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The First [4+2] Cycloaddition of 1-Phenyl-1-benzothiophenium Salts with Dienes

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Supporting Information:
X-Ray Structural Information on Cycloadduct 2a

Contents

Experimental

Data Collection

A colorless prismatic crystal of $C_{20}H_{17}O_3F_3S_2$ having approximate dimensions of 0.30 x 0.30 x 0.15 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC7R diffractometer with filtered Cu-Kα radiation and a rotating anode generator.

Cell constants and an orientation matrix for data collection , obtained from a least-squares refinement using the setting angles of 19 carefully centered reflections in the range $58.60 < 2\theta < 59.52°$ corresponded to a primitive monoclinic cell with dimensions:

$$a = 10.468(2)\ \AA$$
$$b = 12.889(2)\ \AA \qquad \beta = 104.693(9)°$$
$$c = 14.915(1)\ \AA$$
$$V = 1946.5(4)\ \AA^3$$

For Z = 4 and F.W. = 426.47, the calculated density is 1.46 g/cm^3. The systematic absences of:

$$h0l:\ h \neq 2n$$
$$0k0:\ k \neq 2n$$

uniquely determine the space group to be:

$$P2_1/a\ (\#14)$$

The data were collected at a temperature of $23 \pm 1°C$ using the ω-2θ scan technique to a maximum 2θ value of 134.1°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.22° with a take-off angle of 6.0°. Scans of $(1.50 + 0.30 \tan \theta)°$ were made at speeds of 32.0, 16.0, 8.0 and 4.0°/min (in omega) for each 2θ shell (4.0<80.0<100.0<120.0 <135.0°). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 7 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 and the crystal to detector distance was 235 mm, The computer-controlled slits were set to 3.0 mm (horizontal) and 3.0 mm (vertical).

Data Reduction

Of the 3842 reflections which were collected, 3632 were unique ($R_{int} = 0.014$). The intensities of three representative reflection were measured after every 150 reflections. Over the course of data collection, the standards increased by 6.6%. A polynomial correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ, for Cu-Kα radiation is 29.1 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors

ranging from 0.70 to 1.00. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction was applied (coefficient = 2.25721e-05).

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 but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 2720 observed reflections ($I > 3.00\sigma(I)$) and 254 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.062$$

$$R_w = \sqrt{\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2} = 0.096$$

The standard deviation of an observation of unit weight[4] was 1.82. The weighting scheme was based on counting statistics and included a factor (p = 0.088) 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 0.34 and -0.45 $e^-/\mathring{A}^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5] . Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf" 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., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G., (1994), J. Appl. Cryst., 27, 435

(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	$C_{20}H_{17}O_3F_3S_2$
Formula Weight	426.47
Crystal Color, Habit	colorless, prismatic
Crystal Dimensions	0.30 X 0.30 X 0.15 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	19 (58.6 - 59.5°)
Omega Scan Peak Width at Half-height	0.22°
Lattice Parameters	a = 10.468(2) Å b = 12.889(2) Å c = 14.915(1) Å β = 104.693(9)°
	V = 1946.5(4) Å^3
Space Group	$P2_1/a$ (#14)
Z value	4
D_{calc}	1.455 g/cm^3
F_{000}	880.00
μ(CuKα)	29.09 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7R
Radiation	CuKα (λ = 1.54178 Å)
Attenuator	Ni foil (factor = 9.24)

Take-off Angle	6.0°
Detector Aperture	3.0 mm horizontal 3.0 mm vertical
Crystal to Detector Distance	235 mm
Voltage, Current	50kV, 100mA
Temperature	23.0°C
Scan Type	ω-2θ
Scan Rate(in ω)	32,16,8,4°/min for each 2θ shell($4<80<100<120<135°$) (up to 7 scans)
Scan Width	$(1.50 + 0.30 \tan \theta)°$
$2\theta_{max}$	134.1°
No. of Reflections Measured	Total: 3842 Unique: 3632 ($R_{int} = 0.014$)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.6976 - 0.9982) Decay (6.61% increase) Secondary Extinction (coefficient: 2.25721e-05)

