at room temperature. ^{19}F NMR analysis at -60 °C indicated there to be two borane aldehyde adducts in a 2.4:1 ratio. The signals for the major adduct (-133.7, -154.8, -162.4) most closely matched those of *p*-anisaldehyde adduct **4** obtained independently at -60 °C (see section 7 below) while the signals for the minor adduct (-134.0, -153.9, -162.2) most closely matched those of *o*-anisaldehyde adduct **1** obtained at -60 °C (see section 5 below). This identification was confirmed by adding an additional 0.1 mmol of *p*-anisaldehyde to the mixture whereupon the major adduct grew in proportion to the minor adduct.

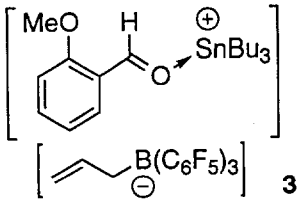
4. $B(C_6F_5)_3$ activation of allyltributyltin:



To a septum-sealed NMR tube containing 51 mg (0.1 mmol) of $B(C_6F_5)_3$ in d^8-toluene cooled to -78 °C was added 32 μL (0.1 mmol) of allyltributylstannane by syringe. The following NMR spectra were collected at -60 °C. ^{1}H NMR: 7.85 (br. s, 1H), 4.20-3.20 (br. m, 4H), 1.30-0.80 (br. m, 27H). ^{13}C NMR (excluding fluorinated aromatic C's): 192.1 (br.), 89.0, 41.0, 28.5, 27.6, 16.8, 13.9. ^{19}F NMR: -132.4 (br. s, 6F, *o*-F's), -159.8 (br.s, 3F, *p*-F's), -164.4 (br. s, 6F, *m*-F's). ^{119}Sn NMR (149.2 MHz): 186.9. ^{11}B NMR(64.2 MHz): -12.2.

In another experiment, the temperature dependence of interaction of $B(C_6F_5)_3$ and allyltributylstannane was determined by warming a d^8-toluene solution of the two reagents from -80 °C to room temperature. The following values for $\__{m,p}$ were obtained at the indicated temperatures: -80 °C, 4.2 ppm; -40 °C, 4.8 ppm; 0 °C, 15.9 ppm; 27 °C, 17.9 ppm. A similar trend was observed for a 5:1 mixture of allyltributylstannane and $B(C_6F_5)_3$.

5. $B(C_6F_5)_3$ activation of allyltributyltin in presence of *o*-anisaldehyde (stannane added to aldehyde adduct):



3

To an NMR tube containing 10 mg (0.02 mmol) of $B(C_6F_5)_3$ was added 14 mg (0.1 mmol) of *o*-anisaldehyde dissolved in d^8-toluene. The fluorescent green solution was cooled in the NMR probe to -60 °C and ^{1}H and ^{19}F NMR were obtained; ^{19}F NMR: -134.0, -153.8, -162.2. ^{1}H NMR (of adduct): 9.93 (s, 1H), 8.21 (d, 1H), 6.83 (t, 1H), 6.31 (t, 1H), 5.52 (d, 1H), 2.53 (s, 3H). The adduct shifts are clearly distinguishable from free *o*-anisaldehyde:. The NMR tube was removed from the probe, cooled in -78 °C cold bath and 32 μL (0.1 mmol) of allyltributylstannane was injected by syringe through the rubber NMR septum. The NMR tube was placed back in NMR probe (at -80 °C) and ^{19}F and ^{1}H NMR spectra were immediately recorded, the former clearly showing a new species being formed. Over time these new ^{19}F signals grow in intensity relative to adduct **1** and upon warming to -60 °C, these signals (-131.1 (br. s, 6F, *o-F's*), -163.3 (t, 3F, *p-F's*), -166.1 (apparent t, 6F, *m-F's*)) predominate to the complete exclusion of **1** (see Figure 2). ^{11}B NMR also supports the formation of anionic borate with a shift of -3.8 ppm.

6. $B(C_6F_5)_3$ activation of allyltributyltin in the presence of *o*-anisaldehyde (aldehyde added to stannane/borane mixture):

To an NMR tube containing 5 mg (0.01 mmol) of $B(C_6F_5)_3$ dissolved in d^8-toluene and cooled to -78 °C was added 32 μL (0.1 mmol) of allyltributylstannane. The NMR tube was immediately transferred to NMR probe precooled to -80 °C and a ^{19}F NMR spectrum was recorded; -132.5 (br. s, 6F, *o-F's*), -159.0 (m, 3F, *p-F's*), -163.9 (m, 6F, *m-F's*). The NMR tube was removed from the probe and then cooled to -78 °C. To this tube was added a solution of *o*-anisaldehyde (14 mg, 0.1 mmol) in d^8-toluene (100 μL) and then immediately placed in NMR probe at -80 °C. A ^{19}F NMR spectrum was collected immediately (1 minute after mixing). Signals for two main compounds were distinguishable. The major compound was assigned as borane:aldehyde adduct **1** (-134.1, -153.8, -162.2). The other set of signals was indicative of allylborate **3** (-131.2, -163.3, -166.1). A third set of signals was also present which match those collected prior to *o*-anisaldehyde addition. After 5 minutes, this third set of signals is gone and the resonances for **3** have grown in intensity relative to those for **1**. The sample was warmed to -40 °C leading to nearly complete conversion of signals for **1** to **3** (-130.9, -163.6, -166.3).

7. $B(C_6F_5)_3$ activation of allyltributyltin in presence of *p*-anisaldehyde:

To an NMR tube containing 10 mg (0.02 mmol) of $B(C_6F_5)_3$ was added 12 μL (0.1 mmol) of *p*-anisaldehyde dissolved in d^8-toluene. The colorless solution was cooled in the NMR probe to -80 °C and ^1H and ^{19}F NMR were obtained; ^{19}F NMR: -133.4, -154.2, -162.0. The ^1H NMR shifts of adduct were readily distinguished from excess *p*-anisaldehyde. The NMR tube was removed from the probe, cooled in a -78 °C cold bath and 32 μL (0.1 mmol) of allyltributylstannane was injected by syringe through a rubber NMR septum. The NMR tube was placed back in NMR probe and ^{19}F and ^1H NMR spectra were immediately recorded, the former clearly showing that no new species had been formed. The sample was warmed to -60 °C with no change in the ^{19}F NMR spectrum apparent. When the sample was warmed to -40 °C, a small set of peaks suggestive of allylborate appear, but are minor compared to those for **4**.

