Supporting Information

Synthesis of 1,3-Bis(methylseleno)-1,3-diphenylpropadiene (1). To a hexane solution (40 mL) of 1,3-diphenylpropyne (1.00 g, 5.21 mmol) was added dropwise *n*-butyllithium (1.54 mol/L, 6.6 mL, 10.2 mmol) under nitrogen, and the solution was stirred for 1 h. *N,N,N',N'*-tetramethylethylenediamine (0.80 mL, 5.32 mmol) was added to the mixture, and stirring was continued for additional 1 h. A benzene solution (20 mL) of dimethyldiselenide (2.06 g, 11.0 mmol) was added dropwise to the solution and stirred for 30 min. Water (100 mL) was added to the solution and product was extracted with benzene. The combined organic extracts were washed with brine and dried over anhydrous magnesium sulfate. After removal of solvent *in vacuo*, the product was purified by silica-gel column chromatography (benzene/hexane = 1/8) to give 1.36 g of **1** (70%).

1,3-Bis(methylseleno)-1,3-diphenylpropadiene (1). Yellow liquid; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 2.14 (s, 6H), 7.26 (t, 2H, J = 7.3 Hz), 7.33 (t, 4H, J = 7.3 Hz), 7.53 (d, 4H, J = 7.3 Hz); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 7.1, 106.9, 127.0, 128.2, 128.6, 135.2, 193.4; IR (neat) ν_{max} 3052, 2926, 1906, 1595, 1491, 1444, 1420, 1273, 1211, 1029, 911, 857, 760, 690 cm^{-1}; UV (cyclohexane) λ_{max} 236 (ε 2.37 x 10^4), 250 (sh, ε 2.14 x 10^4), 298 (sh, ε 1.54 x 10^4) nm; MS *m/z* 378 (M^+, $^{78}Se^{80}Se$), 285, 270, 189. Anal. Calcd for $C_{17}H_{16}Se_2$: C, 53.98; H, 4.26. Found: C, 54.27; H, 4.24.

Synthesis of 1,3-Bis(benzylseleno)-1,3-diphenylpropadiene (2). To a hexane solution (45 mL) of 1,3-diphenylpropyne (1.50 g, 7.81 mmol) was added dropwise *n*-butyllithium (1.54 mol/L, 10.0 mL, 15.4 mmol) under nitrogen, and the solution was stirred for 1 h. *N,N,N',N'*-tetramethylethylenediamine (1.20 mL, 7.98 mmol) was added to the mixture, and stirring was continued for additional 1 h. A benzene solution (45 mL) of benzylselenocyanate (3.34 g, 17.0 mmol) was added dropwise at -20 °C to the solution and allowed to warm to room temperature. Water (100 mL) was added to the solution and product was extracted with benzene. The combined organic extracts were washed with brine and dried over anhydrous magnesium

sulfate. After removal of solvent *in vacuo*, the product was purified by silica-gel column chromatography (benzene/hexane = 1/6) to give 2.60 g of **2** (64%).

1,3-Bis(benzylseleno)-1,3-diphenylpropadiene (2). Mp 100.0-100.7 °C (pale yellow prisms from ethanol-hexane); ^{1}H-NMR (500 MHz, $CDCl_3$) δ 3.90 (s, 4H), 7.16-7.28 (m, 12H), 7.31 (t, 4H, J = 7.7 Hz), 7.46 (d, 4H, J = 7.7 Hz); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 31.1, 103.3, 126.9, 127.4, 128.2, 128.5, 128.7, 129.1, 134.8, 138.0, 197.6; IR (KBr) ν_{max} 3076, 3027, 1904, 1594, 1490, 1453, 1444, 1172, 1029, 912, 862, 761, 697, 629 cm^{-1}; UV (cyclohexane) λ_{max} 229 (sh, ε 3.98 x 10^4), 266 (sh, ε 2.35 x 10^4), 307 (sh, ε 1.38 x 10^4) nm; MS *m/z* 530 (M$^+$, ^{78}Se^{80}Se), 439, 359. Anal. Calcd for $C_{29}H_{24}Se_2$: C, 65.67; H, 4.56. Found: C, 65.79; H, 4.66.