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	0.0880
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I>3.00\sigma(I)$)	2720
No. Variables	254
Reflection/Parameter Ratio	10.71
Residuals: R; Rw	0.062 ; 0.096

Goodness of Fit Indicator	1.82
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.34 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.45 $e^-/\AA^3$

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

atom	x	y	z	B_{eq}
S(1)	0.50014(9)	0.88193(6)	0.22567(6)	4.70(2)
S(2)	0.44111(9)	0.57075(7)	0.24396(6)	4.99(2)
F(1)	0.4918(8)	0.5918(4)	0.4214(3)	14.4(2)
F(2)	0.4282(4)	0.4399(3)	0.3745(3)	10.4(1)
F(3)	0.6195(5)	0.4868(6)	0.3746(5)	17.2(2)
O(1)	0.5329(3)	0.6521(2)	0.2397(2)	6.20(7)
O(2)	0.3110(4)	0.6050(4)	0.2404(4)	9.1(1)
O(3)	0.4483(4)	0.4845(3)	0.1854(3)	7.98(10)
C(1)	0.3244(4)	0.8604(3)	0.1703(2)	4.98(7)
C(2)	0.2564(4)	0.9668(3)	0.1459(3)	5.26(8)
C(3)	0.1992(4)	0.9585(4)	0.0382(3)	5.86(9)
C(4)	0.3139(4)	0.9540(4)	-0.0047(3)	5.86(9)
C(5)	0.3747(5)	0.8639(4)	0.0160(3)	6.09(9)
C(6)	0.2996(5)	0.8039(3)	0.0740(3)	5.99(9)
C(7)	0.1585(5)	0.8446(5)	0.0324(3)	7.0(1)
C(8)	0.3563(4)	1.0509(3)	0.1791(3)	4.94(7)
C(9)	0.3314(5)	1.1580(3)	0.1733(3)	6.5(1)
C(10)	0.4335(8)	1.2273(4)	0.2059(4)	7.7(1)
C(11)	0.5604(7)	1.1924(4)	0.2438(4)	7.5(1)
C(12)	0.5895(5)	1.0876(4)	0.2502(3)	6.19(10)
C(13)	0.4844(4)	1.0190(3)	0.2176(2)	4.78(7)
C(14)	0.5170(4)	0.8634(3)	0.3474(2)	4.80(7)
C(15)	0.4144(5)	0.8860(4)	0.3885(3)	5.95(9)
C(16)	0.4368(6)	0.8723(4)	0.4836(3)	6.9(1)

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

atom	x	y	z	B_{eq}
C(17)	0.5593(6)	0.8401(4)	0.5360(3)	7.3(1)
C(18)	0.6595(5)	0.8193(4)	0.4939(3)	7.2(1)
C(19)	0.6390(4)	0.8300(3)	0.3984(3)	5.86(9)
C(20)	0.4996(6)	0.5196(5)	0.3587(3)	7.5(1)
H(1)	0.2841	0.8230	0.2109	6.0127
H(2)	0.1865	0.9737	0.1754	6.3762
H(3)	0.1313	1.0063	0.0113	7.1128
H(4)	0.3386	1.0071	-0.0412	7.1180
H(5)	0.4511	0.8411	-0.0017	7.3681
H(6)	0.3108	0.7305	0.0759	7.2925
H(7a)	0.0989	0.8282	0.0690	8.3916
H(7b)	0.1220	0.8214	-0.0295	8.3916
H(9)	0.2443	1.1830	0.1472	7.8935
H(10)	0.4170	1.2997	0.2022	9.3946
H(11)	0.6292	1.2412	0.2659	9.0907
H(12)	0.6765	1.0633	0.2757	7.5440
H(15)	0.3314	0.9104	0.3524	7.2274
H(16)	0.3674	0.8849	0.5129	8.3132
H(17)	0.5737	0.8329	0.6010	8.9480
H(18)	0.7426	0.7979	0.5304	8.7613
H(19)	0.7075	0.8145	0.3692	7.1279

