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*Experimental*Data Collection

A yellow, transparent columnar crystal of $C_{52}H_{62}Si_2Lu_2$ having approximate dimensions of $0.45 \times 0.11 \times 0.09$ mm was mounted using oil, (Paratone-N, Exxon) on a glass fiber. All measurements were made on an Enraf-Nonius CAD4 diffractometer with graphite monochromated Mo-K α radiation.

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 $18.3 < 2\theta < 20.3^\circ$ corresponded to a primitive orthorhombic cell with dimensions:

$$\begin{aligned}a &= 10.536(4) \text{ \AA} \\b &= 13.340(3) \text{ \AA} \\c &= 36.820(9) \text{ \AA} \\V &= 5175(2) \text{ \AA}^3\end{aligned}$$

For $Z = 4$ and F.W. = 1093.17, the calculated density is 1.40 g/cm³. The systematic absences of:

$$\begin{aligned}h00: h &\neq 2n \\0k0: k &\neq 2n \\00l: l &\neq 2n\end{aligned}$$

uniquely determine the space group to be:

$$P2_12_12_1 (\#19)$$

The data were collected at a temperature of $-120 \pm 1^\circ\text{C}$ using the ω - θ scan technique to a maximum 2θ value of 45.9° . 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 2.8° . Scans of $(1.00 + 0.35 \tan \theta)^\circ$ were made at variable speed from 3.0 - $16.0^\circ/\text{min}$ (in omega). Moving-crystal moving counter background measurements were made by scanning an additional 25% above and below the scan range. The counter aperture consisted of a variable horizontal slit with a width ranging from 2.0 to 2.5 mm and a vertical slit set to 2.0 mm. The diameter of the incident beam collimator was 0.7 mm and the crystal to detector distance was 21 cm. For intense reflections an attenuator was automatically inserted in front of the detector.

Data Reduction

Of the 4258 reflections which were collected, 4099 were unique ($R_{int} = 0.073$). The intensities of three representative reflection were measured after every 90 minutes of X-ray exposure time. No decay correction was applied.

The linear absorption coefficient, μ , for Mo-K α radiation is 38.7 cm^{-1} . An empirical absorption correction using the program DIFABS¹ was applied which resulted in transmission factors ranging from 0.75 to 1.15. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by and expanded using Fourier techniques³. Carbon atoms were refined isotropically, the remaining non-hydrogen atoms were refined anisotropically, Hydrogen atoms were included but not refined. The Cp ring C8-C12 was placed in a rigid group owing to some disorder. The highest peaks left in the final difference map were located close to C23 and indicating the disorder. The final cycle of full-matrix least-squares refinement⁴ was based on 2978 observed reflections ($I > 3.00\sigma(I)$) and 232 variable parameters and converged (largest parameter shift was 0.01 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o| = 0.061$$

$$R_w = \sqrt{(\Sigma w(|F_o| - |F_c|)^2 / \Sigma w F_o^2)} = 0.079$$

The enantiomer was refined with unweighted and weighted R factors to be 8.6 and 11.6 respectively indicating the other being the correct enantiomer. The standard deviation of an observation of unit weight⁵ was 3.58. The weighting scheme was based on counting statistics and included a factor ($p = 0.005$) to downweight the intense reflections. Plots of $\Sigma w(|F_o| - |F_c|)^2$ versus $|F_o|$, 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 2.03 and $-1.61 e^-/\text{\AA}^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber⁶. Anomalous dispersion effects were included in F_{calc} ⁷; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley⁸. The values for the mass attenuation coefficients are those of Creagh and Hubbel⁹. All calculations were performed using the teXsan¹⁰ crystallographic software package of Molecular Structure Corporation.

References

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

(3) DIRDIF92: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(4) Least-Squares:

Function minimized: $\Sigma w(|F_o| - |F_c|)^2$

$$\text{where } w = \frac{1}{\sigma^2(F_o)} = \frac{4F_o^2}{\sigma^2(F_o^2)}$$

$$\sigma^2(F_o^2) = \frac{S^2(C + R^2B) + (pF_o^2)^2}{L_p^2}$$

S = Scan rate

C = Total integrated peak count

R = Ratio of scan time to background counting time

B = Total background count

L_p = Lorentz-polarization factor

p = p-factor

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

$$\sqrt{\sum w(|F_o| - |F_c|)^2 / (N_o - N_v)}$$

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 | $C_{52}H_{62}Si_2Lu_2$ |
| Formula Weight | 1093.17 |
| Crystal Color, Habit | yellow, columnar |
| Crystal Dimensions | 0.45 X 0.11 X 0.09 mm |
| Crystal System | orthorhombic |
| Lattice Type | Primitive |
| No. of Reflections Used for Unit | |
| Cell Determination (2θ range) | 25 (18.3 - 20.3°) |
| Omega Scan Peak Width | |
| at Half-height | 0.30° |
| Lattice Parameters | $a = 10.536(4)\text{\AA}$ $b = 13.340(3) \text{\AA}$ $c = 36.820(9) \text{\AA}$ |
| | $V = 5175(2) \text{\AA}^3$ |
| Space Group | P2 ₁ 2 ₁ 2 ₁ (#19) |
| Z value | 4 |
| D _{calc} | 1.403 g/cm ³ |
| F ₀₀₀ | 2176.00 |
| $\mu(\text{MoK}\alpha)$ | 38.69 cm ⁻¹ |

B. Intensity Measurements

| | |
|------------------------------|--|
| Diffractometer | CAD4 |
| Radiation | MoK α ($\lambda = 0.71069 \text{ \AA}$) graphite monochromated |
| Attenuator | Zr foil (factor = 22.25) |
| Take-off Angle | 2.8° |
| Detector Aperture | 2.0 - 2.5 mm horizontal 2.0 mm vertical |
| Crystal to Detector Distance | 21 mm |
| Temperature | -120.0°C |
| Scan Type | ω - θ |
| Scan Rate | 3.0°/min (in ω) (up to 0 scans) |
| Scan Width | (1.00 + 0.35 tan θ)° |
| $2\theta_{max}$ | 45.9° |
| No. of Reflections Measured | Total: 4258 Unique: 4099 ($R_{int} = 0.073$) |
| Corrections | Lorentz-polarization Absorption (trans. factors: 0.7472 - 1.1479) |

