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**Supporting Information for the Communication Entitled**

# Synthesis, Structure, and Reducing Ability of a Stable Organotrihydroaluminate Bearing a Novel Bowl-Type Substituent

Kei Goto,* Junji Kobayashi, and Renji Okazaki*

Department of Chemistry, Graduate School of Science, The University of Tokyo

7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

## X-ray Crystallographic Data for $C_{64}H_{80}AlLiO_4$ (6)

*Experimental*

Data Collection

A colorless prismatic crystal of $C_{64}H_{80}AlLiO_4$ having approximate dimensions of 0.70 x 0.40 x 0.30 mm was mounted in a glass capillary. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Mo-K$\alpha$ 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 $24.50 < 2\theta < 33.94°$ corresponded to amonoclinic cell with dimensions:

a = 11.769(2) $\AA$
b = 21.482(3) $\AA$ $\beta = 102.856(9)°$
c = 23.960(2) $\AA$
V = 5905(1) $\AA^3$

For Z = 4 and F.W. = 947.26, the calculated density is 1.07 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 $\omega$-2$\theta$ scan technique to a maximum 2$\theta$ value of 55.0°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.32° with a take-off angle of 6.0°. Scans of (1.26 + 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 2 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 258 mm, and the detector aperture was 9.0 x 13.0 mm (horizontal x vertical).

Data Reduction

Of the 14586 reflections which were collected, 13925 were unique ($R_{int}$ = 0.057). The intensities of three representative reflection were measured after every 150 reflections. Over the course of data collection, the standards decreased by 14.3%. A linear correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, $\mu$, for Mo-K$\alpha$ radiation is 0.8 cm$^{-1}$. An empirical absorption correction using the program DIFABS[1] was applied which resulted in transmission factors ranging from 0.56 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques[3]. The non-hydrogen atoms were refined anisotropically. Some hydrogen atoms were refined isotropically, the rest were included in fixed positions. The final cycle of full-matrix least-squares refinement[4] was based on 3236 observed reflections ($I > 3.00\sigma(I)$) and 643 variable parameters and converged (largest parameter shift was 0.02 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.061$$

$$R_w = \sqrt{(\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2)} = 0.058$$

The standard deviation of an observation of unit weight[5] was 1.63. The weighting scheme was based on counting statistics and included a factor (p = 0.009) 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 0.07 and -0.05 $e^-/\AA^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6] . Anomalous dispersion effects were included in Fcalc[7]; the values for $\Delta$f' and $\Delta$f" were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[9]. All calculations were performed using the teXsan[10] crystallographic software package of Molecular Structure Corporation.

*References*

(1) DIFABS: Walker, N. & Stuart, Acta Cryst. A39, 158-166 (1983). An empirical absorption correction program.

(2) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G. (1994). J. Appl. Cryst., in preparation.

(3) 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.

(4) 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

(5) 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

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

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

(8) 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).

(9) 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).

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

## *EXPERIMENTAL DETAILS*

### A. Crystal Data

| | |
|---|---|
| Empirical Formula | $C_{64}H_{80}AlLiO_4$ |
| Formula Weight | 947.26 |
| Crystal Color, Habit | colorless, prismatic |
| Crystal Dimensions | 0.70 X 0.40 X 0.30 mm |
| Crystal System | monoclinic |
| Lattice Type | Primitive |
| No. of Reflections Used for Unit Cell Determination ($2\theta$ range) | 25 ( 24.5 - 33.9° ) |
| Omega Scan Peak Width at Half-height | 0.32° |
| Lattice Parameters | a = 11.769(2)Å<br>b = 21.482(3) Å<br>c = 23.960(2) Å<br>$\beta$ = 102.856(9)° |
| | V = 5905(1) Å$^3$ |
| Space Group | $P2_1/n$ (#14) |
| Z value | 4 |
| $D_{calc}$ | 1.065 g/cm$^3$ |
| $F_{000}$ | 2048.00 |
| $\mu$(MoK$\alpha$) | 0.78 cm$^{-1}$ |

### B. Intensity Measurements

| | |
|---|---|
| Diffractometer | Rigaku AFC5R |
| Radiation | MoK$\alpha$ ($\lambda$ = 0.71069 Å)<br>graphite monochromated |

| | |
|---|---|
| Attenuator | Zr foil (factors = 1.00, 3.73, 13.44, 49.14) |
| Take-off Angle | 6.0° |
| Detector Aperture | 9.0 mm horizontal<br>13.0 mm vertical |
| Crystal to Detector Distance | 258 mm |
| Temperature | 23.0°C |
| Scan Type | $\omega$-$2\theta$ |
| Scan Rate | 16.0°/min (in $\omega$) (up to 2 scans) |
| Scan Width | $(1.26 + 0.30 \tan \theta)°$ |
| $2\theta_{max}$ | 55.0° |
| No. of Reflections Measured | Total: 14586<br>Unique: 13925 ($R_{int}$ = 0.057) |
| Corrections | Lorentz-polarization<br>Absorption<br>(trans. factors: 0.5583 - 1.0000)<br>Decay (14.33% decline) |

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 | 0.0090 |
| Anomalous Dispersion | All non-hydrogen atoms |
| No. Observations (I>3.00$\sigma$(I)) | 3236 |
| No. Variables | 643 |
| Reflection/Parameter Ratio | 5.03 |
| Residuals: R; Rw | 0.061 ; 0.058 |
| Goodness of Fit Indicator | 1.63 |