Synthesis of 1-Benzylseleno-3-methylseleno-1,3-diphenylpropadiene (3). To a hexane solution (30 mL) of 1,3-diphenylpropyne (1.00 g, 5.21 mmol) was added dropwise *n*-butyllithium (1.54 mol/L, 6.6 mL, 10.2 mmol) under nitrogen, and the solution was stirred for 1 h. *N,N,N',N'*-tetramethylethylenediamine (0.80 mL, 5.32 mmol) was added to the mixture, and stirring was continued for additional 1 h. A benzene solution (30 mL) of dimethyldiselenide (1.06 g, 5.63 mmol) and benzylselenocyanate (1.23 g, 6.26 mmol) was added dropwise to the solution and stirred for 30 min. Water (100 mL) was added to the solution and product was extracted with benzene. The combined organic extracts were washed with brine and dried over anhydrous magnesium sulfate. After removal of solvent *in vacuo*, the product was purified by silica-gel column chromatography (benzene/hexane = 1/8) to give 402 mg of **3** (17%) together with 520 mg of **1** (26%) and 128 mg of **2** (5%).

1-Benzylseleno-3-methylseleno-1,3-diphenylpropadiene (3). Yellow liquid; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 2.06 (s, 3H), 3.97 (s, 2H), 7.14-7.35 (m, 11H), 7.45 (dd, 2H, J = 1.5, 7.8 Hz), 7.54 (dd, 2H, J = 1.2, 7.9 Hz); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 7.2, 31.0, 105.2, 105.3, 126.9, 127.1, 127.2, 128.17, 128.20, 128.5, 128.6, 128.7, 129.1, 134.9, 135.0, 137.9, 195.3; IR (neat) ν_{max} 3057, 3027, 2925, 1906, 1594, 1490, 1445, 1029, 911, 860, 760, 692 cm^{-1}; MS *m/z* 454 (M$^+$, ^{78}Se^{80}Se), 361,

285, 269, 189. Anal. Calcd for $C_{23}H_{20}Se_2$: C, 60.81; H, 4.44. Found: C, 60.90; H, 4.41.

Thermal Reaction of 1,3-Bis(methylseleno)-1,3-diphenylpropadiene (1). A *p*-xylene solution (11 mL) of 1,3-bis(methylseleno)allene **1** (547 mg, 1.45 mmol) was refluxed for 3 d under nitrogen. After removal of solvent *in vacuo*, the residue was subjected to silica-gel short column chromatography (benzene/hexane = 1/3). Products were separated by gel-peameation chromatography (chloroform) to give compounds **4** (34%), **5** (7%), **6** (21%), and **7** (9%) at point of 79% conversion.

***Z,Z*-1,2-Bis(methylselenobenzylidene)-3,4-diphenylcyclobutene (6).** Mp 153.6-155.0 °C (yellow needles from chloroform-methanol); ^{1}H-NMR (500 MHz, $CDCl_3$) δ 1.70 (s, 6H), 6.64 (dd, 4H, J = 1.2, 7.9 Hz), 6.81 (t, 4H, J = 7.9 Hz), 6.90-6.96 (m, 8H), 7.10 (dd, 4H, J = 1.2, 7.7 Hz); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 8.9, 114.8, 126.66, 126.72, 127.1, 127.2, 127.8, 130.3, 131.9, 138.4, 142.2, 151.6; IR (KBr) ν_{max} 3050, 2920, 1600, 1480, 1440, 1410, 1260, 1070, 1025, 910, 770, 700 cm^{-1}; MS *m/z* 568 (M^+, $^{78}Se^{80}Se$), 475, 460, 380. Anal. Calcd for $C_{32}H_{26}Se_2$: C, 67.61; H, 4.61. Found: C, 67.38; H, 4.71.

***E,Z*-1,2-Bis(methylselenobenzylidene)-3,4-diphenylcyclobutene (7).** Mp 112.1-113.8 °C (yellow solid); ^{1}H-NMR (500 MHz, $CDCl_3$) δ 1.26 (s, 3H), 1.53 (s, 3H), 6.59 (dd, 2H, J = 1.1, 7.9 Hz), 6.80 (t, 2H, J = 7.9 Hz), 6.87-6.97 (m, 6H), 7.27-7.34 (m, 4H), 7.41-7.45 (m, 4H), 7.54 (dd, 2H, J = 1.2, 8.3 Hz); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 7.4, 7.8, 116.9, 117.8, 126.6, 126.7, 127.1, 127.2, 127.4, 127.6, 127.7, 127.8, 128.6, 129.1, 130.3, 131.1, 131.9, 133.1, 138.3, 139.7, 140.3, 141.3, 152.5, 152.9; IR (KBr) ν_{max} 3076, 3017, 2999, 1595, 1489, 1442, 1305, 1160, 1070, 1028, 923, 772, 755, 727, 699, 685 cm^{-1}; MS *m/z* 568 (M^+, $^{78}Se^{80}Se$), 475, 460, 380. Anal. Calcd for $C_{32}H_{26}Se_2$: C, 67.61; H, 4.61. Found: C, 67.58; H, 4.64.