C. Structure Solution and Refinement

| | |
|--|--|
| Structure Solution | Direct Methods |
| Refinement | Full-matrix least-squares |
| Function Minimized | $\Sigma w(F_o - F_c)^2$ |
| Least Squares Weights | $\frac{1}{\sigma^2(F_o)} = \frac{4F_o^2}{\sigma^2(F_o^2)}$ |
| p-factor | 0.005 |
| Anomalous Dispersion | All non-hydrogen atoms |
| No. Observations ($I > 3.00\sigma(I)$) | 2978 |
| No. Variables | 232 |
| Reflection/Parameter Ratio | 12.84 |

| | |
|---------------------------------|----------------------------------|
| Residuals: R; R _w | 0.061 ; 0.079 |
| Goodness of Fit Indicator | 3.58 |
| Max Shift/Error in Final Cycle | 0.01 |
| Maximum peak in Final Diff. Map | $2.03 \text{ e}^-/\text{\AA}^3$ |
| Minimum peak in Final Diff. Map | $-1.61 \text{ e}^-/\text{\AA}^3$ |

Table 1. Atomic coordinates and B_{iso}/B_{eq} S15D

| atom | x | y | z | B_{eq} |
|-------|------------|------------|-------------|----------|
| Lu(1) | 0.1729(1) | 0.0257(1) | 0.12688(4) | 1.55(3) |
| Lu(2) | 0.3529(1) | 0.2282(1) | 0.15500(4) | 1.62(3) |
| Si(1) | -0.1133(8) | -0.0765(7) | 0.1135(3) | 1.9(2) |
| Si(2) | 0.6191(9) | 0.3600(8) | 0.1685(3) | 2.3(2) |
| C(1) | -0.161(4) | -0.201(3) | 0.0995(9) | 3.7(9) |
| C(2) | -0.251(3) | 0.005(3) | 0.1205(8) | 1.7(6) |
| C(3) | 0.002(3) | -0.016(3) | 0.0814(8) | 1.2(6) |
| C(4) | 0.113(3) | -0.065(2) | 0.0680(8) | 1.4(7) |
| C(5) | 0.205(3) | 0.003(2) | 0.0551(8) | 1.5(7) |
| C(6) | 0.148(3) | 0.102(2) | 0.0598(8) | 1.7(6) |
| C(7) | 0.025(3) | 0.089(2) | 0.0766(8) | 1.3(7) |
| C(8) | 0.006(1) | -0.083(2) | 0.1533(5) | 1.22 |
| C(9) | 0.116(2) | -0.143(1) | 0.1516(4) | 1.22 |
| C(10) | 0.199(1) | -0.111(1) | 0.1790(5) | 1.22 |
| C(11) | 0.141(2) | -0.031(1) | 0.1975(5) | 1.22 |
| C(12) | 0.022(2) | -0.014(1) | 0.1817(5) | 1.22 |
| C(13) | 0.330(3) | -0.010(2) | 0.0381(7) | 1.6(6) |
| C(14) | 0.325(3) | -0.034(2) | -0.0035(7) | 1.3(6) |
| C(15) | 0.283(3) | -0.140(2) | -0.0112(8) | 1.4(7) |
| C(16) | 0.381(3) | -0.214(3) | 0.0082(8) | 1.9(7) |
| C(17) | 0.384(4) | -0.194(3) | 0.048(1) | 4(1) |
| C(18) | 0.415(3) | -0.082(3) | 0.0584(8) | 1.7(7) |
| C(19) | 0.240(3) | 0.042(3) | -0.0239(8) | 1.7(7) |
| C(20) | 0.305(4) | 0.149(3) | -0.0247(10) | 4.1(10) |

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

| atom | x | y | z | B_{eq} |
|-------|----------|-----------|------------|----------|
| C(21) | 0.228(3) | 0.011(3) | -0.0638(9) | 3.1(8) |
| C(22) | 0.496(4) | -0.259(3) | 0.0682(10) | 4.0(9) |
| C(23) | 0.299(3) | -0.175(3) | 0.1842(9) | 2.5(8) |
| C(24) | 0.404(3) | -0.107(3) | 0.2103(10) | 3.1(9) |
| C(25) | 0.399(3) | -0.212(2) | 0.1550(8) | 1.5(6) |
| C(26) | 0.278(5) | -0.261(4) | 0.215(1) | 8(1) |
| C(27) | 0.644(3) | 0.496(2) | 0.1793(8) | 2.6(7) |
| C(28) | 0.770(3) | 0.293(3) | 0.1625(9) | 2.6(8) |
| C(29) | 0.518(3) | 0.346(3) | 0.1339(8) | 1.9(7) |
| C(30) | 0.388(3) | 0.397(2) | 0.1253(8) | 1.2(6) |
| C(31) | 0.311(3) | 0.346(2) | 0.1029(8) | 2.3(7) |
| C(32) | 0.395(3) | 0.269(3) | 0.0860(8) | 2.0(7) |
| C(33) | 0.511(3) | 0.264(3) | 0.1010(8) | 2.2(7) |
| C(34) | 0.513(3) | 0.294(3) | 0.2004(9) | 2.5(8) |
| C(35) | 0.396(3) | 0.333(3) | 0.2111(9) | 2.2(8) |
| C(36) | 0.313(3) | 0.261(3) | 0.2294(8) | 2.5(7) |
| C(37) | 0.383(3) | 0.173(3) | 0.2218(9) | 2.4(8) |
| C(38) | 0.497(3) | 0.193(3) | 0.2089(9) | 2.7(8) |
| C(39) | 0.185(3) | 0.376(2) | 0.0863(8) | 2.4(7) |
| C(40) | 0.187(3) | 0.445(2) | 0.0533(8) | 2.1(7) |
| C(41) | 0.214(3) | 0.553(2) | 0.0609(9) | 1.9(7) |
| C(42) | 0.105(3) | 0.591(3) | 0.0866(9) | 2.7(8) |
| C(43) | 0.118(4) | 0.526(4) | 0.126(1) | 5(1) |
| C(44) | 0.107(3) | 0.415(2) | 0.1139(7) | 0.7(6) |