| | |
|---|---|
| Max Shift/Error in Final Cycle | 0.02 |
| Maximum peak in Final Diff. Map | 0.07 $e^-/\AA^3$ |
| Minimum peak in Final Diff. Map | -0.05 $e^-/\AA^3$ |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| Al(1) | 0.4674(2) | -0.0359(1) | 0.84021(9) | 4.47(6) |
| O(1) | 0.4479(6) | -0.1485(4) | 0.9700(3) | 8.6(2) |
| O(2) | 0.5575(6) | -0.2463(4) | 0.9365(3) | 8.5(2) |
| O(3) | 0.4855(7) | -0.2072(4) | 0.8094(3) | 9.6(2) |
| O(4) | 0.3109(6) | -0.2165(3) | 0.8598(3) | 8.1(2) |
| C(1) | 0.5441(5) | -0.0241(3) | 0.7734(2) | 3.0(2) |
| C(2) | 0.6643(5) | -0.0095(3) | 0.7841(3) | 3.0(2) |
| C(3) | 0.7266(5) | -0.0077(3) | 0.7412(3) | 3.4(2) |
| C(4) | 0.6724(5) | -0.0189(3) | 0.6838(3) | 3.4(2) |
| C(5) | 0.5553(6) | -0.0321(3) | 0.6726(3) | 3.6(2) |
| C(6) | 0.4919(5) | -0.0347(3) | 0.7153(3) | 3.1(2) |
| C(7) | 0.7406(6) | -0.0188(4) | 0.6364(3) | 4.7(2) |
| C(8) | 0.857(1) | 0.0089(8) | 0.6536(5) | 16.7(6) |
| C(9) | 0.6740(9) | 0.0089(7) | 0.5827(4) | 13.7(5) |
| C(10) | 0.760(1) | -0.0862(6) | 0.6222(5) | 11.7(4) |
| C(11) | 0.3638(5) | -0.0535(3) | 0.6974(3) | 3.8(2) |
| C(12) | 0.7255(5) | 0.0031(3) | 0.8465(3) | 3.9(2) |
| C(13) | 0.2925(5) | -0.0260(3) | 0.6424(3) | 3.6(2) |
| C(14) | 0.2714(6) | 0.0385(4) | 0.6376(3) | 4.2(2) |
| C(15) | 0.2029(7) | 0.0628(4) | 0.5878(4) | 5.1(2) |
| C(16) | 0.1542(7) | 0.0245(5) | 0.5421(3) | 5.8(2) |
| C(17) | 0.1735(6) | -0.0385(4) | 0.5461(3) | 5.0(2) |
| C(18) | 0.2431(5) | -0.0638(3) | 0.5960(3) | 3.9(2) |
| C(19) | 0.3197(7) | 0.0800(3) | 0.6872(3) | 4.6(2) |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| C(20) | 0.4211(7) | 0.1146(4) | 0.6880(4) | 5.3(2) |
| C(21) | 0.4726(8) | 0.1459(4) | 0.7376(5) | 6.8(3) |
| C(22) | 0.427(1) | 0.1444(5) | 0.7852(5) | 7.9(3) |
| C(23) | 0.3232(10) | 0.1138(5) | 0.7828(4) | 7.1(3) |
| C(24) | 0.2675(7) | 0.0824(4) | 0.7341(4) | 5.6(2) |
| C(25) | 0.2558(6) | -0.1334(3) | 0.5995(3) | 4.0(2) |
| C(26) | 0.1892(7) | -0.1679(4) | 0.6298(3) | 4.8(2) |
| C(27) | 0.2042(9) | -0.2310(5) | 0.6353(4) | 6.7(3) |
| C(28) | 0.284(1) | -0.2604(5) | 0.6121(5) | 7.9(3) |
| C(29) | 0.3504(9) | -0.2291(6) | 0.5812(4) | 7.4(3) |
| C(30) | 0.3356(7) | -0.1639(4) | 0.5742(3) | 5.3(2) |
| C(31) | 0.4743(8) | 0.1183(4) | 0.6364(5) | 8.0(3) |
| C(32) | 0.1542(8) | 0.0496(4) | 0.7324(4) | 7.6(3) |
| C(33) | 0.4043(7) | -0.1306(5) | 0.5378(4) | 7.3(3) |
| C(34) | 0.0996(8) | -0.1368(5) | 0.6559(4) | 7.2(3) |
| C(35) | 0.8559(6) | 0.0125(4) | 0.8600(3) | 3.7(2) |
| C(36) | 0.9022(6) | 0.0726(4) | 0.8632(3) | 4.5(2) |
| C(37) | 1.0217(7) | 0.0813(4) | 0.8722(3) | 5.4(2) |
| C(38) | 1.0969(6) | 0.0322(5) | 0.8797(3) | 5.6(2) |
| C(39) | 1.0535(6) | -0.0270(4) | 0.8799(3) | 5.0(2) |
| C(40) | 0.9338(6) | -0.0379(4) | 0.8709(3) | 3.8(2) |
| C(41) | 0.8304(7) | 0.1305(4) | 0.8632(4) | 5.2(2) |
| C(42) | 0.8016(8) | 0.1486(5) | 0.9147(4) | 6.4(3) |
| C(43) | 0.7408(10) | 0.2035(6) | 0.9156(5) | 8.7(4) |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| C(44) | 0.711(1) | 0.2409(5) | 0.8681(7) | 9.2(4) |
| C(45) | 0.7404(10) | 0.2237(5) | 0.8183(5) | 8.2(3) |
| C(46) | 0.8004(8) | 0.1684(4) | 0.8148(4) | 6.3(3) |
| C(47) | 0.8959(6) | -0.1039(4) | 0.8757(3) | 4.2(2) |
| C(48) | 0.8557(6) | -0.1229(4) | 0.9239(3) | 5.1(2) |
| C(49) | 0.8329(8) | -0.1858(6) | 0.9311(4) | 7.0(3) |
| C(50) | 0.8509(9) | -0.2287(5) | 0.8919(5) | 7.9(3) |
| C(51) | 0.8896(8) | -0.2114(4) | 0.8449(4) | 6.5(3) |
| C(52) | 0.9126(6) | -0.1490(4) | 0.8360(3) | 5.0(2) |
| C(53) | 0.8362(9) | 0.1100(5) | 0.9685(4) | 8.8(3) |
| C(54) | 0.8309(10) | 0.1508(4) | 0.7596(4) | 9.0(3) |
| C(55) | 0.9540(8) | -0.1309(4) | 0.7831(4) | 6.9(3) |
| C(56) | 0.8370(7) | -0.0781(5) | 0.9688(3) | 6.7(3) |
| C(57) | 0.443(1) | -0.0852(7) | 0.9854(5) | 13.3(5) |
| C(58) | 0.530(1) | -0.1834(8) | 1.0114(5) | 10.7(5) |
| C(59) | 0.531(1) | -0.2486(7) | 0.9898(6) | 10.7(5) |
| C(60) | 0.577(1) | -0.3067(7) | 0.9163(6) | 11.5(5) |
| C(61) | 0.567(1) | -0.1887(5) | 0.7791(4) | 9.0(4) |
| C(62) | 0.388(2) | -0.2336(8) | 0.7796(6) | 14.2(6) |
| C(63) | 0.292(1) | -0.2332(8) | 0.8029(7) | 13.1(5) |
| C(64) | 0.220(1) | -0.2150(7) | 0.8852(6) | 13.5(5) |
| Li(1) | 0.468(1) | -0.1726(8) | 0.8874(6) | 6.8(4) |
| H(1) | 0.8072 | 0.0026 | 0.7509 | 3.8803 |
| H(2) | 0.5162 | -0.0392 | 0.6339 | 4.0938 |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| H(3) | 0.9006 | -0.0139 | 0.6866 | 19.4102 |
| H(4) | 0.8974 | 0.0045 | 0.6236 | 19.4102 |
| H(5) | 0.8511 | 0.0503 | 0.6634 | 19.4102 |
| H(6) | 0.6589 | 0.0516 | 0.5892 | 15.5089 |
| H(7) | 0.7156 | 0.0058 | 0.5534 | 15.5089 |
| H(8) | 0.6008 | -0.0122 | 0.5709 | 15.5089 |
| H(9) | 0.6872 | -0.1066 | 0.6099 | 13.3932 |
| H(10) | 0.8016 | -0.0882 | 0.5921 | 13.3932 |
| H(11) | 0.8045 | -0.1069 | 0.6549 | 13.3932 |
| H(12) | 0.3605 | -0.0975 | 0.6929 | 3.9125 |
| H(13) | 0.3272 | -0.0419 | 0.7274 | 3.9125 |
| H(14) | 0.6918 | 0.0393 | 0.8588 | 4.5312 |
| H(15) | 0.7107 | -0.0316 | 0.8689 | 4.5312 |
| H(16) | 0.1876 | 0.1067 | 0.5848 | 6.0704 |
| H(17) | 0.1085 | 0.0418 | 0.5078 | 7.0096 |
| H(18) | 0.1375 | -0.0649 | 0.5156 | 5.8204 |
| H(19) | 0.5433 | 0.1689 | 0.7384 | 8.2674 |
| H(20) | 0.4678 | 0.1637 | 0.8192 | 9.2296 |
| H(21) | 0.2900 | 0.1158 | 0.8155 | 8.5308 |
| H(22) | 0.1572 | -0.2547 | 0.6552 | 8.0719 |
| H(23) | 0.2963 | -0.3035 | 0.6173 | 9.2207 |
| H(24) | 0.4060 | -0.2500 | 0.5649 | 8.9179 |
| H(25) | 0.5514 | 0.1017 | 0.6456 | 9.2849 |
| H(26) | 0.4287 | 0.0943 | 0.6058 | 9.2849 |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| H(27) | 0.4769 | 0.1601 | 0.6242 | 9.2849 |
| H(28) | 0.0971 | 0.0787 | 0.7388 | 8.9020 |
| H(29) | 0.1278 | 0.0304 | 0.6963 | 8.9020 |
| H(30) | 0.1651 | 0.0187 | 0.7617 | 8.9020 |
| H(31) | 0.4858 | -0.1354 | 0.5537 | 8.6200 |
| H(32) | 0.3868 | -0.1466 | 0.5000 | 8.6200 |
| H(33) | 0.3864 | -0.0870 | 0.5364 | 8.6200 |
| H(34) | 0.1004 | -0.0927 | 0.6485 | 8.5423 |
| H(35) | 0.0247 | -0.1525 | 0.6393 | 8.5423 |
| H(36) | 0.1171 | -0.1432 | 0.6960 | 8.5423 |
| H(37) | 1.0530 | 0.1222 | 0.8735 | 6.4657 |
| H(38) | 1.1784 | 0.0386 | 0.8847 | 6.3636 |
| H(39) | 1.1062 | -0.0609 | 0.8862 | 5.8597 |
| H(40) | 0.7193 | 0.2167 | 0.9495 | 10.4345 |
| H(41) | 0.6674 | 0.2777 | 0.8681 | 10.7932 |
| H(42) | 0.7233 | 0.2499 | 0.7851 | 9.7771 |
| H(43) | 0.8056 | -0.1994 | 0.9633 | 7.8413 |
| H(44) | 0.8353 | -0.2715 | 0.8974 | 8.9530 |
| H(45) | 0.9017 | -0.2416 | 0.8180 | 7.6937 |
| H(46) | 0.7683 | 0.0976 | 0.9803 | 10.3715 |
| H(47) | 0.8770 | 0.0741 | 0.9600 | 10.3715 |
| H(48) | 0.8850 | 0.1337 | 0.9972 | 10.3715 |
| H(49) | 0.8702 | 0.1121 | 0.7638 | 10.0693 |
| H(50) | 0.7608 | 0.1473 | 0.7307 | 10.0693 |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| H(51) | 0.8789 | 0.1819 | 0.7489 | 10.0693 |
| H(52) | 1.0260 | -0.1508 | 0.7834 | 8.0206 |
| H(53) | 0.8980 | -0.1427 | 0.7499 | 8.0206 |
| H(54) | 0.9649 | -0.0868 | 0.7828 | 8.0206 |
| H(55) | 0.8865 | -0.0888 | 1.0053 | 8.1186 |
| H(56) | 0.8562 | -0.0369 | 0.9595 | 8.1186 |
| H(57) | 0.7584 | -0.0790 | 0.9726 | 8.1186 |
| H(58) | 0.5180 | -0.0671 | 0.9886 | 15.4321 |
| H(59) | 0.3883 | -0.0646 | 0.9562 | 15.4321 |
| H(60) | 0.4203 | -0.0825 | 1.0206 | 15.4321 |
| H(61) | 0.6063 | -0.1671 | 1.0163 | 12.6074 |
| H(62) | 0.5079 | -0.1848 | 1.0470 | 12.6074 |
| H(63) | 0.4560 | -0.2674 | 0.9860 | 13.0812 |
| H(64) | 0.5873 | -0.2734 | 1.0147 | 13.0812 |
| H(65) | 0.5064 | -0.3309 | 0.9124 | 13.6525 |
| H(66) | 0.5937 | -0.3038 | 0.8789 | 13.6525 |
| H(67) | 0.6380 | -0.3269 | 0.9413 | 13.6525 |
| H(68) | 0.5899 | -0.2243 | 0.7599 | 10.6036 |
| H(69) | 0.5338 | -0.1586 | 0.7513 | 10.6036 |
| H(70) | 0.6335 | -0.1720 | 0.8042 | 10.6036 |
| H(71) | 0.3644 | -0.2091 | 0.7457 | 16.1682 |
| H(72) | 0.4047 | -0.2738 | 0.7714 | 16.1682 |
| H(73) | 0.2662 | -0.2770 | 0.8017 | 14.7161 |
| H(74) | 0.2334 | -0.2094 | 0.7818 | 14.7161 |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| H(75) | 0.2466 | -0.2011 | 0.9239 | 15.7292 |
| H(76) | 0.1623 | -0.1871 | 0.8656 | 15.7292 |
| H(77) | 0.1879 | -0.2554 | 0.8855 | 15.7292 |
| H(78) | 0.540(4) | -0.093(2) | 0.877(2) | 4(1) |
| H(79) | 0.480(5) | 0.022(3) | 0.883(2) | 5(1) |
| H(80) | 0.338(6) | -0.056(3) | 0.824(3) | 7(1) |