8. $B(C_6F_5)_3$ activation of allyltributyltin in presence of *o*-anisaldehyde/*p*-anisaldehyde mixture:

A septum-sealed NMR tube was loaded with 0.1 mmol of each of *o*- and *p*-anisaldehyde, 0.02 mmol of $B(C_6F_5)_3$ and d^8-toluene and cooled to -78 °C. Allyltributylstannane (32 μL, 0.1 mmol) was added by syringe and the NMR tube was placed in probe precooled to -80 °C. The sample was warmed to -60 °C and this temperature was maintained for 2 h over which time both ^{19}F and ^1H NMR analysis showed that the initially discernible borane:aldehyde adducts **1** and **4** had both disappeared. The ^{19}F NMR spectrum collected after 2h was comprised primarily of signals attributable to allylborate, -131.2, -163.1, -165.9. The most notable feature of the ^1H NMR spectrum collected after 2 h was the observation of an upfield shift and broadening of both the aldehydic H's (*o*-anisaldehyde shifted from 10.6 to 10.2 ppm, *p*-anisaldehyde shifted from 9.6 to 9.4 ppm).

9. NMR comparison study of the activation of allyltributylstannane in the presence of *o*-anisaldehyde, *p*-anisaldehyde and 1:1 *o*-anisaldehyde/*p*-anisaldehyde mixture.

Two stock solutions were prepared as follows:
Stock solution 1 was prepared by dissolving 51 mg (0.10 mmol) of $B(C_6F_5)_3$ in 1.0 mL of toluene.
Stock solution 2 was prepared by dissolving 27 mg (0.20 mmol) of *o*-anisaldehyde in 600 μL of toluene.

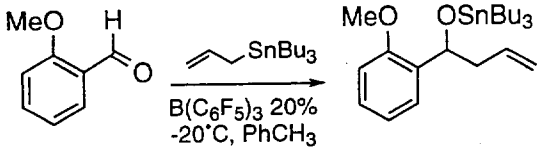
Three NMR tubes were prepared as follows:
Tube 1 - 200 μL (0.02 mmol) of stock solution 1, 300 μL (0.10 mmol) of stock solution 2.
Tube 2 - 200 μL (0.02 mmol) of stock solution 1, 300 μL of toluene, 12 μL (0.10 mmol) of *p*-anisaldehyde.
Tube 3 - 200 μL (0.02 mmol) of stock solution 1, 300 μL (0.10 mmol) of stock solution 2, 12 μL (0.10 mmol) of *p*-anisaldehyde.
To each NMR tube cooled to -78 °C was added 32 μL of allyltributylstannane. Each NMR tube was monitored periodically by ^{19}F NMR to determine whether $B(C_6F_5)_3$ was coordinated to aldehyde or converted to allylborate.
The following results were observed after 65 minutes at -78 °C:
Tube 1: mostly allylborate, some aldehyde adduct remaining.
Tube 2: only aldehyde adduct observable.
Tube 3: mostly aldehyde adduct, but some allylborate formed.
The following results were obtained after warming to -60 °C for 55 minutes:
Tube 1: only allylborate observed.
Tube 2: only aldehyde adduct observed.
Tube 3: mostly allylborate observed.

10. Effect of [aldehyde] on rate of allylation:

Table 1

RCHO	# eq. RCHO	% Reacted after 10 min. (-20 °C)	20 min. (-20 °C)
o-anisaldehyde	1	75%	91%
	2	63%	84%
	4	43%	59%
		30 min. (0 °C)	**60 min. (0 °C)**
p-anisaldehyde	1	34%	52%
	2	24%	40%
	4	16%	27%

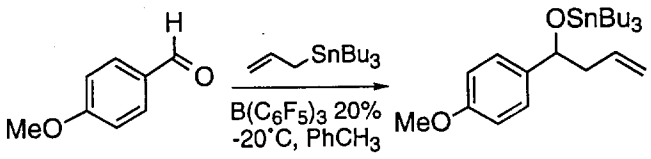
(a)



Two stock solutions were prepared as follows:
Stock solution 1 - 26 mg (0.05 mmol) of $B(C_6F_5)_3$ was dissolved in 500 µL of d^8-toluene.
Stock solution 2 - 136 mg (1.0 mmol) of *o*-anisaldehyde was dissolved in 1.0 mL of d^8-toluene.

Three NMR tubes were prepared as follows:
Tube 1 - 100 µL of sol'n 1, 100 µL of sol'n 2, 300 µL of d^8-toluene.
Tube 2 - 100 µL of sol'n 1, 200 µL of sol'n 2, 200 µL of d^8-toluene.
Tube 3 - 100 µL of sol'n 1, 400 µL of sol'n 2.
To each septum-sealed NMR tube cooled to -78 °C was added 32 µL of allyltributylstannane immediately prior to being placed in NMR probe precooled to -80 °C. In each case, a ^{1}H NMR spectrum indicated no reaction had occurred yet. The sample was warmed in the probe to -20 °C and ^{1}H NMR spectra were collected at identical time intervals for each sample. The results are summarized in Table 1 where the % of allyltributylstannane reacted was determined by integration of the vinylic CH_2 resonances for allyltributylstannane versus that of the allylated product as shown above.

(b)



A stock solution was prepared as follows:
Stock solution 1 - 26 mg (0.05 mmol) of $B(C_6F_5)_3$ was dissolved in 500 µL of d^8-toluene.

Three NMR tubes were prepared as follows:
Tube 1 - 100 µL of sol'n 1, 400 µL of d^8-toluene, 12 µL (0.1 mmol) of *p*-anisaldehyde.
Tube 2 - 100 µL of sol'n 1, 400 µL of d^8-toluene, 24 µL (0.2 mmol) of *p*-anisaldehyde.
Tube 3 - 100 µL of sol'n 1, 400 µL of d^8-toluene, 48 µL (0.4 mmol) of *p*-anisaldehyde.
To each septum-sealed NMR tube cooled to -78 °C was added 32 µL of allyltributylstannane immediately prior to being placed in NMR probe precooled to -80 °C. In each case, a ^{1}H NMR spectrum indicated no reaction had occurred yet. The sample was warmed in the probe to 0 °C and ^{1}H NMR spectra were collected at identical time intervals for each sample. The results are summarized in Table 1 where the % of allyltributylstannane reacted was determined by integration of the allylic CH_2 resonances for allyltributylstannane versus that of the allylated product as shown above.