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	0.0672(5)	0.0559(5)	0.0557(5)	0.0000(3)	0.0163(3)	-0.0003(3)
S(2)	0.0659(5)	0.0625(5)	0.0628(5)	-0.0017(4)	0.0191(4)	0.0034(3)
F(1)	0.304(8)	0.167(4)	0.069(2)	-0.065(5)	0.036(3)	-0.014(2)
F(2)	0.157(3)	0.126(3)	0.099(2)	-0.046(2)	0.014(2)	0.044(2)
F(3)	0.097(3)	0.260(6)	0.248(7)	-0.015(3)	-0.042(3)	0.160(6)
O(1)	0.094(2)	0.062(1)	0.089(2)	-0.014(1)	0.039(2)	-0.005(1)
O(2)	0.077(2)	0.130(3)	0.145(4)	0.028(2)	0.045(2)	0.047(3)
O(3)	0.142(3)	0.074(2)	0.089(2)	-0.028(2)	0.034(2)	-0.024(2)
C(1)	0.073(2)	0.062(2)	0.052(2)	-0.014(2)	0.013(1)	0.001(1)
C(2)	0.060(2)	0.081(2)	0.062(2)	0.000(2)	0.022(1)	-0.001(2)
C(3)	0.064(2)	0.095(3)	0.060(2)	0.004(2)	0.009(2)	0.005(2)
C(4)	0.077(2)	0.092(3)	0.053(2)	0.000(2)	0.015(2)	0.009(2)
C(5)	0.084(3)	0.091(3)	0.058(2)	0.007(2)	0.021(2)	-0.005(2)
C(6)	0.097(3)	0.071(2)	0.057(2)	-0.014(2)	0.015(2)	-0.007(2)
C(7)	0.079(3)	0.122(4)	0.061(2)	-0.023(3)	0.011(2)	-0.011(2)
C(8)	0.073(2)	0.060(2)	0.059(2)	0.003(2)	0.024(2)	0.004(1)
C(9)	0.116(4)	0.064(2)	0.067(2)	0.022(2)	0.025(2)	0.004(2)
C(10)	0.166(6)	0.060(2)	0.072(2)	-0.006(3)	0.042(3)	-0.001(2)
C(11)	0.143(5)	0.065(2)	0.088(3)	-0.036(3)	0.050(3)	-0.008(2)
C(12)	0.085(3)	0.073(2)	0.083(3)	-0.020(2)	0.030(2)	-0.004(2)
C(13)	0.068(2)	0.059(2)	0.058(2)	-0.006(1)	0.023(1)	0.001(1)
C(14)	0.069(2)	0.055(2)	0.056(2)	-0.002(1)	0.013(1)	-0.003(1)
C(15)	0.081(2)	0.084(3)	0.062(2)	0.003(2)	0.020(2)	0.000(2)
C(16)	0.105(3)	0.098(3)	0.064(2)	-0.006(3)	0.030(2)	-0.003(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(17)	0.118(4)	0.102(3)	0.056(2)	-0.004(3)	0.017(2)	0.001(2)
C(18)	0.092(3)	0.101(3)	0.066(2)	0.003(3)	-0.007(2)	0.006(2)
C(19)	0.073(2)	0.080(2)	0.065(2)	0.003(2)	0.009(2)	-0.001(2)
C(20)	0.099(3)	0.102(3)	0.073(3)	-0.029(3)	0.000(2)	0.017(3)