Thermal Reaction of 1,3-Bis(benzylseleno)-1,3-diphenylpropadiene (2). A *p*-xylene solution (21 mL) of 1,3-bis(benzylseleno)allene **2** (426 mg, 0.80 mmol) was refluxed for 1.5 h under nitrogen. After removal of solvent *in vacuo*, the residue was subjected to silica-gel short column chromatography (benzene/hexane = 1/3).

Products were separated by gel-peameation chromatography (chloroform) to give compounds **4** (36%), **5** (8%), **8** (57%), and **9** (25%) at point of 90% conversion.

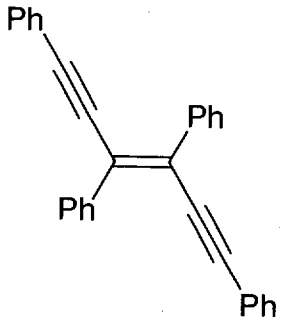
Thermal Reaction of 1-Benzylseleno-3-methylseleno-1,3-diphenylpropadiene (3). A *p*-xylene solution (7.5 mL) of 1,3-bis(alkylseleno)allene **3** (194 mg, 0.42 mmol) was refluxed for 1.5 h under nitrogen. After removal of solvent *in vacuo*, the residue was subjected to silica-gel short column chromatography (benzene/hexane = 1/3). Products were separated by gel-peameation chromatography (chloroform) to give compounds **4** (28%) and **5** (7%) together with large amounts of complex mixture at point of 40% conversion.