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

| atom | x | y | z | B_{eq} |
|-------|----------|----------|------------|----------|
| C(45) | 0.264(3) | 0.404(3) | 0.0225(9) | 2.0(7) |
| C(46) | 0.410(3) | 0.439(2) | 0.0186(8) | 1.7(7) |
| C(47) | 0.205(3) | 0.441(3) | -0.0157(9) | 2.8(8) |
| C(48) | 0.017(3) | 0.563(3) | 0.1480(9) | 2.2(7) |
| C(49) | 0.196(3) | 0.285(3) | 0.2480(9) | 2.6(8) |
| C(50) | 0.113(5) | 0.366(4) | 0.227(1) | 7(1) |
| C(51) | 0.224(4) | 0.306(3) | 0.288(1) | 5(1) |
| C(52) | 0.109(4) | 0.185(4) | 0.247(1) | 6(1) |
| H(1) | -0.21 | -0.23 | 0.12 | 4.50 |
| H(2) | -0.21 | -0.20 | 0.08 | 4.50 |
| H(3) | -0.09 | -0.24 | 0.10 | 4.50 |
| H(4) | -0.22 | 0.07 | 0.13 | 2.07 |
| H(5) | -0.30 | 0.01 | 0.10 | 2.07 |
| H(6) | -0.30 | -0.02 | 0.14 | 2.07 |
| H(7) | 0.12 | -0.14 | 0.07 | 1.70 |
| H(8) | 0.19 | 0.16 | 0.05 | 2.00 |
| H(9) | -0.03 | 0.14 | 0.08 | 1.61 |
| H(10) | 0.37 | 0.05 | 0.04 | 1.97 |
| H(11) | 0.41 | -0.03 | -0.01 | 1.55 |
| H(12) | 0.20 | -0.15 | 0.00 | 1.72 |
| H(13) | 0.28 | -0.15 | -0.04 | 1.72 |
| H(14) | 0.35 | -0.28 | 0.00 | 2.25 |
| H(15) | 0.46 | -0.20 | 0.00 | 2.25 |
| H(16) | 0.30 | -0.21 | 0.06 | 5.01 |

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

| atom | x | y | z | B_{eq} |
|-------|------|-------|-------|----------|
| H(17) | 0.50 | -0.07 | 0.05 | 2.01 |
| H(18) | 0.40 | -0.07 | 0.08 | 2.01 |
| H(19) | 0.38 | 0.14 | -0.04 | 4.88 |
| H(20) | 0.25 | 0.19 | -0.04 | 4.88 |
| H(21) | 0.32 | 0.17 | 0.00 | 4.88 |
| H(22) | 0.19 | -0.05 | -0.07 | 3.69 |
| H(23) | 0.18 | 0.06 | -0.08 | 3.69 |
| H(24) | 0.31 | 0.01 | -0.07 | 3.69 |
| H(25) | 0.48 | -0.33 | 0.06 | 4.86 |
| H(26) | 0.58 | -0.24 | 0.06 | 4.86 |
| H(27) | 0.49 | -0.25 | 0.09 | 4.86 |
| H(28) | 0.47 | -0.15 | 0.22 | 3.67 |
| H(29) | 0.43 | -0.05 | 0.20 | 3.67 |
| H(30) | 0.36 | -0.09 | 0.23 | 3.67 |
| H(31) | 0.46 | -0.25 | 0.17 | 1.83 |
| H(32) | 0.36 | -0.25 | 0.14 | 1.83 |
| H(33) | 0.44 | -0.16 | 0.14 | 1.83 |
| H(34) | 0.24 | -0.23 | 0.24 | 10.46 |
| H(35) | 0.22 | -0.31 | 0.21 | 10.46 |
| H(36) | 0.36 | -0.29 | 0.22 | 10.46 |
| H(37) | 0.70 | 0.50 | 0.20 | 3.09 |
| H(38) | 0.68 | 0.53 | 0.16 | 3.09 |
| H(39) | 0.57 | 0.53 | 0.19 | 3.09 |
| H(40) | 0.75 | 0.22 | 0.16 | 3.17 |

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

| atom | x | y | z | B_{eq} |
|-------|------|------|-------|----------|
| H(41) | 0.81 | 0.32 | 0.14 | 3.17 |
| H(42) | 0.82 | 0.30 | 0.18 | 3.17 |
| H(43) | 0.36 | 0.46 | 0.14 | 1.48 |
| H(44) | 0.37 | 0.23 | 0.07 | 2.46 |
| H(45) | 0.58 | 0.22 | 0.09 | 2.65 |
| H(46) | 0.37 | 0.40 | 0.21 | 2.68 |
| H(47) | 0.35 | 0.11 | 0.23 | 2.89 |
| H(48) | 0.56 | 0.14 | 0.21 | 3.28 |
| H(49) | 0.15 | 0.32 | 0.08 | 2.83 |
| H(50) | 0.10 | 0.44 | 0.04 | 2.48 |
| H(51) | 0.29 | 0.56 | 0.07 | 2.31 |
| H(52) | 0.21 | 0.59 | 0.04 | 2.31 |
| H(53) | 0.11 | 0.66 | 0.09 | 3.21 |
| H(54) | 0.02 | 0.58 | 0.08 | 3.21 |
| H(55) | 0.20 | 0.54 | 0.14 | 6.17 |
| H(56) | 0.02 | 0.41 | 0.11 | 0.80 |
| H(57) | 0.12 | 0.38 | 0.13 | 0.80 |
| H(58) | 0.46 | 0.42 | 0.04 | 2.05 |
| H(59) | 0.45 | 0.41 | 0.00 | 2.05 |
| H(60) | 0.41 | 0.51 | 0.02 | 2.05 |
| H(61) | 0.21 | 0.51 | -0.02 | 3.32 |
| H(62) | 0.25 | 0.41 | -0.04 | 3.32 |
| H(63) | 0.12 | 0.42 | -0.02 | 3.32 |
| H(64) | 0.03 | 0.63 | 0.15 | 2.60 |