---

[1] Blackwell, J. M.; Foster K. L.; Beck, V. H.; Piers, W. E. *J. Org. Chem.* **1999**, *64*, 4887.

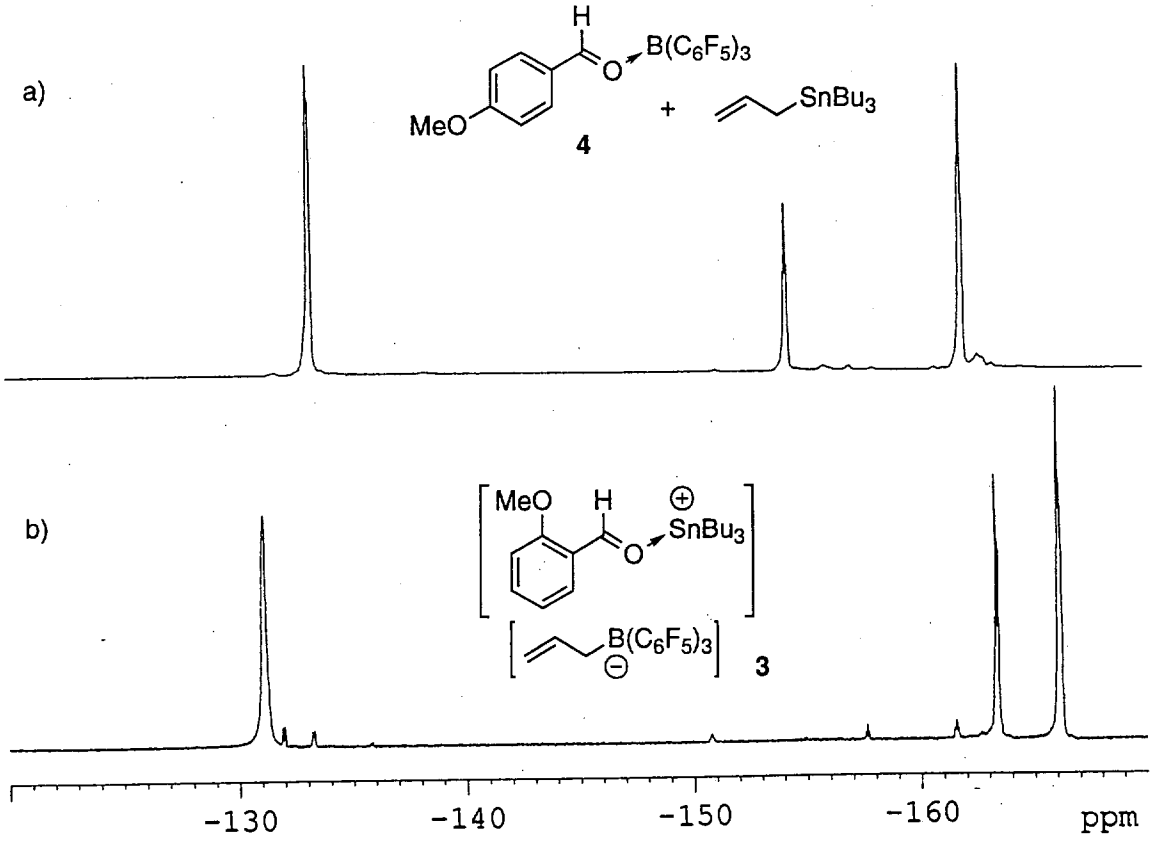


Figure S1. 282 MHz ^{19}F NMR spectra (-60°C) of a) *p*-anisaldehyde and 20% $B(C_6F_5)_3$ to which 1 equivalent of allyltributyltin has been added (time = 15 minutes). The major species in solution is the *p*-anisaldehyde adduct of $B(C_6F_5)_3$, **4**. b) *o*-anisaldehyde and 20% $B(C_6F_5)_3$ to which 1 equivalent of allyltributyltin has been added (time = 15 minutes). The major species in solution is the ion pair consisting of the *o*-anisaldehyde adduct of $[Bu_3Sn]^+$ and $[(C_3H_5)B(C_6F_5)_3]^-$, **3**.