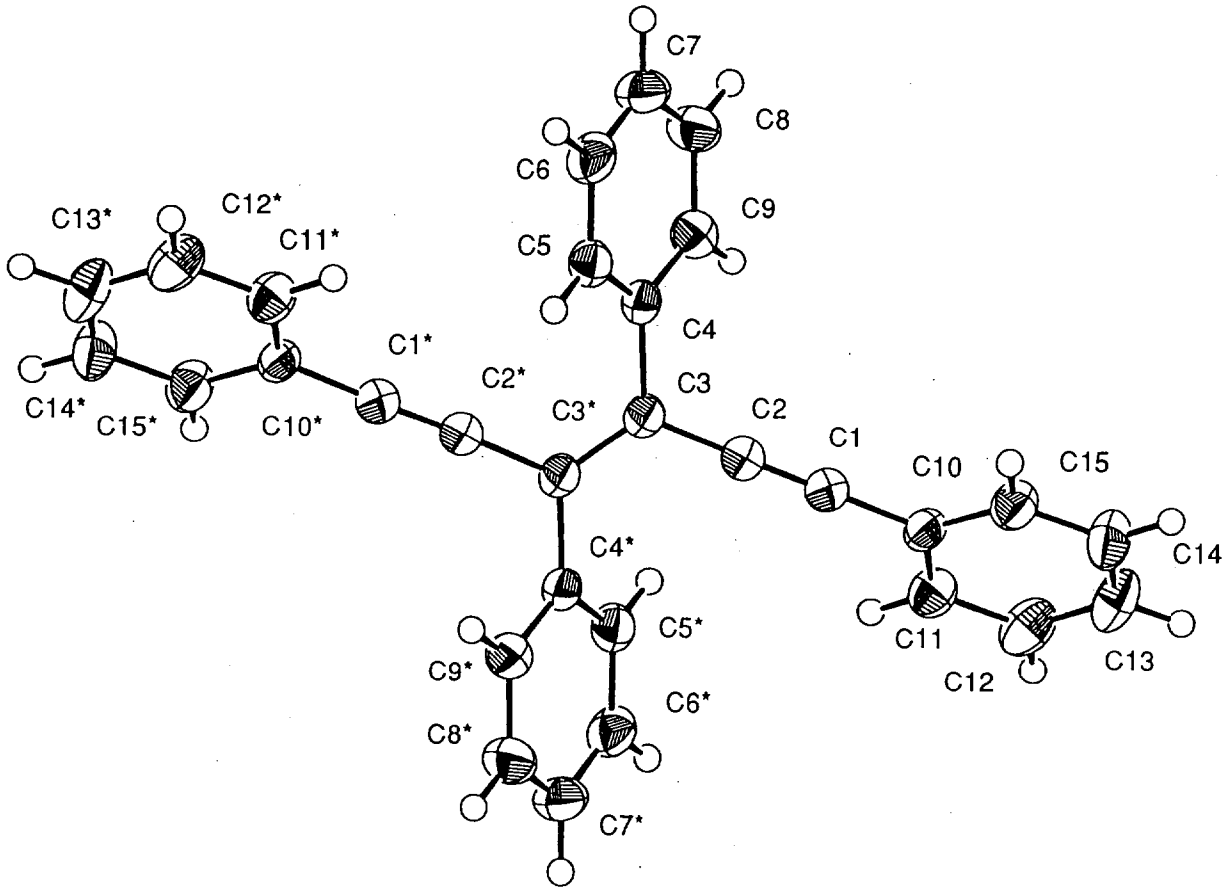
5

X-Ray Structure

of

E-1,3,4,6-Tetraphenyl-3-hexene-1,5-diyne




C7
C8
C6
C9
C5
C4
C3
C2
C1
C10
C15
C14
C11
C12
C13
C4*
C5*
C6*
C7*
C8*
C9*
C3*
C2*
C1*
C10*
C15*
C14*
C11*
C12*
C13*

Experimental

Data Collection

A colorless prismatic crystal of $C_{15}H_{10}$ having approximate dimensions of 0.20 x 0.20 x 0.20 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC7R diffractometer with graphite monochromated Mo-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 25 carefully centered reflections in the range $29.58 < 2\theta < 30.01°$ corresponded to a primitive monoclinic cell with dimensions:

$a = 9.150(2)$ Å

$b = 9.118(2)$ Å $\quad \beta = 99.18(1)°$

$c = 12.576(1)$ Å

$V = 1035.8(3)$ Å^3

For Z = 4 and F.W. = 190.24, the calculated density is 1.22 g/cm^3. The systematic absences of:

h0l: $h+l \neq 2n$

0k0: $k \neq 2n$

uniquely determine the space group to be:

$P2_1/n$ (#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 55.0°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.30° with a take-off angle of 6.0°. Scans of $(1.84 + 0.30 \tan \theta)°$ were made at a speed of 16.0°/min (in omega). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 5 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 0.5 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 2667 reflections which were collected, 2520 were unique ($R_{int} = 0.033$). The intensities of three representative reflection were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ, for Mo-Kα radiation is 0.7 cm^{-1}. Azimuthal scans of several reflections indicated no need for an absorption correction. 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 but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 1735 observed reflections ($I > 3.00\sigma(I)$) and 136 variable parameters and converged (largest parameter shift was 0.02 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.039$$

$$R_w = \sqrt{(\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2)} = 0.037$$

The standard deviation of an observation of unit weight[4] was 2.10. The weighting scheme was based on counting statistics and included a factor (p = 0.002) 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 0.13 and -0.12 $e^-/\AA^3$, 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., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G. (1994). J. Appl. Cryst., in preparation.

(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	$C_{15}H_{10}$
Formula Weight	190.24
Crystal Color, Habit	colorless, prismatic
Crystal Dimensions	0.20 X 0.20 X 0.20 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (29.6 - 30.0°)
Omega Scan Peak Width at Half-height	0.30°
Lattice Parameters	a = 9.150(2)Å b = 9.118(2) Å c = 12.576(1) Å β = 99.18(1)°
	V = 1035.8(3) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.220 g/cm^3
F_{000}	400.00
μ(MoKα)	0.69 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated

Attenuator	Zr foil (factor = 9.00)
Take-off Angle	6.0°
Detector Aperture	3.0 mm horizontal 3.0 mm vertical
Crystal to Detector Distance	235 mm
Voltage, Current	50kV, 200mA
Temperature	23.0°C
Scan Type	ω-2θ
Scan Rate	16.0°/min (in ω) (up to 5 scans)
Scan Width	$(1.84 + 0.30 \tan \theta)°$
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 2667 Unique: 2520 (R_{int} =.0.033)
Corrections	Lorentz-polarization