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

Table 2. Anisotropic Displacement Parameters

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| Al(1) | 0.054(1) | 0.073(2) | 0.046(1) | -0.007(1) | 0.017(1) | -0.004(1) |
| O(1) | 0.133(6) | 0.139(7) | 0.058(4) | -0.048(5) | 0.025(4) | 0.004(5) |
| O(2) | 0.093(5) | 0.132(7) | 0.089(5) | -0.016(5) | 0.003(4) | 0.032(5) |
| O(3) | 0.119(6) | 0.163(7) | 0.080(5) | -0.024(5) | 0.015(5) | -0.020(5) |
| O(4) | 0.091(5) | 0.120(6) | 0.088(5) | -0.034(4) | -0.001(4) | -0.002(4) |
| C(1) | 0.043(4) | 0.033(4) | 0.037(4) | -0.003(3) | 0.007(3) | 0.002(3) |
| C(2) | 0.038(4) | 0.036(4) | 0.039(4) | -0.002(3) | 0.008(3) | 0.002(3) |
| C(3) | 0.029(4) | 0.045(5) | 0.053(5) | -0.001(3) | 0.008(3) | 0.004(4) |
| C(4) | 0.040(4) | 0.047(5) | 0.044(4) | 0.005(3) | 0.012(3) | 0.008(4) |
| C(5) | 0.050(5) | 0.047(5) | 0.040(4) | 0.000(4) | 0.010(3) | -0.001(3) |
| C(6) | 0.036(4) | 0.037(4) | 0.046(4) | 0.001(3) | 0.013(3) | 0.003(4) |
| C(7) | 0.061(5) | 0.078(6) | 0.048(5) | 0.005(5) | 0.028(4) | 0.001(4) |
| C(8) | 0.137(10) | 0.40(2) | 0.134(10) | -0.16(1) | 0.111(9) | -0.10(1) |
| C(9) | 0.130(9) | 0.31(2) | 0.102(8) | 0.10(1) | 0.084(7) | 0.12(1) |
| C(10) | 0.20(1) | 0.15(1) | 0.126(10) | 0.060(10) | 0.107(9) | 0.006(8) |
| C(11) | 0.040(4) | 0.058(5) | 0.046(4) | -0.001(4) | 0.012(3) | -0.005(4) |
| C(12) | 0.042(4) | 0.059(5) | 0.043(4) | -0.011(4) | 0.003(3) | -0.005(4) |
| C(13) | 0.039(4) | 0.049(5) | 0.048(4) | -0.002(4) | 0.010(3) | -0.001(4) |
| C(14) | 0.046(4) | 0.065(6) | 0.049(5) | 0.002(4) | 0.012(4) | 0.004(4) |
| C(15) | 0.063(5) | 0.054(5) | 0.073(6) | 0.010(4) | 0.008(5) | 0.010(5) |
| C(16) | 0.061(5) | 0.090(7) | 0.064(6) | 0.018(5) | 0.000(4) | 0.021(5) |
| C(17) | 0.061(5) | 0.073(6) | 0.053(5) | 0.007(5) | 0.004(4) | 0.006(5) |
| C(18) | 0.038(4) | 0.060(5) | 0.052(5) | 0.005(4) | 0.010(4) | 0.006(4) |
| C(19) | 0.057(5) | 0.046(5) | 0.072(6) | 0.011(4) | 0.014(4) | -0.004(4) |

Table 2. Anisotropic Displacement Parameters (continued)

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| C(20) | 0.058(6) | 0.043(5) | 0.096(7) | 0.005(4) | 0.006(5) | -0.004(5) |
| C(21) | 0.079(7) | 0.046(6) | 0.119(9) | -0.008(5) | -0.009(6) | -0.011(6) |
| C(22) | 0.120(10) | 0.066(7) | 0.101(9) | 0.006(7) | -0.004(7) | -0.023(6) |
| C(23) | 0.110(8) | 0.073(7) | 0.085(8) | 0.017(6) | 0.018(7) | -0.013(6) |
| C(24) | 0.068(6) | 0.064(6) | 0.082(7) | 0.002(5) | 0.019(5) | -0.016(5) |
| C(25) | 0.053(5) | 0.057(5) | 0.037(4) | -0.003(4) | 0.001(4) | -0.007(4) |
| C(26) | 0.064(6) | 0.057(6) | 0.054(5) | -0.015(5) | -0.006(4) | 0.002(4) |
| C(27) | 0.094(8) | 0.075(8) | 0.075(7) | -0.022(6) | -0.004(6) | 0.010(6) |
| C(28) | 0.106(9) | 0.065(7) | 0.112(9) | 0.018(7) | -0.015(7) | 0.001(7) |
| C(29) | 0.086(7) | 0.088(9) | 0.097(8) | 0.025(6) | 0.000(6) | -0.036(6) |
| C(30) | 0.067(6) | 0.079(7) | 0.050(5) | 0.001(5) | 0.000(4) | -0.022(5) |
| C(31) | 0.084(7) | 0.071(7) | 0.16(1) | -0.011(5) | 0.055(7) | 0.006(6) |
| C(32) | 0.088(7) | 0.106(8) | 0.106(7) | 0.013(6) | 0.048(6) | -0.020(6) |
| C(33) | 0.082(6) | 0.121(9) | 0.083(7) | 0.004(6) | 0.032(5) | -0.041(6) |
| C(34) | 0.078(6) | 0.118(8) | 0.086(7) | -0.026(6) | 0.033(5) | -0.001(6) |
| C(35) | 0.048(5) | 0.056(5) | 0.034(4) | -0.010(4) | 0.003(3) | -0.003(4) |
| C(36) | 0.049(5) | 0.069(6) | 0.053(5) | -0.004(5) | 0.012(4) | -0.008(4) |
| C(37) | 0.059(6) | 0.071(6) | 0.076(6) | -0.020(5) | 0.017(5) | -0.008(5) |
| C(38) | 0.038(5) | 0.105(8) | 0.069(6) | -0.020(5) | 0.008(4) | -0.011(6) |
| C(39) | 0.039(5) | 0.091(7) | 0.060(5) | 0.005(5) | 0.007(4) | -0.002(5) |
| C(40) | 0.042(4) | 0.063(5) | 0.033(4) | 0.001(4) | -0.004(3) | -0.001(4) |
| C(41) | 0.059(5) | 0.060(6) | 0.074(6) | -0.016(5) | 0.004(5) | -0.005(5) |
| C(42) | 0.080(7) | 0.074(7) | 0.093(8) | 0.003(5) | 0.023(6) | -0.017(6) |
| C(43) | 0.109(9) | 0.094(9) | 0.13(1) | 0.003(7) | 0.033(8) | -0.035(8) |

Table 2. Anisotropic Displacement Parameters (continued)

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| C(44) | 0.113(9) | 0.064(8) | 0.17(1) | 0.013(6) | 0.028(9) | -0.021(9) |
| C(45) | 0.115(9) | 0.061(7) | 0.12(1) | -0.013(7) | 0.000(7) | -0.003(7) |
| C(46) | 0.083(7) | 0.050(6) | 0.103(8) | -0.015(5) | 0.014(6) | -0.007(6) |
| C(47) | 0.049(5) | 0.062(6) | 0.043(5) | 0.005(4) | 0.000(4) | 0.002(4) |
| C(48) | 0.051(5) | 0.084(7) | 0.055(5) | -0.001(5) | 0.006(4) | 0.008(5) |
| C(49) | 0.075(6) | 0.105(9) | 0.082(8) | 0.009(6) | 0.010(5) | 0.042(6) |
| C(50) | 0.096(8) | 0.075(8) | 0.13(1) | -0.008(6) | 0.024(7) | 0.012(7) |
| C(51) | 0.083(7) | 0.057(7) | 0.105(8) | 0.007(5) | 0.018(6) | 0.001(6) |
| C(52) | 0.062(5) | 0.074(7) | 0.052(5) | 0.013(5) | 0.004(4) | 0.009(5) |
| C(53) | 0.136(9) | 0.128(10) | 0.079(7) | 0.019(7) | 0.037(7) | -0.020(7) |
| C(54) | 0.18(1) | 0.068(7) | 0.090(8) | -0.006(7) | 0.027(8) | 0.017(6) |
| C(55) | 0.112(7) | 0.087(7) | 0.063(6) | 0.021(6) | 0.019(5) | -0.005(5) |
| C(56) | 0.087(6) | 0.119(8) | 0.053(5) | 0.002(6) | 0.022(5) | 0.017(6) |
| C(57) | 0.25(2) | 0.17(1) | 0.11(1) | -0.09(1) | 0.10(1) | -0.056(10) |
| C(58) | 0.13(1) | 0.21(2) | 0.055(8) | -0.04(1) | -0.001(7) | 0.024(9) |
| C(59) | 0.115(10) | 0.20(2) | 0.082(10) | -0.03(1) | 0.001(7) | 0.052(10) |
| C(60) | 0.14(1) | 0.13(1) | 0.16(1) | -0.004(9) | 0.021(9) | 0.03(1) |
| C(61) | 0.16(1) | 0.081(8) | 0.113(9) | 0.039(7) | 0.067(8) | 0.019(6) |
| C(62) | 0.17(2) | 0.24(2) | 0.12(1) | -0.07(1) | 0.00(1) | -0.07(1) |
| C(63) | 0.11(1) | 0.22(2) | 0.14(1) | -0.02(1) | -0.030(9) | -0.08(1) |
| C(64) | 0.074(8) | 0.22(2) | 0.22(2) | -0.014(9) | 0.025(9) | -0.07(1) |
| Li(1) | 0.08(1) | 0.11(1) | 0.055(9) | -0.030(9) | 0.001(8) | 0.004(9) |

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(Å)

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| Al(1) | C(1) | 2.021(6) | Al(1) | H(78) | 1.64(5) |
| Al(1) | H(79) | 1.60(6) | Al(1) | H(80) | 1.55(7) |
| O(1) | C(57) | 1.41(1) | O(1) | C(58) | 1.44(1) |
| O(1) | Li(1) | 2.11(2) | O(2) | C(59) | 1.38(1) |
| O(2) | C(60) | 1.42(1) | O(2) | Li(1) | 2.11(2) |
| O(3) | C(61) | 1.38(1) | O(3) | C(62) | 1.33(1) |
| O(3) | Li(1) | 2.07(2) | O(4) | C(63) | 1.38(1) |
| O(4) | C(64) | 1.35(1) | O(4) | Li(1) | 2.05(1) |
| C(1) | C(2) | 1.414(8) | C(1) | C(6) | 1.409(8) |
| C(2) | C(3) | 1.391(8) | C(2) | C(12) | 1.533(8) |
| C(3) | C(4) | 1.402(8) | C(3) | H(1) | 0.95 |
| C(4) | C(5) | 1.374(8) | C(4) | C(7) | 1.528(8) |
| C(5) | C(6) | 1.396(8) | C(5) | H(2) | 0.95 |
| C(6) | C(11) | 1.528(8) | C(7) | C(8) | 1.46(1) |
| C(7) | C(9) | 1.48(1) | C(7) | C(10) | 1.52(1) |
| C(8) | H(3) | 0.97 | C(8) | H(4) | 0.95 |
| C(8) | H(5) | 0.93 | C(9) | H(6) | 0.95 |
| C(9) | H(7) | 0.94 | C(9) | H(8) | 0.96 |
| C(10) | H(9) | 0.95 | C(10) | H(10) | 0.96 |
| C(10) | H(11) | 0.95 | C(11) | C(13) | 1.515(9) |
| C(11) | H(12) | 0.95 | C(11) | H(13) | 0.95 |
| C(12) | C(35) | 1.509(8) | C(12) | H(14) | 0.95 |
| C(12) | H(15) | 0.96 | C(13) | C(14) | 1.409(9) |
| C(13) | C(18) | 1.396(9) | C(14) | C(15) | 1.387(9) |