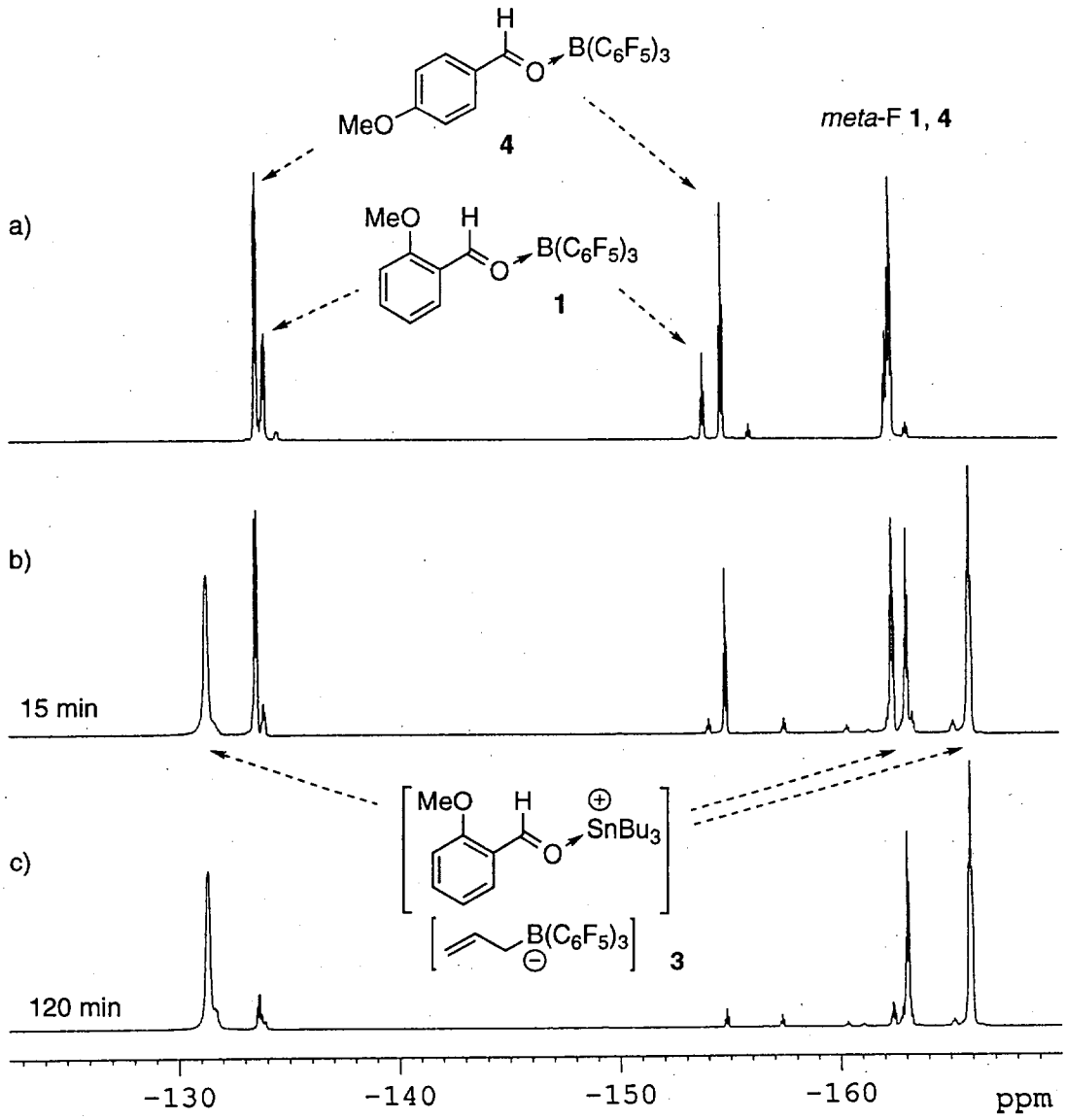


Figure S2. 282 MHz ^{19}F NMR spectra (-60°C) of a) 1:1 *o/p*-anisaldehyde and 20% $B(C_6F_5)_3$ (ratio of **4** to **1** = 2.4:1). b) Sample in a) 15 minutes after one equivalent of allyltributylstannane was added. Adduct **4** remains, while adduct **1** has been converted to ion pair **3**. c) Same sample 120 minutes after addition of allyltributylstannane. Conversion of the borane in the sample to ion pair **3** is complete.

Experimental

Data Collection

A colorless irregular-shaped crystal of $C_{26}H_8BO_2F_{15}.0.5C_7H_8$ having approximate dimensions of 0.45 x 0.42 x 0.38 mm was coated with Paratone-8277 oil (Exxon) and mounted on a glass fiber. All measurements were made on a Rigaku AFC6S diffractometer with graphite monochromated Mo-Kα radiation.

Cell constants and an orientation matrix for data collection , obtained from a least-squares refinement using the setting angles of 24 carefully centered reflections in the range $18.25 < 2\theta < 23.26°$ corresponded to a primitive triclinic cell with dimensions:

a = 11.814(2) $\AA$	α = 110.27(2)°
b = 13.051(3) $\AA$	β = 107.23(2)°
c = 9.819(3) $\AA$	γ = 80.22(2)
V = 1352.7(5) $\AA^3$	

For Z = 2 and F.W. = 694.20, the calculated density is 1.70 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

$P\bar{1}$ (#2)

The data were collected at a temperature of -103 $\pm$ 1°C using the ω-2θ scan technique to a maximum 2θ value of 50.1°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.31° with a take-off angle of 6.0°. Scans of $(1.31 + 0.34 \tan\theta)°$ were made at a speed of 4.0°/min (in omega). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 4 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 400 mm, and the detector aperture was 9.0 x 13.0 mm (horizontal x vertical).

Data Reduction

Of the 5027 reflections which were collected, 4775 were unique (R_{int} = 0.049). The intensities of three representative reflection were measured after every 200 reflections. Over the course of data collection, the standards decreased by 2.6%. A linear correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ, for Mo-Kα radiation is 1.8 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.96 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included at geometrically idealized positions and were not refined. The final cycle of full-matrix least-squares refinement[3] was based on 2036 observed reflections ($I > 3.00\sigma(I)$) and 433 variable parameters and converged (largest parameter shift was 0.02 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.036$$

$$R_w = \sqrt{(\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2)} = 0.025$$

The standard deviation of an observation of unit weight[4] was 1.52. The weighting scheme was based on counting statistics and included a factor (p = 0.007) to downweight the intense reflections. Plots of $\Sigma w(|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.24 and -0.18 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) SIR92: Altomare, A., Cascarano, M., Giacovazzo, C., Guagliardi, A. (1993). J. Appl. Cryst., 26, 343.

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M. (1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $\Sigma w(|Fo| - |Fc|)^2$

where w = $\frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$

$\sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

(4) Standard deviation of an observation of unit weight:

$$\sqrt{\Sigma w(|Fo| - |Fc|)^2/(No - Nv)}$$

where: No = number of observations

Nv = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{29.50}H_{12}BO_2F_{15}$
Formula Weight	694.20
Crystal Color, Habit	colorless, irregular shape
Crystal Dimensions	0.45 X 0.42 X 0.38 mm
Crystal System	triclinic
No. of Reflections Used for Unit	
Cell Determination (2θ range)	24 (18.3 - 23.3°)
Omega Scan Peak Width	
at Half-height	0.31°
Lattice Parameters	a = 11.814(2)Å b = 13.051(3) Å c = 9.819(3) Å α = 110.27(2)° β = 107.23(2)° γ = 80.22(2)° V = 1352.7(5) $Å^3$
Space Group	$P\bar{1}$ (#2)
Z value	2
D_{calc}	1.704 g/cm^3
F_{000}	690.00
μ(MoKα)	1.76 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC6S
Radiation	MoKα (λ = 0.71069 Å)