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	0.0020
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	1735
No. Variables	136
Reflection/Parameter Ratio	12.76
Residuals: R; Rw	0.039 ; 0.037
Goodness of Fit Indicator	2.10
Max Shift/Error in Final Cycle	0.02

Maximum peak in Final Diff. Map	0.13 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.12 $e^-/Å^3$

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

atom	x	y	z	B_{eq}
C(1)	0.1314(2)	0.9732(2)	0.2932(1)	2.91(3)
C(2)	0.1003(2)	0.9777(2)	0.3819(1)	2.84(3)
C(3)	0.0685(2)	0.9819(2)	0.4898(1)	2.61(3)
C(4)	0.1955(2)	0.9461(2)	0.5769(1)	2.64(3)
C(5)	0.1825(2)	0.8445(2)	0.6571(1)	3.22(3)
C(6)	0.3035(2)	0.8110(2)	0.7347(1)	3.90(4)
C(7)	0.4377(2)	0.8792(2)	0.7332(1)	4.16(4)
C(8)	0.4519(2)	0.9796(2)	0.6541(1)	3.93(4)
C(9)	0.3320(2)	1.0122(2)	0.5752(1)	3.27(3)
C(10)	0.1671(2)	0.9821(2)	0.1861(1)	2.73(3)
C(11)	0.1178(2)	1.1020(2)	0.1212(1)	3.33(3)
C(12)	0.1574(2)	1.1166(2)	0.0204(1)	4.10(4)
C(13)	0.2453(2)	1.0125(2)	-0.0171(1)	4.39(4)
C(14)	0.2922(2)	0.8915(2)	0.0452(1)	4.21(4)
C(15)	0.2531(2)	0.8757(2)	0.1463(1)	3.48(4)
H(1)	0.0901	0.7976	0.6588	3.8776
H(2)	0.2940	0.7409	0.7891	4.6805
H(3)	0.5203	0.8569	0.7867	4.9973
H(4)	0.5442	1.0269	0.6534	4.7188
H(5)	0.3434	1.0802	0.5198	3.9305
H(6)	0.0566	1.1740	0.1466	3.9985
H(7)	0.1240	1.1988	-0.0233	4.9330
H(8)	0.2737	1.0237	-0.0861	5.2765
H(9)	0.3518	0.8190	0.0186	5.0404

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

atom	x	y	z	B_{eq}
H(10)	0.2848	0.7919	0.1887	4.1861

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	0.0347(7)	0.0414(9)	0.0342(7)	-0.0010(7)	0.0048(6)	-0.0015(7)
C(2)	0.0338(7)	0.0395(9)	0.0344(7)	0.0008(7)	0.0053(6)	-0.0001(7)
C(3)	0.0358(7)	0.0350(8)	0.0286(7)	-0.0019(6)	0.0060(6)	-0.0004(6)
C(4)	0.0352(7)	0.0358(8)	0.0296(7)	0.0037(6)	0.0057(6)	-0.0037(6)
C(5)	0.0410(8)	0.0448(9)	0.0376(8)	0.0027(7)	0.0101(7)	0.0016(7)
C(6)	0.058(1)	0.054(1)	0.0358(8)	0.0119(9)	0.0066(7)	0.0072(8)
C(7)	0.0475(10)	0.063(1)	0.0431(9)	0.0112(9)	-0.0063(8)	-0.0027(9)
C(8)	0.0369(8)	0.058(1)	0.0523(10)	-0.0013(8)	-0.0006(7)	-0.0056(9)
C(9)	0.0392(8)	0.0445(9)	0.0406(8)	-0.0004(7)	0.0064(7)	0.0012(7)
C(10)	0.0352(7)	0.0405(8)	0.0278(7)	-0.0047(7)	0.0043(6)	-0.0032(6)
C(11)	0.0505(9)	0.0376(9)	0.0385(8)	0.0002(7)	0.0066(7)	-0.0026(7)
C(12)	0.074(1)	0.0431(10)	0.0381(8)	-0.0058(9)	0.0082(8)	0.0074(8)
C(13)	0.079(1)	0.058(1)	0.0339(8)	-0.011(1)	0.0213(8)	-0.0014(9)
C(14)	0.064(1)	0.057(1)	0.0425(9)	0.0066(10)	0.0203(8)	-0.0083(8)
C(15)	0.0529(10)	0.0441(9)	0.0356(8)	0.0071(8)	0.0080(7)	0.0020(7)