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

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| C(14) | C(19) | 1.491(10) | C(15) | C(16) | 1.39(1) |
| C(15) | H(16) | 0.96 | C(16) | C(17) | 1.37(1) |
| C(16) | H(17) | 0.95 | C(17) | C(18) | 1.399(9) |
| C(17) | H(18) | 0.95 | C(18) | C(25) | 1.503(9) |
| C(19) | C(20) | 1.403(10) | C(19) | C(24) | 1.396(10) |
| C(20) | C(21) | 1.38(1) | C(20) | C(31) | 1.51(1) |
| C(21) | C(22) | 1.36(1) | C(21) | H(19) | 0.96 |
| C(22) | C(23) | 1.38(1) | C(22) | H(20) | 0.95 |
| C(23) | C(24) | 1.38(1) | C(23) | H(21) | 0.95 |
| C(24) | C(32) | 1.50(1) | C(25) | C(26) | 1.394(9) |
| C(25) | C(30) | 1.390(10) | C(26) | C(27) | 1.37(1) |
| C(26) | C(34) | 1.50(1) | C(27) | C(28) | 1.35(1) |
| C(27) | H(22) | 0.95 | C(28) | C(29) | 1.36(1) |
| C(28) | H(23) | 0.94 | C(29) | C(30) | 1.42(1) |
| C(29) | H(24) | 0.95 | C(30) | C(33) | 1.50(1) |
| C(31) | H(25) | 0.95 | C(31) | H(26) | 0.96 |
| C(31) | H(27) | 0.95 | C(32) | H(28) | 0.95 |
| C(32) | H(29) | 0.95 | C(32) | H(30) | 0.95 |
| C(33) | H(31) | 0.96 | C(33) | H(32) | 0.95 |
| C(33) | H(33) | 0.96 | C(34) | H(34) | 0.96 |
| C(34) | H(35) | 0.95 | C(34) | H(36) | 0.95 |
| C(35) | C(36) | 1.397(9) | C(35) | C(40) | 1.406(9) |
| C(36) | C(37) | 1.387(10) | C(36) | C(41) | 1.50(1) |
| C(37) | C(38) | 1.36(1) | C(37) | H(37) | 0.95 |

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

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| C(38) | C(39) | 1.37(1) | C(38) | H(38) | 0.95 |
| C(39) | C(40) | 1.396(9) | C(39) | H(39) | 0.95 |
| C(40) | C(47) | 1.498(9) | C(41) | C(42) | 1.41(1) |
| C(41) | C(46) | 1.40(1) | C(42) | C(43) | 1.38(1) |
| C(42) | C(53) | 1.51(1) | C(43) | C(44) | 1.37(1) |
| C(43) | H(40) | 0.95 | C(44) | C(45) | 1.37(1) |
| C(44) | H(41) | 0.94 | C(45) | C(46) | 1.39(1) |
| C(45) | H(42) | 0.96 | C(46) | C(54) | 1.49(1) |
| C(47) | C(48) | 1.403(10) | C(47) | C(52) | 1.403(10) |
| C(48) | C(49) | 1.40(1) | C(48) | C(56) | 1.50(1) |
| C(49) | C(50) | 1.36(1) | C(49) | H(43) | 0.95 |
| C(50) | C(51) | 1.36(1) | C(50) | H(44) | 0.95 |
| C(51) | C(52) | 1.39(1) | C(51) | H(45) | 0.95 |
| C(52) | C(55) | 1.51(1) | C(53) | H(46) | 0.94 |
| C(53) | H(47) | 0.95 | C(53) | H(48) | 0.94 |
| C(54) | H(49) | 0.95 | C(54) | H(50) | 0.96 |
| C(54) | H(51) | 0.95 | C(55) | H(52) | 0.95 |
| C(55) | H(53) | 0.95 | C(55) | H(54) | 0.96 |
| C(56) | H(55) | 0.97 | C(56) | H(56) | 0.95 |
| C(56) | H(57) | 0.95 | C(57) | H(58) | 0.95 |
| C(57) | H(59) | 0.95 | C(57) | H(60) | 0.94 |
| C(58) | C(59) | 1.49(2) | C(58) | H(61) | 0.94 |
| C(58) | H(62) | 0.95 | C(59) | H(63) | 0.95 |
| C(59) | H(64) | 0.95 | C(60) | H(65) | 0.97 |

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

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| C(60) | H(66) | 0.96 | C(60) | H(67) | 0.93 |
| C(61) | H(68) | 0.96 | C(61) | H(69) | 0.95 |
| C(61) | H(70) | 0.94 | C(62) | C(63) | 1.37(2) |
| C(62) | H(71) | 0.96 | C(62) | H(72) | 0.91 |
| C(63) | H(73) | 0.99 | C(63) | H(74) | 0.92 |
| C(64) | H(75) | 0.96 | C(64) | H(76) | 0.95 |
| C(64) | H(77) | 0.95 | | | |

Table 4. Bond Angles(°)

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| C(1) | Al(1) | H(78) | 104(1) | C(1) | Al(1) | H(79) | 114(2) |
| C(1) | Al(1) | H(80) | 114(2) | H(78) | Al(1) | H(79) | 106(2) |
| H(78) | Al(1) | H(80) | 106(3) | H(79) | Al(1) | H(80) | 109(3) |
| C(57) | O(1) | C(58) | 112.6(10) | C(57) | O(1) | Li(1) | 120.1(8) |
| C(58) | O(1) | Li(1) | 108.8(8) | C(59) | O(2) | C(60) | 111(1) |
| C(59) | O(2) | Li(1) | 110.6(9) | C(60) | O(2) | Li(1) | 126.5(8) |
| C(61) | O(3) | C(62) | 117(1) | C(61) | O(3) | Li(1) | 126.4(8) |
| C(62) | O(3) | Li(1) | 112.9(9) | C(63) | O(4) | C(64) | 119.1(10) |
| C(63) | O(4) | Li(1) | 111.9(8) | C(64) | O(4) | Li(1) | 126.4(9) |
| Al(1) | C(1) | C(2) | 119.3(4) | Al(1) | C(1) | C(6) | 126.0(5) |
| C(2) | C(1) | C(6) | 114.4(5) | C(1) | C(2) | C(3) | 122.9(6) |
| C(1) | C(2) | C(12) | 116.8(5) | C(3) | C(2) | C(12) | 120.3(6) |
| C(2) | C(3) | C(4) | 121.4(6) | C(2) | C(3) | H(1) | 119.2 |
| C(4) | C(3) | H(1) | 119.4 | C(3) | C(4) | C(5) | 116.4(6) |
| C(3) | C(4) | C(7) | 121.9(6) | C(5) | C(4) | C(7) | 121.7(6) |
| C(4) | C(5) | C(6) | 122.7(6) | C(4) | C(5) | H(2) | 118.1 |
| C(6) | C(5) | H(2) | 119.2 | C(1) | C(6) | C(5) | 122.1(6) |
| C(1) | C(6) | C(11) | 120.4(5) | C(5) | C(6) | C(11) | 117.4(6) |
| C(4) | C(7) | C(8) | 113.8(7) | C(4) | C(7) | C(9) | 112.6(7) |
| C(4) | C(7) | C(10) | 107.2(7) | C(8) | C(7) | C(9) | 111.3(9) |
| C(8) | C(7) | C(10) | 105.8(10) | C(9) | C(7) | C(10) | 105.4(9) |
| C(7) | C(8) | H(3) | 108.5 | C(7) | C(8) | H(4) | 109.9 |
| C(7) | C(8) | H(5) | 110.3 | H(3) | C(8) | H(4) | 107.3 |
| H(3) | C(8) | H(5) | 109.5 | H(4) | C(8) | H(5) | 111.3 |

Table 4. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| C(7) | C(9) | H(6) | 109.0 | C(7) | C(9) | H(7) | 111.0 |
| C(7) | C(9) | H(8) | 109.5 | H(6) | C(9) | H(7) | 109.6 |
| H(6) | C(9) | H(8) | 108.4 | H(7) | C(9) | H(8) | 109.3 |
| C(7) | C(10) | H(9) | 109.8 | C(7) | C(10) | H(10) | 109.8 |
| C(7) | C(10) | H(11) | 110.2 | H(9) | C(10) | H(10) | 108.7 |
| H(9) | C(10) | H(11) | 109.5 | H(10) | C(10) | H(11) | 108.8 |
| C(6) | C(11) | C(13) | 117.5(5) | C(6) | C(11) | H(12) | 107.9 |
| C(6) | C(11) | H(13) | 107.7 | C(13) | C(11) | H(12) | 106.7 |
| C(13) | C(11) | H(13) | 107.5 | H(12) | C(11) | H(13) | 109.4 |
| C(2) | C(12) | C(35) | 117.9(5) | C(2) | C(12) | H(14) | 108.0 |
| C(2) | C(12) | H(15) | 107.7 | C(35) | C(12) | H(14) | 107.4 |
| C(35) | C(12) | H(15) | 106.7 | H(14) | C(12) | H(15) | 108.9 |
| C(11) | C(13) | C(14) | 120.4(6) | C(11) | C(13) | C(18) | 121.3(6) |
| C(14) | C(13) | C(18) | 118.2(6) | C(13) | C(14) | C(15) | 119.9(7) |
| C(13) | C(14) | C(19) | 119.6(6) | C(15) | C(14) | C(19) | 120.4(7) |
| C(14) | C(15) | C(16) | 121.0(7) | C(14) | C(15) | H(16) | 119.8 |
| C(16) | C(15) | H(16) | 119.2 | C(15) | C(16) | C(17) | 119.8(7) |
| C(15) | C(16) | H(17) | 120.2 | C(17) | C(16) | H(17) | 119.9 |
| C(16) | C(17) | C(18) | 120.0(7) | C(16) | C(17) | H(18) | 119.8 |
| C(18) | C(17) | H(18) | 120.1 | C(13) | C(18) | C(17) | 121.0(7) |
| C(13) | C(18) | C(25) | 121.0(6) | C(17) | C(18) | C(25) | 117.8(7) |
| C(14) | C(19) | C(20) | 120.0(7) | C(14) | C(19) | C(24) | 120.3(7) |
| C(20) | C(19) | C(24) | 119.6(8) | C(19) | C(20) | C(21) | 118.6(9) |
| C(19) | C(20) | C(31) | 121.5(8) | C(21) | C(20) | C(31) | 119.9(9) |