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

| atom | x | y | z | B_{eq} |
|-------|-------|------|------|----------|
| H(65) | -0.06 | 0.56 | 0.13 | 2.60 |
| H(66) | 0.01 | 0.52 | 0.17 | 2.60 |
| H(67) | 0.16 | 0.43 | 0.23 | 9.01 |
| H(68) | 0.10 | 0.34 | 0.20 | 9.01 |
| H(69) | 0.03 | 0.37 | 0.24 | 9.01 |
| H(70) | 0.26 | 0.25 | 0.30 | 6.59 |
| H(71) | 0.28 | 0.36 | 0.29 | 6.59 |
| H(72) | 0.15 | 0.32 | 0.30 | 6.59 |
| H(73) | 0.03 | 0.20 | 0.26 | 7.92 |
| H(74) | 0.09 | 0.17 | 0.22 | 7.92 |
| H(75) | 0.15 | 0.13 | 0.26 | 7.92 |

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

Table 2. Anisotropic Displacement Parameters S15D

| atom | U_{11} | U_{22} | U_{33} | U_{12} | U_{13} | U_{23} |
|-------|-----------|-----------|-----------|------------|------------|------------|
| Lu(1) | 0.0209(7) | 0.0177(8) | 0.0204(8) | -0.0017(8) | -0.0031(7) | -0.0012(8) |
| Lu(2) | 0.0191(7) | 0.0212(8) | 0.0212(8) | -0.0041(8) | -0.0002(8) | -0.0033(7) |
| Si(1) | 0.016(5) | 0.022(6) | 0.033(6) | -0.004(5) | -0.002(4) | -0.001(5) |
| Si(2) | 0.020(6) | 0.036(7) | 0.032(6) | -0.006(5) | -0.012(4) | -0.007(5) |

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 S15D |
|-------|-------|----------|-------|-------|---------------|
| Lu(1) | Lu(2) | 3.459(2) | Lu(1) | C(3) | 2.53(3) |
| Lu(1) | C(4) | 2.56(3) | Lu(1) | C(5) | 2.68(3) |
| Lu(1) | C(6) | 2.68(3) | Lu(1) | C(7) | 2.56(3) |
| Lu(1) | C(9) | 2.50(2) | Lu(1) | C(10) | 2.66(2) |
| Lu(1) | C(11) | 2.73(2) | Lu(1) | C(12) | 2.62(2) |
| Lu(1) | C(8) | 2.47(2) | Lu(2) | C(29) | 2.46(3) |
| Lu(2) | C(30) | 2.53(3) | Lu(2) | C(31) | 2.52(3) |
| Lu(2) | C(32) | 2.64(3) | Lu(2) | C(33) | 2.64(3) |
| Lu(2) | C(34) | 2.53(3) | Lu(2) | C(35) | 2.53(3) |
| Lu(2) | C(37) | 2.59(3) | Lu(2) | C(38) | 2.54(3) |
| Si(1) | C(1) | 1.81(4) | Si(1) | C(2) | 1.83(3) |
| Si(1) | C(3) | 1.87(3) | Si(1) | C(8) | 1.93(2) |
| Si(2) | C(27) | 1.88(3) | Si(2) | C(28) | 1.83(3) |
| Si(2) | C(29) | 1.67(3) | Si(2) | C(34) | 1.84(4) |
| C(3) | C(4) | 1.43(4) | C(3) | C(7) | 1.43(5) |
| C(4) | C(5) | 1.41(4) | C(5) | C(6) | 1.45(4) |
| C(5) | C(13) | 1.47(4) | C(6) | C(7) | 1.45(5) |
| C(13) | C(14) | 1.57(4) | C(13) | C(18) | 1.52(4) |
| C(14) | C(15) | 1.51(4) | C(14) | C(19) | 1.55(4) |
| C(15) | C(16) | 1.60(4) | C(16) | C(17) | 1.50(5) |
| C(17) | C(18) | 1.58(5) | C(17) | C(22) | 1.64(5) |
| C(19) | C(20) | 1.58(5) | C(19) | C(21) | 1.53(5) |
| C(23) | C(24) | 1.72(5) | C(23) | C(25) | 1.58(4) |
| C(23) | C(26) | 1.61(6) | C(23) | C(10) | 1.38(4) |

Table 3. Bond Lengths(Å) (continued)

| atom | atom | distance | atom | atom | distance |
|-------|-------|----------|-------|-------|----------|
| C(29) | C(30) | 1.57(4) | C(29) | C(33) | 1.63(5) |
| C(30) | C(31) | 1.34(4) | C(31) | C(32) | 1.50(5) |
| C(31) | C(39) | 1.51(5) | C(32) | C(33) | 1.34(4) |
| C(34) | C(35) | 1.39(5) | C(34) | C(38) | 1.40(5) |
| C(35) | C(36) | 1.46(5) | C(36) | C(37) | 1.42(5) |
| C(36) | C(49) | 1.44(5) | C(37) | C(38) | 1.32(5) |
| C(39) | C(40) | 1.52(4) | C(39) | C(44) | 1.40(4) |
| C(40) | C(41) | 1.49(5) | C(40) | C(45) | 1.50(5) |
| C(41) | C(42) | 1.58(5) | C(42) | C(43) | 1.70(6) |
| C(43) | C(44) | 1.54(6) | C(43) | C(48) | 1.43(5) |
| C(45) | C(46) | 1.62(5) | C(45) | C(47) | 1.61(5) |
| C(49) | C(50) | 1.58(6) | C(49) | C(51) | 1.54(5) |
| C(49) | C(52) | 1.62(6) | C(9) | C(10) | 1.40(2) |
| C(9) | C(8) | 1.40(2) | C(10) | C(11) | 1.40(3) |
| C(11) | C(12) | 1.40(3) | C(12) | C(8) | 1.40(3) |