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
S(1)	C(1)	1.836(4)	S(1)	C(13)	1.776(4)
S(1)	C(14)	1.795(4)	S(2)	O(1)	1.435(3)
S(2)	O(2)	1.419(4)	S(2)	O(3)	1.427(3)
S(2)	C(20)	1.791(5)	F(1)	C(20)	1.336(8)
F(2)	C(20)	1.326(6)	F(3)	C(20)	1.288(8)
C(1)	C(2)	1.546(6)	C(1)	C(6)	1.571(5)
C(2)	C(3)	1.569(5)	C(2)	C(8)	1.500(6)
C(3)	C(4)	1.498(6)	C(3)	C(7)	1.525(7)
C(4)	C(5)	1.323(6)	C(5)	C(6)	1.518(6)
C(6)	C(7)	1.542(7)	C(8)	C(9)	1.403(5)
C(8)	C(13)	1.380(5)	C(9)	C(10)	1.383(8)
C(10)	C(11)	1.380(9)	C(11)	C(12)	1.383(7)
C(12)	C(13)	1.399(6)	C(14)	C(15)	1.395(6)
C(14)	C(19)	1.379(6)	C(15)	C(16)	1.388(6)
C(16)	C(17)	1.385(8)	C(17)	C(18)	1.378(8)
C(18)	C(19)	1.393(6)			

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.95	C(2)	H(2)	0.95
C(3)	H(3)	0.95	C(4)	H(4)	0.95
C(5)	H(5)	0.95	C(6)	H(6)	0.95
C(7)	H(7a)	0.95	C(7)	H(7b)	0.95
C(9)	H(9)	0.95	C(10)	H(10)	0.95
C(11)	H(11)	0.95	C(12)	H(12)	0.95
C(15)	H(15)	0.95	C(16)	H(16)	0.95
C(17)	H(17)	0.95	C(18)	H(18)	0.94
C(19)	H(19)	0.95			