Table 4. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| C(20) | C(21) | C(22) | 122.0(9) | C(20) | C(21) | H(19) | 118.5 |
| C(22) | C(21) | H(19) | 119.5 | C(21) | C(22) | C(23) | 119.1(10) |
| C(21) | C(22) | H(20) | 119.7 | C(23) | C(22) | H(20) | 121.2 |
| C(22) | C(23) | C(24) | 121.2(9) | C(22) | C(23) | H(21) | 117.8 |
| C(24) | C(23) | H(21) | 120.9 | C(19) | C(24) | C(23) | 119.2(8) |
| C(19) | C(24) | C(32) | 120.6(8) | C(23) | C(24) | C(32) | 120.2(9) |
| C(18) | C(25) | C(26) | 119.9(7) | C(18) | C(25) | C(30) | 120.8(7) |
| C(26) | C(25) | C(30) | 119.4(7) | C(25) | C(26) | C(27) | 120.0(8) |
| C(25) | C(26) | C(34) | 120.6(8) | C(27) | C(26) | C(34) | 119.3(9) |
| C(26) | C(27) | C(28) | 120.6(9) | C(26) | C(27) | H(22) | 120.0 |
| C(28) | C(27) | H(22) | 119.4 | C(27) | C(28) | C(29) | 121.8(10) |
| C(27) | C(28) | H(23) | 120.2 | C(29) | C(28) | H(23) | 118.1 |
| C(28) | C(29) | C(30) | 118.8(9) | C(28) | C(29) | H(24) | 121.4 |
| C(30) | C(29) | H(24) | 119.8 | C(25) | C(30) | C(29) | 119.4(8) |
| C(25) | C(30) | C(33) | 122.3(8) | C(29) | C(30) | C(33) | 118.2(9) |
| C(20) | C(31) | H(25) | 109.8 | C(20) | C(31) | H(26) | 109.6 |
| C(20) | C(31) | H(27) | 110.4 | H(25) | C(31) | H(26) | 108.6 |
| H(25) | C(31) | H(27) | 109.4 | H(26) | C(31) | H(27) | 109.1 |
| C(24) | C(32) | H(28) | 110.0 | C(24) | C(32) | H(29) | 109.7 |
| C(24) | C(32) | H(30) | 109.5 | H(28) | C(32) | H(29) | 109.4 |
| H(28) | C(32) | H(30) | 108.8 | H(29) | C(32) | H(30) | 109.4 |
| C(30) | C(33) | H(31) | 109.9 | C(30) | C(33) | H(32) | 110.6 |
| C(30) | C(33) | H(33) | 110.1 | H(31) | C(33) | H(32) | 109.1 |
| H(31) | C(33) | H(33) | 108.3 | H(32) | C(33) | H(33) | 108.8 |

Table 4. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| C(26) | C(34) | H(34) | 109.0 | C(26) | C(34) | H(35) | 110.0 |
| C(26) | C(34) | H(36) | 110.2 | H(34) | C(34) | H(35) | 108.7 |
| H(34) | C(34) | H(36) | 108.7 | H(35) | C(34) | H(36) | 110.2 |
| C(12) | C(35) | C(36) | 120.1(6) | C(12) | C(35) | C(40) | 121.8(6) |
| C(36) | C(35) | C(40) | 118.1(6) | C(35) | C(36) | C(37) | 120.2(7) |
| C(35) | C(36) | C(41) | 123.5(7) | C(37) | C(36) | C(41) | 116.0(7) |
| C(36) | C(37) | C(38) | 121.5(7) | C(36) | C(37) | H(37) | 120.1 |
| C(38) | C(37) | H(37) | 118.4 | C(37) | C(38) | C(39) | 119.1(7) |
| C(37) | C(38) | H(38) | 120.9 | C(39) | C(38) | H(38) | 120.0 |
| C(38) | C(39) | C(40) | 121.3(7) | C(38) | C(39) | H(39) | 118.9 |
| C(40) | C(39) | H(39) | 119.9 | C(35) | C(40) | C(39) | 119.6(7) |
| C(35) | C(40) | C(47) | 123.3(6) | C(39) | C(40) | C(47) | 117.0(7) |
| C(36) | C(41) | C(42) | 118.2(8) | C(36) | C(41) | C(46) | 121.4(8) |
| C(42) | C(41) | C(46) | 120.2(9) | C(41) | C(42) | C(43) | 118.4(10) |
| C(41) | C(42) | C(53) | 121.7(9) | C(43) | C(42) | C(53) | 119.8(10) |
| C(42) | C(43) | C(44) | 121(1) | C(42) | C(43) | H(40) | 120.4 |
| C(44) | C(43) | H(40) | 118.0 | C(43) | C(44) | C(45) | 119(1) |
| C(43) | C(44) | H(41) | 121.9 | C(45) | C(44) | H(41) | 118.2 |
| C(44) | C(45) | C(46) | 121(1) | C(44) | C(45) | H(42) | 121.3 |
| C(46) | C(45) | H(42) | 117.6 | C(41) | C(46) | C(45) | 118.9(10) |
| C(41) | C(46) | C(54) | 121.4(9) | C(45) | C(46) | C(54) | 119(1) |
| C(40) | C(47) | C(48) | 120.0(7) | C(40) | C(47) | C(52) | 120.8(7) |
| C(48) | C(47) | C(52) | 118.7(7) | C(47) | C(48) | C(49) | 119.6(8) |
| C(47) | C(48) | C(56) | 122.4(8) | C(49) | C(48) | C(56) | 118.1(8) |

Table 4. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| C(48) | C(49) | C(50) | 120.3(9) | C(48) | C(49) | H(43) | 120.6 |
| C(50) | C(49) | H(43) | 119.1 | C(49) | C(50) | C(51) | 121.2(10) |
| C(49) | C(50) | H(44) | 119.6 | C(51) | C(50) | H(44) | 119.2 |
| C(50) | C(51) | C(52) | 120.2(9) | C(50) | C(51) | H(45) | 120.5 |
| C(52) | C(51) | H(45) | 119.3 | C(47) | C(52) | C(51) | 119.9(8) |
| C(47) | C(52) | C(55) | 120.8(8) | C(51) | C(52) | C(55) | 119.3(8) |
| C(42) | C(53) | H(46) | 109.0 | C(42) | C(53) | H(47) | 108.3 |
| C(42) | C(53) | H(48) | 109.3 | H(46) | C(53) | H(47) | 109.8 |
| H(46) | C(53) | H(48) | 110.7 | H(47) | C(53) | H(48) | 109.8 |
| C(46) | C(54) | H(49) | 109.8 | C(46) | C(54) | H(50) | 108.9 |
| C(46) | C(54) | H(51) | 109.7 | H(49) | C(54) | H(50) | 109.3 |
| H(49) | C(54) | H(51) | 110.0 | H(50) | C(54) | H(51) | 109.2 |
| C(52) | C(55) | H(52) | 109.3 | C(52) | C(55) | H(53) | 110.0 |
| C(52) | C(55) | H(54) | 109.4 | H(52) | C(55) | H(53) | 109.9 |
| H(52) | C(55) | H(54) | 109.1 | H(53) | C(55) | H(54) | 109.2 |
| C(48) | C(56) | H(55) | 110.1 | C(48) | C(56) | H(56) | 110.4 |
| C(48) | C(56) | H(57) | 111.0 | H(55) | C(56) | H(56) | 107.9 |
| H(55) | C(56) | H(57) | 108.2 | H(56) | C(56) | H(57) | 109.2 |
| O(1) | C(57) | H(58) | 108.9 | O(1) | C(57) | H(59) | 108.5 |
| O(1) | C(57) | H(60) | 109.3 | H(58) | C(57) | H(59) | 109.5 |
| H(58) | C(57) | H(60) | 110.0 | H(59) | C(57) | H(60) | 110.5 |
| O(1) | C(58) | C(59) | 107.7(10) | O(1) | C(58) | H(61) | 111.6 |
| O(1) | C(58) | H(62) | 110.9 | C(59) | C(58) | H(61) | 108.5 |
| C(59) | C(58) | H(62) | 107.6 | H(61) | C(58) | H(62) | 110.3 |