	graphite monochromated
Temperature	-103.0°C
Scan Type	ω-2θ
Scan Rate	4.0°/min (in ω) (up to 4 scans)
Scan Width	$(1.31 + 0.34 \tan \theta)°$
$2\theta_{max}$	50.1°
No. of Reflections Measured	Total: 5027 Unique: 4775 ($R_{int} = 0.049$)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.9561 - 1.0000) Decay (2.56%)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$
p-factor	0.0070
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	2036
No. Variables	433
Reflection/Parameter Ratio	4.70
Residuals: R; Rw	0.036 ; 0.025
Goodness of Fit Indicator	1.52
Max Shift/Error in Final Cycle	0.02
Maximum peak in Final Diff. Map	0.24 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.18 $e^-/\AA^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
F(1)	0.2082(2)	-0.0849(2)	0.5535(3)	4.58(8)	
F(2)	0.3030(2)	-0.1395(2)	0.3243(3)	5.66(8)	
F(3)	0.4161(2)	0.0091(2)	0.2833(3)	6.09(9)	
F(4)	0.4341(3)	0.2129(2)	0.4841(3)	6.13(9)	
F(5)	0.3363(2)	0.2719(2)	0.7136(3)	4.23(7)	
F(6)	0.0510(2)	0.1596(2)	0.4942(3)	3.68(7)	
F(7)	-0.1432(2)	0.2921(2)	0.4560(3)	3.94(7)	
F(8)	-0.2193(2)	0.4315(2)	0.6957(3)	4.46(7)	
F(9)	-0.0967(2)	0.4326(2)	0.9775(3)	4.30(7)	
F(10)	0.0968(2)	0.2967(2)	1.0194(3)	3.47(7)	
F(11)	-0.0360(2)	0.0598(2)	0.7485(3)	3.74(7)	
F(12)	-0.0692(2)	-0.1063(2)	0.8244(3)	4.55(8)	
F(13)	0.1187(2)	-0.2229(2)	0.9540(3)	5.04(8)	
F(14)	0.3430(2)	-0.1717(2)	0.9987(3)	4.75(8)	
F(15)	0.3794(2)	-0.0104(2)	0.9129(3)	4.11(7)	
O(1)	0.2999(2)	0.1954(2)	0.9306(3)	2.32(7)	
O(2)	0.3665(2)	0.5036(2)	1.0596(3)	3.40(8)	
C(1)	0.3163(3)	0.2963(3)	0.9833(4)	2.2(1)	
C(2)	0.4092(3)	0.3385(3)	1.1123(5)	2.3(1)	
C(3)	0.4325(4)	0.4484(4)	1.1528(5)	2.5(1)	
C(4)	0.5211(4)	0.4911(4)	1.2792(5)	3.5(1)	
C(5)	0.5865(4)	0.4248(4)	1.3611(5)	4.6(1)	
C(6)	0.5649(4)	0.3155(4)	1.3219(5)	4.2(1)	
C(7)	0.4773(4)	0.2724(3)	1.1976(5)	3.1(1)	

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C(8)	0.3774(4)	0.6194(4)	1.1021(6)	4.8(1)	
C(9)	0.2679(3)	0.0958(3)	0.6505(5)	2.3(1)	
C(10)	0.2648(4)	-0.0069(4)	0.5439(5)	3.0(1)	
C(11)	0.3123(4)	-0.0379(4)	0.4234(5)	3.5(1)	
C(12)	0.3686(4)	0.0365(4)	0.4007(5)	4.1(1)	
C(13)	0.3776(4)	0.1393(4)	0.5026(6)	3.8(1)	
C(14)	0.3272(4)	0.1657(4)	0.6209(5)	3.0(1)	
C(15)	0.0878(3)	0.2242(3)	0.7602(5)	2.0(1)	
C(16)	0.0198(4)	0.2272(3)	0.6192(5)	2.5(1)	
C(17)	-0.0816(4)	0.2954(4)	0.5971(5)	2.8(1)	
C(18)	-0.1206(4)	0.3640(4)	0.7165(5)	3.0(1)	
C(19)	-0.0580(4)	0.3642(3)	0.8581(5)	2.6(1)	
C(20)	0.0414(4)	0.2948(3)	0.8753(5)	2.5(1)	
C(21)	0.1744(4)	0.0371(3)	0.8327(4)	2.2(1)	
C(22)	0.0628(4)	0.0060(3)	0.8122(5)	2.6(1)	
C(23)	0.0427(4)	-0.0804(4)	0.8499(5)	3.1(1)	
C(24)	0.1359(5)	-0.1393(4)	0.9143(5)	3.3(1)	
C(25)	0.2488(4)	-0.1127(4)	0.9371(5)	3.1(1)	
C(26)	0.2658(4)	-0.0279(3)	0.8953(5)	2.8(1)	
C(27)	0.173(1)	0.363(1)	0.429(2)	8.4(6)	1/2
C(28)	0.090(1)	0.4272(7)	0.459(2)	10.0(4)	
C(29)	-0.012(2)	0.445(1)	0.353(1)	10.9(4)	
C(30)	-0.104(1)	0.514(1)	0.384(2)	11.7(5)	
B(1)	0.2015(4)	0.1368(4)	0.7859(5)	2.3(1)	

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H(1)	0.2650	0.3452	0.9355	2.6760	
H(2)	0.5367	0.5659	1.3094	4.2410	
H(3)	0.6485	0.4543	1.4471	5.5409	
H(4)	0.6108	0.2715	1.3811	5.0278	
H(5)	0.4624	0.1976	1.1688	3.7296	
H(6)	0.4573	0.6318	1.1143	5.8054	
H(7)	0.3263	0.6474	1.0262	5.8054	
H(8)	0.3560	0.6553	1.1942	5.8054	
H(9)	0.1476	0.2904	0.3826	10.0726	1/2
H(10)	0.2036	0.3809	0.3607	10.0726	1/2
H(11)	0.2340	0.3658	0.5178	10.0726	1/2
H(12)	-0.0170	0.4054	0.2500	13.0006	
H(13)	-0.1740	0.5237	0.3099	14.1191	
H(14)	-0.1533	0.6262	0.5746	11.5770	1/2