Table 4. Bond Lengths(Å)

| atom | atom | distance | atom | atom | distance S15D |
|-------|-------|----------|-------|-------|---------------|
| C(1) | H(1) | 0.95 | C(1) | H(2) | 0.95 |
| C(1) | H(3) | 0.95 | C(2) | H(4) | 0.95 |
| C(2) | H(5) | 0.95 | C(2) | H(6) | 0.95 |
| C(4) | H(7) | 0.95 | C(6) | H(8) | 0.95 |
| C(7) | H(9) | 0.95 | C(13) | H(10) | 0.95 |
| C(14) | H(11) | 0.95 | C(15) | H(12) | 0.95 |
| C(15) | H(13) | 0.95 | C(16) | H(14) | 0.95 |
| C(16) | H(15) | 0.95 | C(17) | H(16) | 0.95 |
| C(18) | H(17) | 0.95 | C(18) | H(18) | 0.95 |
| C(20) | H(19) | 0.95 | C(20) | H(20) | 0.95 |
| C(20) | H(21) | 0.95 | C(21) | H(22) | 0.95 |
| C(21) | H(23) | 0.95 | C(21) | H(24) | 0.95 |
| C(22) | H(25) | 0.95 | C(22) | H(26) | 0.95 |
| C(22) | H(27) | 0.95 | C(24) | H(28) | 0.95 |
| C(24) | H(29) | 0.95 | C(24) | H(30) | 0.95 |
| C(25) | H(31) | 0.95 | C(25) | H(32) | 0.95 |
| C(25) | H(33) | 0.95 | C(26) | H(34) | 0.94 |
| C(26) | H(35) | 0.95 | C(26) | H(36) | 0.95 |
| C(27) | H(37) | 0.95 | C(27) | H(38) | 0.95 |
| C(27) | H(39) | 0.95 | C(28) | H(40) | 0.95 |
| C(28) | H(41) | 0.95 | C(28) | H(42) | 0.95 |
| C(30) | H(43) | 0.95 | C(32) | H(44) | 0.95 |
| C(33) | H(45) | 0.95 | C(35) | H(46) | 0.95 |
| C(37) | H(47) | 0.95 | C(38) | H(48) | 0.95 |

Table 4. Bond Lengths(Å) (continued)

| atom | atom | distance | atom | atom | distance |
|-------|-------|----------|-------|-------|----------|
| C(39) | H(49) | 0.95 | C(40) | H(50) | 0.95 |
| C(41) | H(51) | 0.95 | C(41) | H(52) | 0.95 |
| C(42) | H(53) | 0.95 | C(42) | H(54) | 0.95 |
| C(43) | H(55) | 0.95 | C(44) | H(56) | 0.95 |
| C(44) | H(57) | 0.95 | C(46) | H(58) | 0.95 |
| C(46) | H(59) | 0.95 | C(46) | H(60) | 0.95 |
| C(47) | H(61) | 0.95 | C(47) | H(62) | 0.95 |
| C(47) | H(63) | 0.95 | C(48) | H(64) | 0.95 |
| C(48) | H(65) | 0.95 | C(48) | H(66) | 0.95 |
| C(50) | H(67) | 0.95 | C(50) | H(68) | 0.95 |
| C(50) | H(69) | 0.95 | C(51) | H(70) | 0.95 |
| C(51) | H(71) | 0.95 | C(51) | H(72) | 0.95 |
| C(52) | H(73) | 0.95 | C(52) | H(74) | 0.95 |
| C(52) | H(75) | 0.95 | | | |

Table 5. Bond Angles($^{\circ}$)

| atom | atom | atom | angle | atom | atom | atom | angle S15D |
|-------|-------|-------|----------|-------|-------|-------|------------|
| Lu(2) | Lu(1) | C(3) | 139.8(8) | Lu(2) | Lu(1) | C(4) | 139.2(7) |
| Lu(2) | Lu(1) | C(5) | 108.3(7) | Lu(2) | Lu(1) | C(6) | 92.0(7) |
| Lu(2) | Lu(1) | C(7) | 107.1(7) | Lu(2) | Lu(1) | C(9) | 136.5(4) |
| Lu(2) | Lu(1) | C(10) | 105.2(4) | Lu(2) | Lu(1) | C(11) | 90.0(4) |
| Lu(2) | Lu(1) | C(12) | 105.1(4) | Lu(2) | Lu(1) | C(8) | 136.7(4) |
| C(3) | Lu(1) | C(4) | 32.6(10) | C(3) | Lu(1) | C(5) | 53.9(9) |
| C(3) | Lu(1) | C(6) | 53.3(10) | C(3) | Lu(1) | C(7) | 32(1) |
| C(3) | Lu(1) | C(9) | 82.5(8) | C(3) | Lu(1) | C(10) | 113.6(8) |
| C(3) | Lu(1) | C(11) | 118.8(8) | C(3) | Lu(1) | C(12) | 91.8(8) |
| C(3) | Lu(1) | C(8) | 67.9(8) | C(4) | Lu(1) | C(5) | 31.1(9) |
| C(4) | Lu(1) | C(6) | 51.4(10) | C(4) | Lu(1) | C(7) | 52.7(10) |
| C(4) | Lu(1) | C(9) | 79.9(8) | C(4) | Lu(1) | C(10) | 108.2(8) |
| C(4) | Lu(1) | C(11) | 130.1(8) | C(4) | Lu(1) | C(12) | 113.9(8) |
| C(4) | Lu(1) | C(8) | 83.2(8) | C(5) | Lu(1) | C(6) | 31.5(9) |
| C(5) | Lu(1) | C(7) | 53.2(9) | C(5) | Lu(1) | C(9) | 106.8(8) |
| C(5) | Lu(1) | C(10) | 128.5(8) | C(5) | Lu(1) | C(11) | 157.4(8) |
| C(5) | Lu(1) | C(12) | 144.2(8) | C(5) | Lu(1) | C(8) | 114.2(8) |
| C(6) | Lu(1) | C(7) | 31.9(10) | C(6) | Lu(1) | C(9) | 130.7(8) |
| C(6) | Lu(1) | C(10) | 158.9(8) | C(6) | Lu(1) | C(11) | 165.9(8) |
| C(6) | Lu(1) | C(12) | 136.5(8) | C(6) | Lu(1) | C(8) | 120.9(8) |
| C(7) | Lu(1) | C(9) | 114.3(8) | C(7) | Lu(1) | C(10) | 143.9(8) |
| C(7) | Lu(1) | C(11) | 134.7(8) | C(7) | Lu(1) | C(12) | 104.7(8) |
| C(7) | Lu(1) | C(8) | 92.6(8) | C(9) | Lu(1) | C(10) | 31.3(5) |
| C(9) | Lu(1) | C(11) | 51.1(6) | C(9) | Lu(1) | C(12) | 52.5(5) |