Table 4. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| O(2) | C(59) | C(58) | 107(1) | O(2) | C(59) | H(63) | 108.7 |
| O(2) | C(59) | H(64) | 109.0 | C(58) | C(59) | H(63) | 111.1 |
| C(58) | C(59) | H(64) | 111.3 | H(63) | C(59) | H(64) | 109.0 |
| O(2) | C(60) | H(65) | 109.0 | O(2) | C(60) | H(66) | 109.9 |
| O(2) | C(60) | H(67) | 111.4 | H(65) | C(60) | H(66) | 107.1 |
| H(65) | C(60) | H(67) | 109.5 | H(66) | C(60) | H(67) | 109.8 |
| O(3) | C(61) | H(68) | 108.8 | O(3) | C(61) | H(69) | 109.7 |
| O(3) | C(61) | H(70) | 110.3 | H(68) | C(61) | H(69) | 108.8 |
| H(68) | C(61) | H(70) | 109.1 | H(69) | C(61) | H(70) | 110.2 |
| O(3) | C(62) | C(63) | 117(1) | O(3) | C(62) | H(71) | 105.9 |
| O(3) | C(62) | H(72) | 108.6 | C(63) | C(62) | H(71) | 103.3 |
| C(63) | C(62) | H(72) | 109.2 | H(71) | C(62) | H(72) | 111.8 |
| O(4) | C(63) | C(62) | 116(1) | O(4) | C(63) | H(73) | 104.7 |
| O(4) | C(63) | H(74) | 109.5 | C(62) | C(63) | H(73) | 105.2 |
| C(62) | C(63) | H(74) | 111.8 | H(73) | C(63) | H(74) | 108.9 |
| O(4) | C(64) | H(75) | 108.6 | O(4) | C(64) | H(76) | 110.1 |
| O(4) | C(64) | H(77) | 109.6 | H(75) | C(64) | H(76) | 109.2 |
| H(75) | C(64) | H(77) | 109.1 | H(76) | C(64) | H(77) | 110.2 |
| O(1) | Li(1) | O(2) | 78.9(6) | O(1) | Li(1) | O(3) | 173.2(9) |
| O(1) | Li(1) | O(4) | 98.0(7) | O(2) | Li(1) | O(3) | 95.4(8) |
| O(2) | Li(1) | O(4) | 98.0(7) | O(3) | Li(1) | O(4) | 78.9(6) |

Table 5. Torsion Angles(°)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|---|---|
| Al(1) | C(1) | C(2) | C(3) | 172.4(5) | Al(1) | C(1) | C(2) | C(12) | -6.3(7) |
| Al(1) | C(1) | C(6) | C(5) | -172.6(5) | Al(1) | C(1) | C(6) | C(11) | 3.7(9) |
| O(1) | C(58) | C(59) | O(2) | 57(1) | O(1) | Li(1) | O(2) | C(59) | 15.3(8) |
| O(1) | Li(1) | O(2) | C(60) | 155.5(9) | O(1) | Li(1) | O(3) | C(61) | -133(6) |
| O(1) | Li(1) | O(3) | C(62) | 68(7) | O(1) | Li(1) | O(4) | C(63) | 174.1(9) |
| O(1) | Li(1) | O(4) | C(64) | 12(1) | O(2) | Li(1) | O(1) | C(57) | 147.7(9) |
| O(2) | Li(1) | O(1) | C(58) | 16.0(8) | O(2) | Li(1) | O(3) | C(61) | -99.4(9) |
| O(2) | Li(1) | O(3) | C(62) | 102(1) | O(2) | Li(1) | O(4) | C(63) | -106.0(10) |
| O(2) | Li(1) | O(4) | C(64) | 92(1) | O(3) | C(62) | C(63) | O(4) | -12(2) |
| O(3) | Li(1) | O(1) | C(57) | -177(6) | O(3) | Li(1) | O(1) | C(58) | 50(7) |
| O(3) | Li(1) | O(2) | C(59) | -160.8(8) | O(3) | Li(1) | O(2) | C(60) | -20(1) |
| O(3) | Li(1) | O(4) | C(63) | -12(1) | O(3) | Li(1) | O(4) | C(64) | -173(1) |
| O(4) | Li(1) | O(1) | C(57) | -115(1) | O(4) | Li(1) | O(1) | C(58) | 112.6(9) |
| O(4) | Li(1) | O(2) | C(59) | -81.3(9) | O(4) | Li(1) | O(2) | C(60) | 58(1) |
| O(4) | Li(1) | O(3) | C(61) | 163.5(9) | O(4) | Li(1) | O(3) | C(62) | 5(1) |
| C(1) | C(2) | C(3) | C(4) | 1(1) | C(1) | C(2) | C(12) | C(35) | 174.1(6) |
| C(1) | C(6) | C(5) | C(4) | 0(1) | C(1) | C(6) | C(11) | C(13) | 141.4(6) |
| C(2) | C(1) | C(6) | C(5) | 1.2(9) | C(2) | C(1) | C(6) | C(11) | 177.5(6) |
| C(2) | C(3) | C(4) | C(5) | -0.4(10) | C(2) | C(3) | C(4) | C(7) | -178.3(7) |
| C(2) | C(12) | C(35) | C(36) | 95.7(8) | C(2) | C(12) | C(35) | C(40) | -85.8(8) |
| C(3) | C(2) | C(1) | C(6) | -1.9(9) | C(3) | C(2) | C(12) | C(35) | -4.6(9) |
| C(3) | C(4) | C(5) | C(6) | 0(1) | C(3) | C(4) | C(7) | C(8) | -14(1) |
| C(3) | C(4) | C(7) | C(9) | -142.5(9) | C(3) | C(4) | C(7) | C(10) | 102.0(9) |
| C(4) | C(3) | C(2) | C(12) | -179.8(6) | C(4) | C(5) | C(6) | C(11) | -176.6(6) |

Table 5. Torsion Angles(°) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|---|---|
| C(5) | C(4) | C(7) | C(8) | 167.6(10) | C(5) | C(4) | C(7) | C(9) | 39(1) |
| C(5) | C(4) | C(7) | C(10) | -75.7(10) | C(5) | C(6) | C(11) | C(13) | -42.2(9) |
| C(6) | C(1) | C(2) | C(12) | 179.5(6) | C(6) | C(5) | C(4) | C(7) | 177.7(7) |
| C(6) | C(11) | C(13) | C(14) | -64.8(8) | C(6) | C(11) | C(13) | C(18) | 117.3(7) |
| C(11) | C(13) | C(14) | C(15) | -177.9(6) | C(11) | C(13) | C(14) | C(19) | 0.0(10) |
| C(11) | C(13) | C(18) | C(17) | 177.4(6) | C(11) | C(13) | C(18) | C(25) | 1.9(10) |
| C(12) | C(35) | C(36) | C(37) | -176.1(6) | C(12) | C(35) | C(36) | C(41) | 9(1) |
| C(12) | C(35) | C(40) | C(39) | 176.4(6) | C(12) | C(35) | C(40) | C(47) | -6(1) |
| C(13) | C(14) | C(15) | C(16) | 0(1) | C(13) | C(14) | C(19) | C(20) | 100.7(8) |
| C(13) | C(14) | C(19) | C(24) | -76.3(9) | C(13) | C(18) | C(17) | C(16) | 0(1) |
| C(13) | C(18) | C(25) | C(26) | 76.0(9) | C(13) | C(18) | C(25) | C(30) | -102.2(8) |
| C(14) | C(13) | C(18) | C(17) | -0.6(10) | C(14) | C(13) | C(18) | C(25) | -176.1(6) |
| C(14) | C(15) | C(16) | C(17) | 0(1) | C(14) | C(19) | C(20) | C(21) | -171.2(7) |
| C(14) | C(19) | C(20) | C(31) | 8(1) | C(14) | C(19) | C(24) | C(23) | 170.5(7) |
| C(14) | C(19) | C(24) | C(32) | -7(1) | C(15) | C(14) | C(13) | C(18) | 0(1) |
| C(15) | C(14) | C(19) | C(20) | -81.5(9) | C(15) | C(14) | C(19) | C(24) | 101.6(9) |
| C(15) | C(16) | C(17) | C(18) | 0(1) | C(16) | C(15) | C(14) | C(19) | -177.8(7) |
| C(16) | C(17) | C(18) | C(25) | 176.5(7) | C(17) | C(18) | C(25) | C(26) | -99.7(8) |
| C(17) | C(18) | C(25) | C(30) | 82.1(9) | C(18) | C(13) | C(14) | C(19) | 178.0(6) |
| C(18) | C(25) | C(26) | C(27) | -177.1(7) | C(18) | C(25) | C(26) | C(34) | 3(1) |
| C(18) | C(25) | C(30) | C(29) | 176.3(7) | C(18) | C(25) | C(30) | C(33) | -5(1) |
| C(19) | C(20) | C(21) | C(22) | 0(1) | C(19) | C(24) | C(23) | C(22) | 2(1) |
| C(20) | C(19) | C(24) | C(23) | -6(1) | C(20) | C(19) | C(24) | C(32) | 175.4(7) |
| C(20) | C(21) | C(22) | C(23) | -3(1) | C(21) | C(20) | C(19) | C(24) | 5(1) |

Table 5. Torsion Angles(°) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|---|---|
| C(21) | C(22) | C(23) | C(24) | 3(1) | C(22) | C(21) | C(20) | C(31) | 179.5(9) |
| C(22) | C(23) | C(24) | C(32) | -179.8(9) | C(24) | C(19) | C(20) | C(31) | -174.3(8) |
| C(25) | C(26) | C(27) | C(28) | 0(1) | C(25) | C(30) | C(29) | C(28) | 0(1) |
| C(26) | C(25) | C(30) | C(29) | -1(1) | C(26) | C(25) | C(30) | C(33) | 175.8(7) |
| C(26) | C(27) | C(28) | C(29) | -2(1) | C(27) | C(26) | C(25) | C(30) | 1(1) |
| C(27) | C(28) | C(29) | C(30) | 1(1) | C(28) | C(27) | C(26) | C(34) | 179.9(8) |
| C(28) | C(29) | C(30) | C(33) | -177.1(9) | C(30) | C(25) | C(26) | C(34) | -177.9(7) |
| C(35) | C(36) | C(37) | C(38) | -2(1) | C(35) | C(36) | C(41) | C(42) | 80.2(9) |
| C(35) | C(36) | C(41) | C(46) | -104.7(9) | C(35) | C(40) | C(39) | C(38) | 1(1) |
| C(35) | C(40) | C(47) | C(48) | -72.0(9) | C(35) | C(40) | C(47) | C(52) | 115.5(8) |
| C(36) | C(35) | C(40) | C(39) | -5.1(10) | C(36) | C(35) | C(40) | C(47) | 172.4(6) |
| C(36) | C(37) | C(38) | C(39) | -1(1) | C(36) | C(41) | C(42) | C(43) | 176.7(8) |
| C(36) | C(41) | C(42) | C(53) | -2(1) | C(36) | C(41) | C(46) | C(45) | -175.7(8) |
| C(36) | C(41) | C(46) | C(54) | 4(1) | C(37) | C(36) | C(35) | C(40) | 5(1) |
| C(37) | C(36) | C(41) | C(42) | -93.9(9) | C(37) | C(36) | C(41) | C(46) | 81.1(9) |
| C(37) | C(38) | C(39) | C(40) | 1(1) | C(38) | C(37) | C(36) | C(41) | 172.4(8) |
| C(38) | C(39) | C(40) | C(47) | -176.1(7) | C(39) | C(40) | C(47) | C(48) | 105.6(8) |
| C(39) | C(40) | C(47) | C(52) | -66.9(9) | C(40) | C(35) | C(36) | C(41) | -168.6(7) |
| C(40) | C(47) | C(48) | C(49) | -172.9(7) | C(40) | C(47) | C(48) | C(56) | 6(1) |
| C(40) | C(47) | C(52) | C(51) | 172.4(7) | C(40) | C(47) | C(52) | C(55) | -8(1) |
| C(41) | C(42) | C(43) | C(44) | -1(1) | C(41) | C(46) | C(45) | C(44) | 0(1) |
| C(42) | C(41) | C(46) | C(45) | 0(1) | C(42) | C(41) | C(46) | C(54) | 179.4(8) |
| C(42) | C(43) | C(44) | C(45) | 0(1) | C(43) | C(42) | C(41) | C(46) | 1(1) |
| C(43) | C(44) | C(45) | C(46) | 0(1) | C(44) | C(43) | C(42) | C(53) | 177(1) |