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
C(1)	C(2)	1.195(2)	C(1)	C(10)	1.438(2)
C(2)	C(3)	1.433(2)	C(3)	C(3)	1.359(3)
C(3)	C(4)	1.501(2)	C(4)	C(5)	1.388(2)
C(4)	C(9)	1.390(2)	C(5)	C(6)	1.390(2)
C(5)	H(1)	0.97	C(6)	C(7)	1.380(3)
C(6)	H(2)	0.97	C(7)	C(8)	1.372(3)
C(7)	H(3)	0.97	C(8)	C(9)	1.389(2)
C(8)	H(4)	0.97	C(9)	H(5)	0.97
C(10)	C(11)	1.396(2)	C(10)	C(15)	1.391(2)
C(11)	C(12)	1.380(2)	C(11)	H(6)	0.97
C(12)	C(13)	1.375(3)	C(12)	H(7)	0.97
C(13)	C(14)	1.382(3)	C(13)	H(8)	0.96
C(14)	C(15)	1.382(2)	C(14)	H(9)	0.96
C(15)	H(10)	0.97			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(1)	C(10)	174.7(2)	C(1)	C(2)	C(3)	177.9(2)
C(2)	C(3)	C(3)	121.2(2)	C(2)	C(3)	C(4)	115.8(1)
C(3)	C(3)	C(4)	123.0(2)	C(3)	C(4)	C(5)	121.9(1)
C(3)	C(4)	C(9)	119.1(1)	C(5)	C(4)	C(9)	118.9(1)
C(4)	C(5)	C(6)	120.3(2)	C(4)	C(5)	H(1)	119.5
C(6)	C(5)	H(1)	120.1	C(5)	C(6)	C(7)	120.2(2)
C(5)	C(6)	H(2)	119.8	C(7)	C(6)	H(2)	120.0
C(6)	C(7)	C(8)	119.9(2)	C(6)	C(7)	H(3)	120.3
C(8)	C(7)	H(3)	119.9	C(7)	C(8)	C(9)	120.4(2)
C(7)	C(8)	H(4)	120.1	C(9)	C(8)	H(4)	119.5
C(4)	C(9)	C(8)	120.2(2)	C(4)	C(9)	H(5)	119.4
C(8)	C(9)	H(5)	120.4	C(1)	C(10)	C(11)	119.4(1)
C(1)	C(10)	C(15)	121.6(1)	C(11)	C(10)	C(15)	119.0(1)
C(10)	C(11)	C(12)	120.3(2)	C(10)	C(11)	H(6)	119.4
C(12)	C(11)	H(6)	120.3	C(11)	C(12)	C(13)	120.1(2)
C(11)	C(12)	H(7)	120.1	C(13)	C(12)	H(7)	119.7
C(12)	C(13)	C(14)	120.2(2)	C(12)	C(13)	H(8)	120.2
C(14)	C(13)	H(8)	119.6	C(13)	C(14)	C(15)	120.1(2)
C(13)	C(14)	H(9)	119.7	C(15)	C(14)	H(9)	120.2
C(10)	C(15)	C(14)	120.2(2)	C(10)	C(15)	H(10)	119.7
C(14)	C(15)	H(10)	120.2				

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(1)	C(2)	C(3)	C(3)	178(4)	C(1)	C(2)	C(3)	C(4)	0(4)
C(1)	C(10)	C(11)	C(12)	176.5(2)	C(1)	C(10)	C(15)	C(14)	-176.4(2)
C(2)	C(1)	C(10)	C(11)	-23(1)	C(2)	C(1)	C(10)	C(15)	155(1)
C(2)	C(3)	C(3)	C(2)	-180.0	C(2)	C(3)	C(3)	C(4)	0.9(3)
C(2)	C(3)	C(4)	C(5)	-130.3(2)	C(2)	C(3)	C(4)	C(9)	47.2(2)
C(3)	C(2)	C(1)	C(10)	-110(4)	C(3)	C(4)	C(5)	C(6)	178.2(1)
C(3)	C(4)	C(9)	C(8)	-179.2(1)	C(4)	C(3)	C(3)	C(4)	-180.0
C(4)	C(5)	C(6)	C(7)	0.4(3)	C(4)	C(9)	C(8)	C(7)	1.4(3)
C(5)	C(4)	C(9)	C(8)	-1.6(2)	C(5)	C(6)	C(7)	C(8)	-0.6(3)
C(6)	C(5)	C(4)	C(9)	0.6(2)	C(6)	C(7)	C(8)	C(9)	-0.4(3)
C(10)	C(11)	C(12)	C(13)	0.4(3)	C(10)	C(15)	C(14)	C(13)	-0.6(3)
C(11)	C(10)	C(15)	C(14)	2.0(2)	C(11)	C(12)	C(13)	C(14)	1.0(3)
C(12)	C(11)	C(10)	C(15)	-1.9(2)	C(12)	C(13)	C(14)	C(15)	-0.9(3)