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F(1)	0.084(2)	0.036(2)	0.053(2)	-0.023(2)	0.025(2)	-0.004(1)
F(2)	0.090(2)	0.048(2)	0.060(2)	-0.006(2)	0.031(2)	-0.013(2)
F(3)	0.080(2)	0.097(3)	0.057(2)	-0.011(2)	0.042(2)	0.003(2)
F(4)	0.095(2)	0.083(2)	0.075(2)	-0.040(2)	0.045(2)	0.013(2)
F(5)	0.079(2)	0.036(2)	0.052(2)	-0.023(1)	0.027(2)	0.006(1)
F(6)	0.045(2)	0.052(2)	0.030(2)	-0.001(1)	0.001(1)	0.005(1)
F(7)	0.044(2)	0.063(2)	0.042(2)	-0.004(1)	-0.001(1)	0.025(2)
F(8)	0.041(2)	0.064(2)	0.066(2)	0.016(1)	0.014(2)	0.031(2)
F(9)	0.047(2)	0.054(2)	0.054(2)	0.007(1)	0.022(2)	0.004(2)
F(10)	0.038(2)	0.059(2)	0.030(2)	0.000(1)	0.007(1)	0.010(1)
F(11)	0.030(2)	0.045(2)	0.065(2)	-0.011(1)	0.003(1)	0.019(2)
F(12)	0.058(2)	0.058(2)	0.064(2)	-0.029(2)	0.024(2)	0.011(2)
F(13)	0.092(2)	0.048(2)	0.066(2)	-0.021(2)	0.023(2)	0.027(2)
F(14)	0.071(2)	0.042(2)	0.069(2)	0.002(2)	0.008(2)	0.030(2)
F(15)	0.034(2)	0.043(2)	0.081(2)	-0.004(1)	0.004(1)	0.031(2)
O(1)	0.028(2)	0.025(2)	0.031(2)	-0.007(1)	0.002(1)	0.007(1)
O(2)	0.043(2)	0.027(2)	0.055(2)	-0.006(2)	0.001(2)	0.015(2)
C(1)	0.028(3)	0.026(3)	0.030(3)	-0.002(2)	0.009(2)	0.008(2)
C(2)	0.023(3)	0.030(3)	0.031(3)	-0.005(2)	0.003(2)	0.007(2)
C(3)	0.029(3)	0.033(3)	0.033(3)	-0.002(2)	0.011(2)	0.007(2)
C(4)	0.047(3)	0.037(3)	0.043(3)	-0.018(3)	0.004(3)	0.003(3)
C(5)	0.052(4)	0.072(4)	0.042(3)	-0.029(3)	-0.012(3)	0.014(3)
C(6)	0.042(3)	0.067(4)	0.050(3)	-0.015(3)	-0.011(3)	0.032(3)
C(7)	0.037(3)	0.036(3)	0.041(3)	-0.009(2)	0.001(2)	0.012(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(8)	0.063(4)	0.029(3)	0.091(4)	-0.008(3)	0.012(3)	0.022(3)
C(9)	0.023(3)	0.024(3)	0.038(3)	-0.003(2)	0.002(2)	0.009(2)
C(10)	0.036(3)	0.033(3)	0.046(3)	-0.006(2)	0.011(3)	0.013(3)
C(11)	0.049(3)	0.034(3)	0.039(3)	0.002(3)	0.013(3)	-0.003(3)
C(12)	0.049(4)	0.065(4)	0.039(3)	-0.002(3)	0.023(3)	0.004(3)
C(13)	0.049(3)	0.057(4)	0.045(4)	-0.016(3)	0.019(3)	0.013(3)
C(14)	0.036(3)	0.033(3)	0.040(3)	-0.006(2)	0.008(3)	0.005(3)
C(15)	0.023(2)	0.022(3)	0.029(3)	-0.008(2)	0.005(2)	0.005(2)
C(16)	0.034(3)	0.026(3)	0.030(3)	-0.004(2)	0.009(2)	0.003(2)
C(17)	0.034(3)	0.042(3)	0.035(3)	-0.008(2)	0.004(3)	0.018(3)
C(18)	0.021(3)	0.042(3)	0.055(4)	0.002(2)	0.004(3)	0.027(3)
C(19)	0.030(3)	0.028(3)	0.041(3)	0.001(2)	0.014(3)	0.007(3)
C(20)	0.028(3)	0.034(3)	0.030(3)	-0.009(2)	0.000(2)	0.010(2)
C(21)	0.033(3)	0.021(3)	0.026(3)	-0.006(2)	0.006(2)	0.000(2)
C(22)	0.037(3)	0.028(3)	0.027(3)	-0.003(2)	0.003(2)	0.005(2)
C(23)	0.042(3)	0.037(3)	0.038(3)	-0.019(3)	0.013(3)	0.001(3)
C(24)	0.065(4)	0.031(3)	0.037(3)	-0.013(3)	0.017(3)	0.011(2)
C(25)	0.051(3)	0.030(3)	0.038(3)	0.000(3)	0.005(3)	0.018(2)
C(26)	0.034(3)	0.031(3)	0.040(3)	-0.009(2)	0.008(2)	0.008(2)
C(27)	0.10(1)	0.08(1)	0.16(2)	-0.024(9)	0.01(1)	0.06(1)
C(28)	0.21(2)	0.065(7)	0.141(9)	-0.060(8)	0.12(1)	-0.007(8)
C(29)	0.23(2)	0.12(1)	0.088(8)	-0.12(1)	0.06(1)	0.002(7)
C(30)	0.22(1)	0.105(8)	0.16(1)	-0.078(8)	0.116(9)	0.013(8)
B(1)	0.026(3)	0.025(3)	0.029(3)	-0.006(2)	0.000(2)	0.002(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
F(1)	C(10)	1.352(4)	F(2)	C(11)	1.345(5)
F(3)	C(12)	1.341(5)	F(4)	C(13)	1.345(5)
F(5)	C(14)	1.371(4)	F(6)	C(16)	1.352(4)
F(7)	C(17)	1.350(4)	F(8)	C(18)	1.346(4)
F(9)	C(19)	1.355(4)	F(10)	C(20)	1.366(4)
F(11)	C(22)	1.357(4)	F(12)	C(23)	1.350(4)
F(13)	C(24)	1.342(5)	F(14)	C(25)	1.353(4)
F(15)	C(26)	1.350(4)	O(1)	C(1)	1.262(4)
O(1)	B(1)	1.589(5)	O(2)	C(3)	1.345(5)
O(2)	C(8)	1.439(5)	C(1)	C(2)	1.418(5)
C(2)	C(3)	1.402(5)	C(2)	C(7)	1.400(5)
C(3)	C(4)	1.377(5)	C(4)	C(5)	1.372(6)
C(5)	C(6)	1.389(6)	C(6)	C(7)	1.360(5)
C(9)	C(10)	1.384(5)	C(9)	C(14)	1.389(5)
C(9)	B(1)	1.628(6)	C(10)	C(11)	1.365(6)
C(11)	C(12)	1.376(6)	C(12)	C(13)	1.367(6)
C(13)	C(14)	1.373(5)	C(15)	C(16)	1.390(5)
C(15)	C(20)	1.378(5)	C(15)	B(1)	1.628(6)
C(16)	C(17)	1.375(5)	C(17)	C(18)	1.357(6)
C(18)	C(19)	1.367(5)	C(19)	C(20)	1.362(5)
C(21)	C(22)	1.383(5)	C(21)	C(26)	1.385(5)
C(21)	B(1)	1.628(6)	C(22)	C(23)	1.376(5)
C(23)	C(24)	1.357(6)	C(24)	C(25)	1.369(6)
C(25)	C(26)	1.368(5)	C(27)	C(28)	1.21(1)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(28)	C(29)	1.38(1)	C(28)	C(30*)	1.44(1)
C(29)	C(30)	1.33(1)			