Table 5. Torsion Angles(°) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|---|---|
| C(44) | C(45) | C(46) | C(54) | 179(1) | C(46) | C(41) | C(42) | C(53) | -177.9(8) |
| C(47) | C(48) | C(49) | C(50) | 0(1) | C(47) | C(52) | C(51) | C(50) | 0(1) |
| C(48) | C(47) | C(52) | C(51) | 0(1) | C(48) | C(47) | C(52) | C(55) | 179.1(7) |
| C(48) | C(49) | C(50) | C(51) | 0(1) | C(49) | C(48) | C(47) | C(52) | 0(1) |
| C(49) | C(50) | C(51) | C(52) | 0(1) | C(50) | C(49) | C(48) | C(56) | -178.6(9) |
| C(50) | C(51) | C(52) | C(55) | -179.2(9) | C(52) | C(47) | C(48) | C(56) | 179.2(7) |
| C(57) | O(1) | C(58) | C(59) | -178.3(10) | C(58) | C(59) | O(2) | C(60) | 171(1) |
| C(58) | C(59) | O(2) | Li(1) | -42(1) | C(59) | C(58) | O(1) | Li(1) | -42(1) |
| C(61) | O(3) | C(62) | C(63) | -158(1) | C(62) | C(63) | O(4) | C(64) | 179(1) |
| C(62) | C(63) | O(4) | Li(1) | 16(2) | C(63) | C(62) | O(3) | Li(1) | 1(2) |

Table 6. Non-bonded Contacts out to 3.60 Å

| atom | atom | distance | ADC | atom | atom | distance | ADC |
|---|---|---|---|---|---|---|---|
| O(1) | H(46) | 3.23 | 65703 | O(1) | H(40) | 3.38 | 65703 |
| O(3) | H(51) | 3.34 | 64602 | C(8) | H(29) | 3.16 | 65501 |
| C(8) | H(28) | 3.44 | 65501 | C(9) | H(33) | 3.25 | 65603 |
| C(9) | H(32) | 3.54 | 65603 | C(10) | H(41) | 3.04 | 64602 |
| C(10) | H(35) | 3.37 | 65501 | C(15) | H(65) | 3.36 | 55602 |
| C(16) | H(7) | 3.09 | 65603 | C(16) | H(17) | 3.37 | 55603 |
| C(16) | H(18) | 3.51 | 55603 | C(17) | H(7) | 3.04 | 65603 |
| C(17) | H(17) | 3.28 | 55603 | C(19) | H(73) | 3.26 | 55602 |
| C(20) | H(73) | 3.25 | 55602 | C(20) | H(77) | 3.40 | 55602 |
| C(21) | H(73) | 3.22 | 55602 | C(21) | H(45) | 3.27 | 65602 |
| C(22) | H(22) | 2.89 | 55602 | C(22) | H(73) | 3.20 | 55602 |
| C(23) | H(73) | 3.12 | 55602 | C(23) | H(22) | 3.18 | 55602 |
| C(23) | H(23) | 3.52 | 55602 | C(24) | H(73) | 3.14 | 55602 |
| C(25) | H(64) | 3.20 | 44404 | C(26) | H(64) | 3.03 | 44404 |
| C(27) | H(64) | 2.91 | 44404 | C(27) | H(62) | 3.30 | 44404 |
| C(27) | H(20) | 3.37 | 54602 | C(27) | H(21) | 3.49 | 54602 |
| C(27) | H(61) | 3.58 | 44404 | C(28) | H(64) | 2.99 | 44404 |
| C(28) | H(37) | 3.14 | 64602 | C(28) | H(61) | 3.15 | 44404 |
| C(28) | H(21) | 3.40 | 54602 | C(28) | H(62) | 3.49 | 44404 |
| C(29) | H(64) | 3.15 | 44404 | C(29) | H(43) | 3.15 | 44404 |
| C(29) | H(37) | 3.48 | 64602 | C(30) | H(64) | 3.25 | 44404 |
| C(30) | H(67) | 3.51 | 44404 | C(31) | H(77) | 3.29 | 55602 |
| C(31) | H(45) | 3.42 | 65602 | C(31) | H(44) | 3.48 | 65602 |
| C(32) | H(3) | 3.24 | 45501 | C(32) | H(5) | 3.58 | 45501 |

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

| atom | atom | distance | ADC | atom | atom | distance | ADC |
|---|---|---|---|---|---|---|---|
| C(33) | H(6) | 3.42 | 65603 | C(33) | H(7) | 3.55 | 65603 |
| C(33) | H(67) | 3.58 | 44404 | C(34) | H(52) | 3.37 | 45501 |
| C(34) | H(11) | 3.53 | 45501 | C(34) | H(41) | 3.57 | 54602 |
| C(36) | H(55) | 3.57 | 75703 | C(37) | H(55) | 2.90 | 75703 |
| C(37) | H(23) | 3.25 | 65602 | C(37) | H(28) | 3.50 | 65501 |
| C(38) | H(55) | 2.98 | 75703 | C(38) | H(30) | 3.12 | 65501 |
| C(38) | H(21) | 3.51 | 65501 | C(38) | H(28) | 3.52 | 65501 |
| C(39) | H(30) | 3.52 | 65501 | C(43) | H(62) | 3.27 | 65703 |
| C(44) | H(11) | 3.31 | 65602 | C(44) | H(9) | 3.49 | 65602 |
| C(44) | H(35) | 3.57 | 55602 | C(45) | H(68) | 3.23 | 65602 |
| C(45) | H(45) | 3.41 | 65602 | C(45) | H(53) | 3.52 | 65602 |
| C(46) | H(68) | 3.35 | 65602 | C(47) | H(48) | 3.58 | 75703 |
| C(48) | H(48) | 3.22 | 75703 | C(49) | H(24) | 3.42 | 54504 |
| C(49) | H(48) | 3.56 | 75703 | C(50) | H(27) | 3.21 | 64602 |
| C(51) | H(27) | 3.18 | 64602 | C(51) | H(76) | 3.18 | 65501 |
| C(51) | H(42) | 3.21 | 64602 | C(51) | H(19) | 3.45 | 64602 |
| C(51) | H(77) | 3.56 | 65501 | C(52) | H(76) | 2.98 | 65501 |
| C(53) | H(60) | 3.14 | 65703 | C(53) | H(55) | 3.22 | 75703 |
| C(53) | H(75) | 3.54 | 65703 | C(53) | H(39) | 3.56 | 75703 |
| C(54) | H(68) | 2.91 | 65602 | C(55) | H(76) | 3.04 | 65501 |
| C(55) | H(36) | 3.14 | 65501 | C(55) | H(42) | 3.47 | 64602 |
| C(56) | H(48) | 3.41 | 75703 | C(56) | H(47) | 3.42 | 75703 |
| C(57) | H(46) | 2.80 | 65703 | C(57) | H(58) | 3.34 | 65703 |
| C(57) | H(79) | 3.37(6) | 65703 | C(58) | H(40) | 3.35 | 65703 |

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

| atom | atom | distance | ADC | atom | atom | distance | ADC |
|---|---|---|---|---|---|---|---|
| C(58) | H(23) | 3.57 | 54504 | C(61) | H(51) | 2.96 | 64602 |
| C(61) | H(42) | 3.45 | 64602 | C(62) | H(51) | 3.48 | 64602 |
| C(63) | H(52) | 3.54 | 45501 | C(64) | H(52) | 3.25 | 45501 |
| C(64) | H(27) | 3.52 | 54602 | C(64) | H(39) | 3.57 | 45501 |
| H(3) | H(29) | 2.80 | 65501 | H(3) | H(28) | 3.10 | 65501 |
| H(3) | H(34) | 3.19 | 65501 | H(3) | H(30) | 3.31 | 65501 |
| H(4) | H(29) | 2.93 | 65501 | H(4) | H(34) | 3.13 | 65501 |
| H(4) | H(17) | 3.29 | 65603 | H(4) | H(18) | 3.52 | 65603 |
| H(4) | H(28) | 3.58 | 65501 | H(5) | H(28) | 3.11 | 65501 |
| H(5) | H(29) | 3.20 | 65501 | H(5) | H(66) | 3.40 | 65602 |
| H(6) | H(32) | 2.92 | 65603 | H(6) | H(33) | 3.03 | 65603 |
| H(7) | H(33) | 2.82 | 65603 | H(7) | H(18) | 2.93 | 65603 |
| H(7) | H(17) | 2.97 | 65603 | H(7) | H(32) | 3.40 | 65603 |
| H(8) | H(33) | 3.37 | 65603 | H(9) | H(41) | 3.00 | 64602 |
| H(10) | H(35) | 2.96 | 65501 | H(10) | H(17) | 2.99 | 65603 |
| H(10) | H(41) | 3.03 | 64602 | H(10) | H(34) | 3.48 | 65501 |
| H(11) | H(41) | 2.58 | 64602 | H(11) | H(35) | 2.87 | 65501 |
| H(11) | H(42) | 3.44 | 64602 | H(11) | H(34) | 3.53 | 65501 |
| H(14) | H(60) | 3.56 | 65703 | H(16) | H(65) | 2.66 | 55602 |
| H(16) | H(77) | 3.31 | 55602 | H(16) | H(63) | 3.43 | 55602 |
| H(17) | H(18) | 2.87 | 55603 | H(17) | H(17) | 3.08 | 55603 |
| H(18) | H(67) | 2.93 | 44404 | H(18) | H(65) | 3.43 | 44404 |
| H(18) | H(64) | 3.52 | 44404 | H(19) | H(45) | 2.52 | 65602 |
| H(20) | H(22) | 2.45 | 55602 | H(20) | H(62) | 3.19 | 65703 |