Table 6. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC
C(1)	H(4)	2.92	67403
C(1)	H(3)	3.17	46404
C(2)	H(3)	3.31	46404
C(2)	H(9)	3.35	55302
C(3)	H(9)	3.16	55302
C(4)	H(7)	2.93	54302
C(4)	C(12)	3.585(2)	54302
C(5)	H(8)	3.10	54302
C(5)	H(9)	3.56	46504
C(6)	H(7)	3.00	54302
C(6)	H(8)	3.23	54302
C(7)	H(7)	3.06	54302
C(8)	H(7)	3.04	54302
C(8)	H(6)	3.30	57504
C(8)	H(10)	3.53	67403
C(9)	H(2)	3.02	55402
C(9)	H(9)	3.38	55302
C(9)	H(6)	3.54	57504
C(10)	H(3)	3.17	67403
C(10)	H(7)	3.49	57303
C(11)	H(3)	3.34	67403
C(11)	H(4)	3.48	47404
C(12)	H(3)	3.50	67403
C(13)	H(6)	3.42	57303
C(1)	H(10)	3.00	55302
C(2)	H(10)	3.22	55302
C(2)	H(4)	3.34	67403
C(2)	H(2)	3.48	46404
C(3)	H(9)	3.43	46504
C(4)	H(2)	3.15	55402
C(5)	H(7)	2.94	54302
C(5)	C(12)	3.533(2)	54302
C(5)	H(8)	3.59	55601
C(6)	H(8)	3.01	55601
C(6)	H(9)	3.52	55601
C(7)	H(8)	3.19	55601
C(8)	H(5)	3.14	67403
C(8)	H(2)	3.42	55402
C(9)	H(7)	2.96	54302
C(9)	H(4)	3.26	67403
C(9)	H(5)	3.47	67403
C(10)	H(4)	3.05	67403
C(10)	H(10)	3.22	55302
C(11)	H(10)	2.95	55302
C(11)	C(12)	3.473(2)	57303
C(11)	C(13)	3.529(3)	57303
C(12)	C(12)	3.553(4)	57303
C(13)	H(3)	3.51	67403

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(13)	H(2)	3.55	55401	C(14)	H(5)	3.14	54302
C(14)	H(1)	3.33	56404	C(14)	H(3)	3.38	67403
C(14)	H(2)	3.49	55401	C(15)	H(4)	3.01	67403
C(15)	H(3)	3.21	67403	C(15)	H(5)	3.42	54302
C(15)	H(6)	3.42	54302	C(15)	H(1)	3.43	56404
C(15)	H(7)	3.60	57303	H(1)	H(9)	2.76	46504
H(1)	H(10)	2.97	46504	H(1)	H(8)	3.00	54302
H(1)	H(7)	3.47	54302	H(2)	H(9)	2.92	55601
H(2)	H(8)	3.03	55601	H(2)	H(8)	3.21	54302
H(2)	H(5)	3.23	54402	H(2)	H(7)	3.56	54302
H(3)	H(10)	3.18	56504	H(3)	H(8)	3.32	55601
H(3)	H(9)	3.51	55601	H(4)	H(5)	2.71	67403
H(4)	H(6)	2.72	57504	H(4)	H(10)	2.84	67403
H(4)	H(7)	3.49	57504	H(5)	H(9)	2.81	55302
H(5)	H(6)	3.22	57504	H(5)	H(10)	3.31	55302
H(5)	H(5)	3.33	67403	H(5)	H(7)	3.36	57504
H(5)	H(7)	3.49	54302	H(6)	H(10)	2.55	55302
H(6)	H(8)	3.49	57303				

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