Symmetry operation for the starred atom: -x, 1-y, 1-z

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	O(1)	B(1)	127.0(3)	C(3)	O(2)	C(8)	118.7(3)
O(1)	C(1)	C(2)	121.6(4)	C(1)	C(2)	C(3)	118.6(4)
C(1)	C(2)	C(7)	121.2(4)	C(3)	C(2)	C(7)	120.2(4)
O(2)	C(3)	C(2)	115.8(4)	O(2)	C(3)	C(4)	124.9(4)
C(2)	C(3)	C(4)	119.3(4)	C(3)	C(4)	C(5)	119.4(4)
C(4)	C(5)	C(6)	122.0(4)	C(5)	C(6)	C(7)	119.2(4)
C(2)	C(7)	C(6)	119.9(4)	C(10)	C(9)	C(14)	111.3(4)
C(10)	C(9)	B(1)	126.0(4)	C(14)	C(9)	B(1)	122.5(4)
F(1)	C(10)	C(9)	119.3(4)	F(1)	C(10)	C(11)	115.0(4)
C(9)	C(10)	C(11)	125.6(4)	F(2)	C(11)	C(10)	121.1(5)
F(2)	C(11)	C(12)	119.2(5)	C(10)	C(11)	C(12)	119.6(5)
F(3)	C(12)	C(11)	121.3(5)	F(3)	C(12)	C(13)	120.2(5)
C(11)	C(12)	C(13)	118.4(5)	F(4)	C(13)	C(12)	119.5(5)
F(4)	C(13)	C(14)	121.4(4)	C(12)	C(13)	C(14)	119.1(5)
F(5)	C(14)	C(9)	119.2(4)	F(5)	C(14)	C(13)	115.0(4)
C(9)	C(14)	C(13)	125.8(4)	C(16)	C(15)	C(20)	112.9(4)
C(16)	C(15)	B(1)	123.5(4)	C(20)	C(15)	B(1)	123.2(4)
F(6)	C(16)	C(15)	120.2(4)	F(6)	C(16)	C(17)	116.3(4)
C(15)	C(16)	C(17)	123.5(4)	F(7)	C(17)	C(16)	119.7(4)
F(7)	C(17)	C(18)	120.2(4)	C(16)	C(17)	C(18)	120.0(4)
F(8)	C(18)	C(17)	120.4(4)	F(8)	C(18)	C(19)	120.5(4)
C(17)	C(18)	C(19)	119.2(4)	F(9)	C(19)	C(18)	119.3(4)
F(9)	C(19)	C(20)	121.6(4)	C(18)	C(19)	C(20)	119.0(4)
F(10)	C(20)	C(15)	119.0(4)	F(10)	C(20)	C(19)	115.7(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(15)	C(20)	C(19)	125.3(4)	C(22)	C(21)	C(26)	113.2(4)
C(22)	C(21)	B(1)	125.5(4)	C(26)	C(21)	B(1)	121.3(4)
F(11)	C(22)	C(21)	120.4(4)	F(11)	C(22)	C(23)	115.4(4)
C(21)	C(22)	C(23)	124.1(4)	F(12)	C(23)	C(22)	120.4(4)
F(12)	C(23)	C(24)	119.7(4)	C(22)	C(23)	C(24)	119.9(4)
F(13)	C(24)	C(23)	121.0(5)	F(13)	C(24)	C(25)	120.2(5)
C(23)	C(24)	C(25)	118.8(4)	F(14)	C(25)	C(24)	119.7(4)
F(14)	C(25)	C(26)	120.4(4)	C(24)	C(25)	C(26)	119.9(4)
F(15)	C(26)	C(21)	119.2(4)	F(15)	C(26)	C(25)	116.7(4)
C(21)	C(26)	C(25)	124.0(4)	C(27)	C(28)	C(29)	124(2)
C(27)	C(28)	C(30*)	115(2)	C(29)	C(28)	C(30*)	121(1)
C(28)	C(29)	C(30)	124(1)	C(28)	C(30)	C(29)	115(1)
O(1)	B(1)	C(9)	104.5(3)	O(1)	B(1)	C(15)	108.9(3)
O(1)	B(1)	C(21)	101.6(3)	C(9)	B(1)	C(15)	113.3(4)
C(9)	B(1)	C(21)	113.5(4)	C(15)	B(1)	C(21)	113.8(4)