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

| atom | atom | distance | ADC | atom | atom | distance | ADC |
|---|---|---|---|---|---|---|---|
| H(21) | H(23) | 2.71 | 55602 | H(21) | H(38) | 2.86 | 45501 |
| H(21) | H(22) | 2.90 | 55602 | H(21) | H(37) | 3.39 | 45501 |
| H(21) | H(73) | 3.58 | 55602 | H(22) | H(62) | 3.08 | 44404 |
| H(22) | H(64) | 3.34 | 44404 | H(23) | H(37) | 2.36 | 64602 |
| H(23) | H(61) | 2.98 | 44404 | H(23) | H(38) | 3.41 | 64602 |
| H(23) | H(62) | 3.45 | 44404 | H(23) | H(64) | 3.48 | 44404 |
| H(24) | H(43) | 2.69 | 44404 | H(24) | H(37) | 3.10 | 64602 |
| H(25) | H(44) | 3.30 | 65602 | H(25) | H(45) | 3.49 | 65602 |
| H(26) | H(77) | 3.53 | 55602 | H(27) | H(77) | 2.63 | 55602 |
| H(27) | H(45) | 2.74 | 65602 | H(27) | H(44) | 2.80 | 65602 |
| H(28) | H(49) | 2.95 | 45501 | H(28) | H(72) | 3.18 | 55602 |
| H(28) | H(51) | 3.44 | 45501 | H(28) | H(37) | 3.51 | 45501 |
| H(28) | H(38) | 3.52 | 45501 | H(30) | H(38) | 2.95 | 45501 |
| H(30) | H(54) | 3.39 | 45501 | H(32) | H(44) | 2.97 | 44404 |
| H(32) | H(67) | 3.01 | 44404 | H(32) | H(43) | 3.50 | 44404 |
| H(35) | H(41) | 2.68 | 54602 | H(35) | H(53) | 3.32 | 45501 |
| H(35) | H(52) | 3.45 | 45501 | H(36) | H(52) | 2.56 | 45501 |
| H(36) | H(53) | 3.13 | 45501 | H(36) | H(54) | 3.27 | 45501 |
| H(37) | H(55) | 2.92 | 75703 | H(38) | H(55) | 3.09 | 75703 |
| H(38) | H(80) | 3.32 | 65501 | H(38) | H(57) | 3.44 | 75703 |
| H(38) | H(59) | 3.47 | 65501 | H(38) | H(79) | 3.58 | 65501 |
| H(39) | H(76) | 2.86 | 65501 | H(39) | H(48) | 3.18 | 75703 |
| H(39) | H(46) | 3.31 | 75703 | H(39) | H(59) | 3.37 | 65501 |
| H(39) | H(80) | 3.39 | 65501 | H(39) | H(75) | 3.46 | 65501 |

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

| atom | atom | distance | ADC | atom | atom | distance | ADC |
|---|---|---|---|---|---|---|---|
| H(40) | H(62) | 2.78 | 65703 | H(40) | H(75) | 2.99 | 65703 |
| H(40) | H(63) | 3.04 | 65703 | H(40) | H(60) | 3.47 | 65703 |
| H(41) | H(53) | 3.25 | 65602 | H(42) | H(45) | 2.59 | 65602 |
| H(42) | H(68) | 2.71 | 65602 | H(42) | H(53) | 2.75 | 65602 |
| H(42) | H(70) | 3.44 | 65602 | H(44) | H(50) | 3.49 | 64602 |
| H(45) | H(50) | 3.12 | 64602 | H(45) | H(76) | 3.24 | 65501 |
| H(45) | H(77) | 3.41 | 65501 | H(46) | H(60) | 2.24 | 65703 |
| H(46) | H(59) | 2.73 | 65703 | H(46) | H(75) | 3.23 | 65703 |
| H(47) | H(55) | 2.74 | 75703 | H(47) | H(56) | 3.40 | 75703 |
| H(48) | H(55) | 2.87 | 75703 | H(48) | H(75) | 3.06 | 65703 |
| H(50) | H(68) | 3.25 | 65602 | H(50) | H(66) | 3.60 | 65602 |
| H(51) | H(68) | 2.07 | 65602 | H(51) | H(72) | 2.86 | 65602 |
| H(51) | H(66) | 3.16 | 65602 | H(51) | H(70) | 3.38 | 65602 |
| H(51) | H(69) | 3.58 | 65602 | H(52) | H(76) | 2.38 | 65501 |
| H(52) | H(74) | 2.75 | 65501 | H(52) | H(77) | 3.55 | 65501 |
| H(54) | H(76) | 3.45 | 65501 | H(58) | H(58) | 2.98 | 65703 |
| H(58) | H(59) | 3.21 | 65703 | H(58) | H(79) | 3.22 | 65703 |
| H(58) | H(60) | 3.31 | 65703 | H(60) | H(79) | 2.68 | 65703 |

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 |

Special Contacts

| atom | atom | distance | ADC(*) | atom | atom | distance | ADC(*) |
|---|---|---|---|---|---|---|---|
| Li(1) | H(78) | 1.94(5) | 1 | | | | |

Contacts out to 2.00 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

(*)footnote

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(1st digit) + TB(2nd digit) + TC(3rd digit) + SN(4th and 5th digit). TA, TB, & 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.

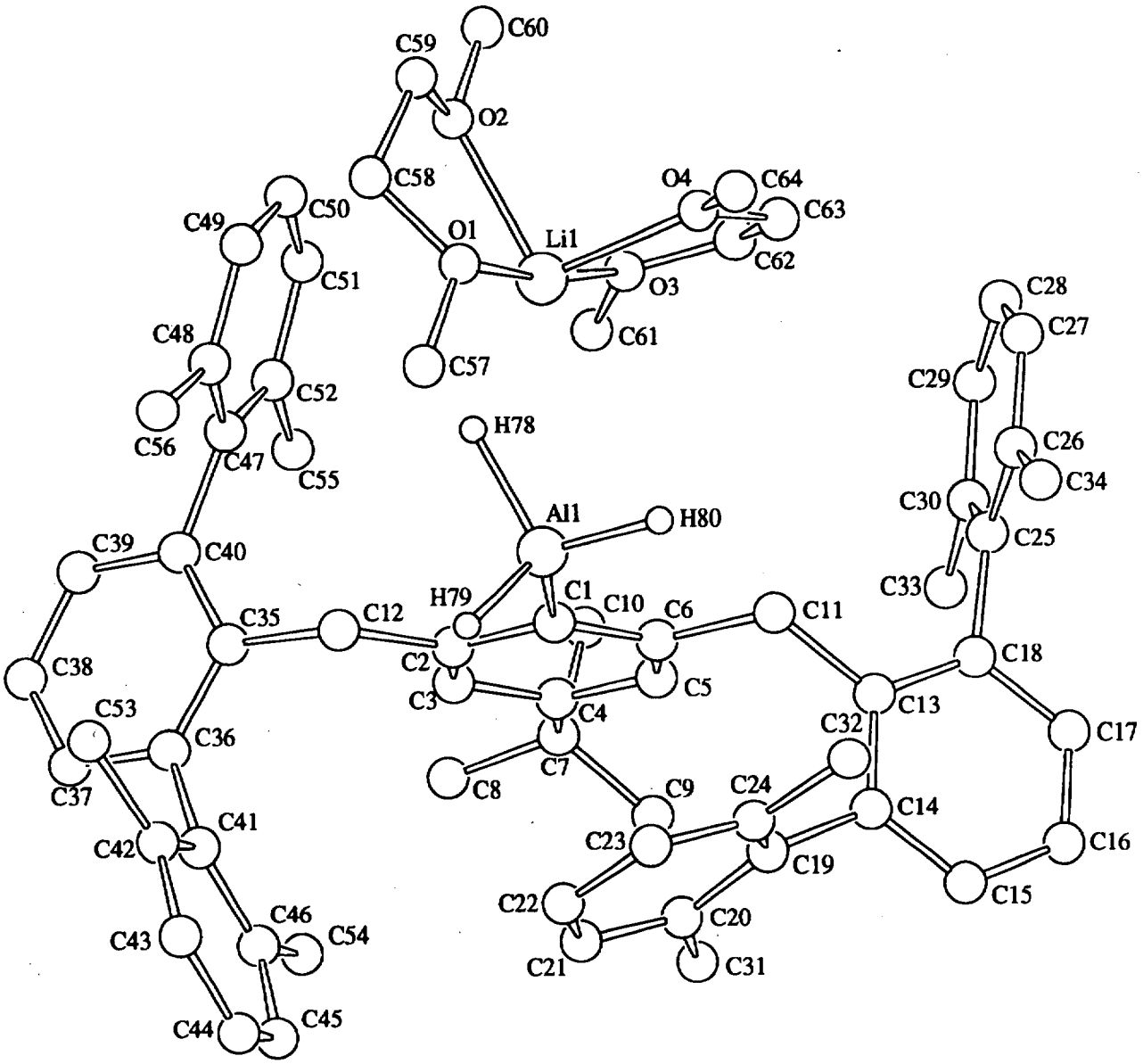
The SN or symmetry operator number refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of the symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell (TA=5,TB=5,TC=5) and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always ADC=55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of that atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through 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 (i.e.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 |




Atom numbering scheme for **6**