Table 5. Bond Angles($^{\circ}$) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|----------|-------|-------|-------|----------|
| C(9) | Lu(1) | C(8) | 32.7(6) | C(10) | Lu(1) | C(11) | 30.1(6) |
| C(10) | Lu(1) | C(12) | 50.8(5) | C(10) | Lu(1) | C(8) | 52.2(5) |
| C(11) | Lu(1) | C(12) | 30.2(6) | C(11) | Lu(1) | C(8) | 51.3(6) |
| C(12) | Lu(1) | C(8) | 31.7(6) | Lu(1) | Lu(2) | C(29) | 142.1(7) |
| Lu(1) | Lu(2) | C(30) | 130.2(7) | Lu(1) | Lu(2) | C(31) | 99.4(8) |
| Lu(1) | Lu(2) | C(32) | 88.0(7) | Lu(1) | Lu(2) | C(33) | 105.2(7) |
| Lu(1) | Lu(2) | C(34) | 146.5(8) | Lu(1) | Lu(2) | C(35) | 140.6(8) |
| Lu(1) | Lu(2) | C(37) | 97.3(8) | Lu(1) | Lu(2) | C(38) | 114.7(8) |
| C(29) | Lu(2) | C(30) | 36.5(10) | C(29) | Lu(2) | C(31) | 59(1) |
| C(29) | Lu(2) | C(32) | 56(1) | C(29) | Lu(2) | C(33) | 37(1) |
| C(29) | Lu(2) | C(34) | 61(1) | C(29) | Lu(2) | C(35) | 77(1) |
| C(29) | Lu(2) | C(37) | 113(1) | C(29) | Lu(2) | C(38) | 86(1) |
| C(30) | Lu(2) | C(31) | 30(1) | C(30) | Lu(2) | C(32) | 51(1) |
| C(30) | Lu(2) | C(33) | 54(1) | C(30) | Lu(2) | C(34) | 83(1) |
| C(30) | Lu(2) | C(35) | 80(1) | C(30) | Lu(2) | C(37) | 130(1) |
| C(30) | Lu(2) | C(38) | 114(1) | C(31) | Lu(2) | C(32) | 33(1) |
| C(31) | Lu(2) | C(33) | 54(1) | C(31) | Lu(2) | C(34) | 113(1) |
| C(31) | Lu(2) | C(35) | 107(1) | C(31) | Lu(2) | C(37) | 157(1) |
| C(31) | Lu(2) | C(38) | 144(1) | C(32) | Lu(2) | C(33) | 29.5(9) |
| C(32) | Lu(2) | C(34) | 116(1) | C(32) | Lu(2) | C(35) | 129(1) |
| C(32) | Lu(2) | C(37) | 162(1) | C(32) | Lu(2) | C(38) | 133(1) |
| C(33) | Lu(2) | C(34) | 90(1) | C(33) | Lu(2) | C(35) | 113(1) |
| C(33) | Lu(2) | C(37) | 133(1) | C(33) | Lu(2) | C(38) | 104(1) |
| C(34) | Lu(2) | C(35) | 31(1) | C(34) | Lu(2) | C(37) | 52(1) |

Table 5. Bond Angles($^{\circ}$) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|--------|-------|-------|-------|--------|
| C(34) | Lu(2) | C(38) | 31(1) | C(35) | Lu(2) | C(37) | 50(1) |
| C(35) | Lu(2) | C(38) | 50(1) | C(37) | Lu(2) | C(38) | 29(1) |
| C(1) | Si(1) | C(2) | 111(1) | C(1) | Si(1) | C(3) | 113(1) |
| C(1) | Si(1) | C(8) | 110(1) | C(2) | Si(1) | C(3) | 110(1) |
| C(2) | Si(1) | C(8) | 115(1) | C(3) | Si(1) | C(8) | 94(1) |
| C(27) | Si(2) | C(28) | 111(1) | C(27) | Si(2) | C(29) | 111(1) |
| C(27) | Si(2) | C(34) | 114(1) | C(28) | Si(2) | C(29) | 114(1) |
| C(28) | Si(2) | C(34) | 111(1) | C(29) | Si(2) | C(34) | 92(1) |
| Lu(1) | C(3) | Si(1) | 97(1) | Lu(1) | C(3) | C(4) | 75(1) |
| Lu(1) | C(3) | C(7) | 75(1) | Si(1) | C(3) | C(4) | 123(2) |
| Si(1) | C(3) | C(7) | 127(2) | C(4) | C(3) | C(7) | 105(2) |
| Lu(1) | C(4) | C(3) | 72(1) | Lu(1) | C(4) | C(5) | 79(1) |
| C(3) | C(4) | C(5) | 112(2) | Lu(1) | C(5) | C(4) | 69(1) |
| Lu(1) | C(5) | C(6) | 74(1) | Lu(1) | C(5) | C(13) | 123(1) |
| C(4) | C(5) | C(6) | 105(2) | C(4) | C(5) | C(13) | 133(2) |
| C(6) | C(5) | C(13) | 121(2) | Lu(1) | C(6) | C(5) | 74(1) |
| Lu(1) | C(6) | C(7) | 69(1) | C(5) | C(6) | C(7) | 108(2) |
| Lu(1) | C(7) | C(3) | 72(1) | Lu(1) | C(7) | C(6) | 78(1) |
| C(3) | C(7) | C(6) | 108(2) | C(5) | C(13) | C(14) | 114(2) |
| C(5) | C(13) | C(18) | 113(2) | C(14) | C(13) | C(18) | 111(2) |
| C(13) | C(14) | C(15) | 112(2) | C(13) | C(14) | C(19) | 110(2) |
| C(15) | C(14) | C(19) | 110(2) | C(14) | C(15) | C(16) | 107(2) |
| C(15) | C(16) | C(17) | 110(2) | C(16) | C(17) | C(18) | 114(2) |
| C(16) | C(17) | C(22) | 111(2) | C(18) | C(17) | C(22) | 104(2) |