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	S(1)	C(13)	93.1(2)	C(1)	S(1)	C(14)	105.4(2)
C(13)	S(1)	C(14)	100.6(2)	O(1)	S(2)	O(2)	114.7(2)
O(1)	S(2)	O(3)	113.7(2)	O(1)	S(2)	C(20)	104.0(2)
O(2)	S(2)	O(3)	114.7(3)	O(2)	S(2)	C(20)	104.0(3)
O(3)	S(2)	C(20)	103.9(3)	S(1)	C(1)	C(2)	108.7(2)
S(1)	C(1)	C(6)	113.3(3)	C(2)	C(1)	C(6)	103.7(3)
C(1)	C(2)	C(3)	102.3(3)	C(1)	C(2)	C(8)	108.8(3)
C(3)	C(2)	C(8)	116.1(3)	C(2)	C(3)	C(4)	107.5(3)
C(2)	C(3)	C(7)	98.7(3)	C(4)	C(3)	C(7)	100.4(4)
C(3)	C(4)	C(5)	109.0(4)	C(4)	C(5)	C(6)	107.0(4)
C(1)	C(6)	C(5)	107.2(3)	C(1)	C(6)	C(7)	97.4(4)
C(5)	C(6)	C(7)	100.3(4)	C(3)	C(7)	C(6)	94.6(3)
C(2)	C(8)	C(9)	126.0(4)	C(2)	C(8)	C(13)	116.4(3)
C(9)	C(8)	C(13)	117.6(4)	C(8)	C(9)	C(10)	120.0(5)
C(9)	C(10)	C(11)	120.7(4)	C(10)	C(11)	C(12)	121.2(5)
C(11)	C(12)	C(13)	117.0(5)	S(1)	C(13)	C(8)	112.8(3)
S(1)	C(13)	C(12)	123.6(3)	C(8)	C(13)	C(12)	123.5(4)
S(1)	C(14)	C(15)	121.8(3)	S(1)	C(14)	C(19)	116.0(3)
C(15)	C(14)	C(19)	122.1(4)	C(14)	C(15)	C(16)	118.2(4)
C(15)	C(16)	C(17)	120.5(4)	C(16)	C(17)	C(18)	120.2(4)
C(17)	C(18)	C(19)	120.6(4)	C(14)	C(19)	C(18)	118.4(4)
S(2)	C(20)	F(1)	110.2(4)	S(2)	C(20)	F(2)	112.6(3)
S(2)	C(20)	F(3)	112.2(5)	F(1)	C(20)	F(2)	106.1(5)
F(1)	C(20)	F(3)	109.3(6)	F(2)	C(20)	F(3)	106.2(5)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
S(1)	C(1)	H(1)	110.2	C(2)	C(1)	H(1)	110.2
C(6)	C(1)	H(1)	110.5	C(1)	C(2)	H(2)	109.8
C(3)	C(2)	H(2)	110.0	C(8)	C(2)	H(2)	109.6
C(2)	C(3)	H(3)	116.1	C(4)	C(3)	H(3)	116.1
C(7)	C(3)	H(3)	115.6	C(3)	C(4)	H(4)	125.4
C(5)	C(4)	H(4)	125.6	C(4)	C(5)	H(5)	126.5
C(6)	C(5)	H(5)	126.5	C(1)	C(6)	H(6)	116.2
C(5)	C(6)	H(6)	116.4	C(7)	C(6)	H(6)	116.6
C(3)	C(7)	H(7a)	113.4	C(3)	C(7)	H(7b)	113.3
C(6)	C(7)	H(7a)	113.2	C(6)	C(7)	H(7b)	112.9
H(7a)	C(7)	H(7b)	109.0	C(8)	C(9)	H(9)	120.1
C(10)	C(9)	H(9)	119.9	C(9)	C(10)	H(10)	120.2
C(11)	C(10)	H(10)	119.1	C(10)	C(11)	H(11)	119.6
C(12)	C(11)	H(11)	119.2	C(11)	C(12)	H(12)	121.6
C(13)	C(12)	H(12)	121.5	C(14)	C(15)	H(15)	120.9
C(16)	C(15)	H(15)	120.9	C(15)	C(16)	H(16)	119.7
C(17)	C(16)	H(16)	119.8	C(16)	C(17)	H(17)	119.4
C(18)	C(17)	H(17)	120.4	C(17)	C(18)	H(18)	119.4
C(19)	C(18)	H(18)	120.0	C(14)	C(19)	H(19)	121.0
C(18)	C(19)	H(19)	120.7				

Table 7. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
S(1)	O(1)	2.983(3)	1	S(1)	O(2)	3.210(4)	56504
F(1)	F(2)	2.974(5)	66603	F(1)	F(1)	3.306(10)	66603
F(1)	C(18)	3.448(8)	1	F(1)	C(19)	3.491(7)	1
F(1)	C(20)	3.560(6)	66603	F(2)	C(12)	3.578(7)	46504
F(3)	C(18)	3.399(7)	64602	F(3)	C(15)	3.455(7)	56504
O(1)	C(14)	3.188(4)	1	O(1)	C(19)	3.280(5)	1
O(1)	C(2)	3.381(5)	56504	O(1)	C(1)	3.449(5)	1
O(1)	C(1)	3.466(5)	56504	O(1)	C(6)	3.583(6)	1
O(2)	C(19)	3.412(6)	46504	O(2)	C(12)	3.425(7)	46504
O(2)	C(1)	3.468(6)	1	O(2)	C(6)	3.550(6)	1
O(3)	C(3)	3.317(5)	54502	O(3)	C(10)	3.337(6)	54501
O(3)	C(4)	3.347(6)	54502	O(3)	C(2)	3.479(6)	56504
C(16)	C(16)	3.54(1)	67603				

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ± 4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	X,	Y,	Z	(2)	1/2-X,	1/2+Y,	-Z
(3)	-X,	-Y,	-Z	(4)	1/2+X,	1/2-Y,	Z