Symmetry operation for the starred atoms: -x, 1-y, 1-z

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(1)	C(10)	C(9)	C(14)	-178.6(4)	F(1)	C(10)	C(9)	B(1)	-4.0(7)
F(1)	C(10)	C(11)	F(2)	-0.7(6)	F(1)	C(10)	C(11)	C(12)	178.0(4)
F(2)	C(11)	C(10)	C(9)	-178.9(4)	F(2)	C(11)	C(12)	F(3)	-1.1(7)
F(2)	C(11)	C(12)	C(13)	-179.8(4)	F(3)	C(12)	C(11)	C(10)	-179.8(4)
F(3)	C(12)	C(13)	F(4)	0.2(8)	F(3)	C(12)	C(13)	C(14)	179.3(4)
F(4)	C(13)	C(12)	C(11)	178.9(4)	F(4)	C(13)	C(14)	F(5)	1.7(7)
F(4)	C(13)	C(14)	C(9)	-179.5(4)	F(5)	C(14)	C(9)	C(10)	178.5(4)
F(5)	C(14)	C(9)	B(1)	3.7(6)	F(5)	C(14)	C(13)	C(12)	-177.3(4)
F(6)	C(16)	C(15)	C(20)	-177.5(4)	F(6)	C(16)	C(15)	B(1)	-4.1(6)
F(6)	C(16)	C(17)	F(7)	-0.2(6)	F(6)	C(16)	C(17)	C(18)	178.5(4)
F(7)	C(17)	C(16)	C(15)	-179.2(4)	F(7)	C(17)	C(18)	F(8)	-1.8(6)
F(7)	C(17)	C(18)	C(19)	178.7(4)	F(8)	C(18)	C(17)	C(16)	179.6(4)
F(8)	C(18)	C(19)	F(9)	0.4(6)	F(8)	C(18)	C(19)	C(20)	179.9(4)
F(9)	C(19)	C(18)	C(17)	-180.0(4)	F(9)	C(19)	C(20)	F(10)	1.7(6)
F(9)	C(19)	C(20)	C(15)	-178.8(4)	F(10)	C(20)	C(15)	C(16)	177.3(3)
F(10)	C(20)	C(15)	B(1)	3.9(6)	F(10)	C(20)	C(19)	C(18)	-177.7(4)
F(11)	C(22)	C(21)	C(26)	-178.3(4)	F(11)	C(22)	C(21)	B(1)	0.0(6)
F(11)	C(22)	C(23)	F(12)	-0.6(6)	F(11)	C(22)	C(23)	C(24)	-180.0(4)
F(12)	C(23)	C(22)	C(21)	-179.2(4)	F(12)	C(23)	C(24)	F(13)	-0.3(7)
F(12)	C(23)	C(24)	C(25)	179.1(4)	F(13)	C(24)	C(23)	C(22)	179.1(4)
F(13)	C(24)	C(25)	F(14)	0.6(7)	F(13)	C(24)	C(25)	C(26)	179.5(4)
F(14)	C(25)	C(24)	C(23)	-178.8(4)	F(14)	C(25)	C(26)	F(15)	2.7(6)
F(14)	C(25)	C(26)	C(21)	-179.5(4)	F(15)	C(26)	C(21)	C(22)	176.0(4)
F(15)	C(26)	C(21)	B(1)	-2.3(6)	F(15)	C(26)	C(25)	C(24)	-176.2(4)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(1)	C(1)	C(2)	C(3)	171.5(4)	O(1)	C(1)	C(2)	C(7)	-8.1(6)
O(1)	B(1)	C(9)	C(10)	133.6(4)	O(1)	B(1)	C(9)	C(14)	-52.4(5)
O(1)	B(1)	C(15)	C(16)	144.0(4)	O(1)	B(1)	C(15)	C(20)	-43.3(5)
O(1)	B(1)	C(21)	C(22)	135.4(4)	O(1)	B(1)	C(21)	C(26)	-46.5(5)
O(2)	C(3)	C(2)	C(1)	-3.0(6)	O(2)	C(3)	C(2)	C(7)	176.7(4)
O(2)	C(3)	C(4)	C(5)	-176.6(4)	C(1)	O(1)	B(1)	C(9)	94.2(4)
C(1)	O(1)	B(1)	C(15)	-27.2(5)	C(1)	O(1)	B(1)	C(21)	-147.6(4)
C(1)	C(2)	C(3)	C(4)	178.9(4)	C(1)	C(2)	C(7)	C(6)	-179.2(4)
C(2)	C(1)	O(1)	B(1)	-178.7(4)	C(2)	C(3)	O(2)	C(8)	173.9(4)
C(2)	C(3)	C(4)	C(5)	1.4(7)	C(2)	C(7)	C(6)	C(5)	-0.9(8)
C(3)	C(2)	C(7)	C(6)	1.2(7)	C(3)	C(4)	C(5)	C(6)	-1.1(8)
C(4)	C(3)	O(2)	C(8)	-8.1(6)	C(4)	C(3)	C(2)	C(7)	-1.5(6)
C(4)	C(5)	C(6)	C(7)	0.8(8)	C(9)	C(10)	C(11)	C(12)	-0.2(8)
C(9)	C(14)	C(13)	C(12)	1.4(8)	C(9)	B(1)	C(15)	C(16)	28.2(6)
C(9)	B(1)	C(15)	C(20)	-159.1(4)	C(9)	B(1)	C(21)	C(22)	-113.1(5)
C(9)	B(1)	C(21)	C(26)	65.1(5)	C(10)	C(9)	C(14)	C(13)	-0.1(6)
C(10)	C(9)	B(1)	C(15)	-108.0(5)	C(10)	C(9)	B(1)	C(21)	23.8(6)
C(10)	C(11)	C(12)	C(13)	1.5(7)	C(11)	C(10)	C(9)	C(14)	-0.4(6)
C(11)	C(10)	C(9)	B(1)	174.2(4)	C(11)	C(12)	C(13)	C(14)	-2.0(8)
C(13)	C(14)	C(9)	B(1)	-175.0(4)	C(14)	C(9)	B(1)	C(15)	66.0(5)
C(14)	C(9)	B(1)	C(21)	-162.1(4)	C(15)	C(16)	C(17)	C(18)	-0.5(7)
C(15)	C(20)	C(19)	C(18)	1.8(7)	C(15)	B(1)	C(21)	C(22)	18.5(6)
C(15)	B(1)	C(21)	C(26)	-163.4(4)	C(16)	C(15)	C(20)	C(19)	-2.1(6)
C(16)	C(15)	B(1)	C(21)	-103.5(5)	C(16)	C(17)	C(18)	C(19)	0.0(7)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(17)	C(16)	C(15)	C(20)	1.5(6)	C(17)	C(16)	C(15)	B(1)	174.9(4)
C(17)	C(18)	C(19)	C(20)	-0.6(7)	C(19)	C(20)	C(15)	B(1)	-175.5(4)
C(20)	C(15)	B(1)	C(21)	69.2(5)	C(21)	C(22)	C(23)	C(24)	1.5(7)
C(21)	C(26)	C(25)	C(24)	1.6(7)	C(22)	C(21)	C(26)	C(25)	-1.7(6)
C(22)	C(23)	C(24)	C(25)	-1.6(7)	C(23)	C(22)	C(21)	C(26)	0.1(6)
C(23)	C(22)	C(21)	B(1)	178.4(4)	C(23)	C(24)	C(25)	C(26)	0.1(7)
C(25)	C(26)	C(21)	B(1)	179.9(4)	C(27)	C(28)	C(29)	C(30)	179(1)
C(27)	C(28)	C(30)	C(29)	-179(1)					