Table 5. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|--------|-------|-------|-------|--------|
| C(13) | C(18) | C(17) | 111(2) | C(14) | C(19) | C(20) | 110(2) |
| C(14) | C(19) | C(21) | 109(2) | C(20) | C(19) | C(21) | 105(2) |
| C(24) | C(23) | C(25) | 96(2) | C(24) | C(23) | C(26) | 94(2) |
| C(24) | C(23) | C(10) | 103(2) | C(25) | C(23) | C(26) | 110(3) |
| C(25) | C(23) | C(10) | 127(2) | C(26) | C(23) | C(10) | 115(2) |
| Lu(2) | C(29) | Si(2) | 106(1) | Lu(2) | C(29) | C(30) | 74(1) |
| Lu(2) | C(29) | C(33) | 77(1) | Si(2) | C(29) | C(30) | 131(2) |
| Si(2) | C(29) | C(33) | 131(2) | C(30) | C(29) | C(33) | 96(2) |
| Lu(2) | C(30) | C(29) | 69(1) | Lu(2) | C(30) | C(31) | 74(1) |
| C(29) | C(30) | C(31) | 115(2) | Lu(2) | C(31) | C(30) | 75(1) |
| Lu(2) | C(31) | C(32) | 77(1) | Lu(2) | C(31) | C(39) | 128(2) |
| C(30) | C(31) | C(32) | 104(2) | C(30) | C(31) | C(39) | 129(2) |
| C(32) | C(31) | C(39) | 122(2) | Lu(2) | C(32) | C(31) | 68(1) |
| Lu(2) | C(32) | C(33) | 75(1) | C(31) | C(32) | C(33) | 113(2) |
| Lu(2) | C(33) | C(29) | 65(1) | Lu(2) | C(33) | C(32) | 75(1) |
| C(29) | C(33) | C(32) | 108(2) | Lu(2) | C(34) | Si(2) | 98(1) |
| Lu(2) | C(34) | C(35) | 74(1) | Lu(2) | C(34) | C(38) | 74(2) |
| Si(2) | C(34) | C(35) | 122(2) | Si(2) | C(34) | C(38) | 132(2) |
| C(35) | C(34) | C(38) | 100(3) | Lu(2) | C(35) | C(34) | 74(1) |
| Lu(2) | C(35) | C(36) | 84(1) | C(34) | C(35) | C(36) | 114(3) |
| C(35) | C(36) | C(37) | 98(2) | C(35) | C(36) | C(49) | 125(3) |
| C(37) | C(36) | C(49) | 135(3) | Lu(2) | C(37) | C(36) | 83(1) |
| Lu(2) | C(37) | C(38) | 73(2) | C(36) | C(37) | C(38) | 111(3) |
| Lu(2) | C(38) | C(34) | 73(2) | Lu(2) | C(38) | C(37) | 76(2) |

Table 5. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|----------|-------|-------|-------|----------|
| C(34) | C(38) | C(37) | 112(3) | C(31) | C(39) | C(40) | 118(2) |
| C(31) | C(39) | C(44) | 108(2) | C(40) | C(39) | C(44) | 111(2) |
| C(39) | C(40) | C(41) | 115(2) | C(39) | C(40) | C(45) | 113(2) |
| C(41) | C(40) | C(45) | 113(2) | C(40) | C(41) | C(42) | 106(2) |
| C(41) | C(42) | C(43) | 106(2) | C(42) | C(43) | C(44) | 103(2) |
| C(42) | C(43) | C(48) | 104(3) | C(44) | C(43) | C(48) | 116(3) |
| C(39) | C(44) | C(43) | 121(2) | C(40) | C(45) | C(46) | 118(2) |
| C(40) | C(45) | C(47) | 109(2) | C(46) | C(45) | C(47) | 101(2) |
| C(36) | C(49) | C(50) | 113(3) | C(36) | C(49) | C(51) | 109(2) |
| C(36) | C(49) | C(52) | 107(3) | C(50) | C(49) | C(51) | 116(3) |
| C(50) | C(49) | C(52) | 103(3) | C(51) | C(49) | C(52) | 105(3) |
| Lu(1) | C(9) | C(10) | 80(1) | Lu(1) | C(9) | C(8) | 72.8(10) |
| C(10) | C(9) | C(8) | 107(1) | Lu(1) | C(10) | C(23) | 127(1) |
| Lu(1) | C(10) | C(9) | 68.0(10) | Lu(1) | C(10) | C(11) | 77(1) |
| C(23) | C(10) | C(9) | 112(2) | C(23) | C(10) | C(11) | 137(2) |
| C(9) | C(10) | C(11) | 107(1) | Lu(1) | C(11) | C(10) | 72(1) |
| Lu(1) | C(11) | C(12) | 70(1) | C(10) | C(11) | C(12) | 108(1) |
| Lu(1) | C(12) | C(11) | 79(1) | Lu(1) | C(12) | C(8) | 68(1) |
| C(11) | C(12) | C(8) | 107(1) | Lu(1) | C(8) | Si(1) | 98.0(8) |
| Lu(1) | C(8) | C(9) | 74.5(9) | Lu(1) | C(8) | C(12) | 80(1) |
| Si(1) | C(8) | C(9) | 121(1) | Si(1) | C(8) | C(12) | 127(1) |
| C(9) | C(8) | C(12) | 108(1) | | | | |

Table 6. Bond Angles($^{\circ}$)

| atom | atom | atom | angle | atom | atom | atom | angle S15D |
|-------|-------|-------|-------|-------|-------|-------|------------|
| Si(1) | C(1) | H(1) | 109.5 | Si(1) | C(1) | H(2) | 109.5 |
| Si(1) | C(1) | H(3) | 109.5 | H(1) | C(1) | H(2) | 109.4 |
| H(1) | C(1) | H(3) | 109.5 | H(2) | C(1) | H(3) | 109.4 |
| Si(1) | C(2) | H(4) | 109.5 | Si(1) | C(2) | H(5) | 109.5 |
| Si(1) | C(2) | H(6) | 109.5 | H(4) | C(2) | H(5) | 109.5 |
| H(4) | C(2) | H(6) | 109.5 | H(5) | C(2) | H(6) | 109.5 |
| Lu(1) | C(4) | H(7) | 116.5 | C(3) | C(4) | H(7) | 123.7 |
| C(5) | C(4) | H(7) | 123.7 | Lu(1) | C(6) | H(8) | 122.1 |
| C(5) | C(6) | H(8) | 125.9 | C(7) | C(6) | H(8) | 125.9 |
| Lu(1) | C(7) | H(9) | 115.5 | C(3) | C(7) | H(9) | 125.6 |
| C(6) | C(7) | H(9) | 125.5 | C(5) | C(13) | H(10) | 105.5 |
| C(14) | C(13) | H(10) | 105.5 | C(18) | C(13) | H(10) | 105.5 |
| C(13) | C(14) | H(11) | 107.4 | C(15) | C(14) | H(11) | 107.4 |
| C(19) | C(14) | H(11) | 107.4 | C(14) | C(15) | H(12) | 109.9 |
| C(14) | C(15) | H(13) | 109.9 | C(16) | C(15) | H(12) | 109.8 |
| C(16) | C(15) | H(13) | 109.9 | H(12) | C(15) | H(13) | 109.5 |
| C(15) | C(16) | H(14) | 109.3 | C(15) | C(16) | H(15) | 109.3 |
| C(17) | C(16) | H(14) | 109.4 | C(17) | C(16) | H(15) | 109.3 |
| H(14) | C(16) | H(15) | 109.5 | C(16) | C(17) | H(16) | 108.9 |
| C(18) | C(17) | H(16) | 109.0 | C(22) | C(17) | H(16) | 109.0 |
| C(13) | C(18) | H(17) | 109.0 | C(13) | C(18) | H(18) | 109.0 |
| C(17) | C(18) | H(17) | 109.1 | C(17) | C(18) | H(18) | 109.0 |
| H(17) | C(18) | H(18) | 109.4 | C(19) | C(20) | H(19) | 109.5 |
| C(19) | C(20) | H(20) | 109.5 | C(19) | C(20) | H(21) | 109.5 |

Table 6. Bond Angles($^{\circ}$) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|-------|-------|-------|-------|-------|
| H(19) | C(20) | H(20) | 109.4 | H(19) | C(20) | H(21) | 109.4 |
| H(20) | C(20) | H(21) | 109.4 | C(19) | C(21) | H(22) | 109.5 |
| C(19) | C(21) | H(23) | 109.5 | C(19) | C(21) | H(24) | 109.5 |
| H(22) | C(21) | H(23) | 109.4 | H(22) | C(21) | H(24) | 109.4 |
| H(23) | C(21) | H(24) | 109.5 | C(17) | C(22) | H(25) | 109.4 |
| C(17) | C(22) | H(26) | 109.5 | C(17) | C(22) | H(27) | 109.5 |
| H(25) | C(22) | H(26) | 109.4 | H(25) | C(22) | H(27) | 109.5 |
| H(26) | C(22) | H(27) | 109.5 | C(23) | C(24) | H(28) | 109.5 |
| C(23) | C(24) | H(29) | 109.6 | C(23) | C(24) | H(30) | 109.5 |
| H(28) | C(24) | H(29) | 109.4 | H(28) | C(24) | H(30) | 109.5 |
| H(29) | C(24) | H(30) | 109.4 | C(23) | C(25) | H(31) | 109.4 |
| C(23) | C(25) | H(32) | 109.5 | C(23) | C(25) | H(33) | 109.5 |
| H(31) | C(25) | H(32) | 109.5 | H(31) | C(25) | H(33) | 109.4 |
| H(32) | C(25) | H(33) | 109.5 | C(23) | C(26) | H(34) | 109.6 |
| C(23) | C(26) | H(35) | 109.2 | C(23) | C(26) | H(36) | 109.0 |
| H(34) | C(26) | H(35) | 110.0 | H(34) | C(26) | H(36) | 109.8 |
| H(35) | C(26) | H(36) | 109.2 | Si(2) | C(27) | H(37) | 109.5 |
| Si(2) | C(27) | H(38) | 109.5 | Si(2) | C(27) | H(39) | 109.5 |
| H(37) | C(27) | H(38) | 109.4 | H(37) | C(27) | H(39) | 109.4 |
| H(38) | C(27) | H(39) | 109.5 | Si(2) | C(28) | H(40) | 109.5 |
| Si(2) | C(28) | H(41) | 109.5 | Si(2) | C(28) | H(42) | 109.5 |
| H(40) | C(28) | H(41) | 109.4 | H(40) | C(28) | H(42) | 109.5 |
| H(41) | C(28) | H(42) | 109.4 | Lu(2) | C(30) | H(43) | 126.1 |
| C(29) | C(30) | H(43) | 122.2 | C(31) | C(30) | H(43) | 122.3 |

Table 6. Bond Angles($^{\circ}$) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|-------|-------|-------|-------|-------|
| Lu(2) | C(32) | H(44) | 124.2 | C(31) | C(32) | H(44) | 123.2 |
| C(33) | C(32) | H(44) | 123.2 | Lu(2) | C(33) | H(45) | 124.5 |
| C(29) | C(33) | H(45) | 125.9 | C(32) | C(33) | H(45) | 125.8 |
| Lu(2) | C(35) | H(46) | 109.7 | C(34) | C(35) | H(46) | 122.6 |
| C(36) | C(35) | H(46) | 122.6 | Lu(2) | C(37) | H(47) | 111.1 |
| C(36) | C(37) | H(47) | 124.1 | C(38) | C(37) | H(47) | 124.2 |
| Lu(2) | C(38) | H(48) | 117.2 | C(34) | C(38) | H(48) | 123.6 |
| C(37) | C(38) | H(48) | 123.5 | C(31) | C(39) | H(49) | 106.1 |
| C(40) | C(39) | H(49) | 106.1 | C(44) | C(39) | H(49) | 106.2 |
| C(39) | C(40) | H(50) | 104.5 | C(41) | C(40) | H(50) | 104.6 |
| C(45) | C(40) | H(50) | 104.6 | C(40) | C(41) | H(51) | 110.2 |
| C(40) | C(41) | H(52) | 110.2 | C(42) | C(41) | H(51) | 110.3 |
| C(42) | C(41) | H(52) | 110.2 | H(51) | C(41) | H(52) | 109.3 |
| C(41) | C(42) | H(53) | 110.1 | C(41) | C(42) | H(54) | 110.2 |
| C(43) | C(42) | H(53) | 110.1 | C(43) | C(42) | H(54) | 110.2 |
| H(53) | C(42) | H(54) | 109.5 | C(42) | C(43) | H(55) | 110.6 |
| C(44) | C(43) | H(55) | 110.8 | C(48) | C(43) | H(55) | 110.9 |
| C(39) | C(44) | H(56) | 109.4 | C(39) | C(44) | H(57) | 106.5 |
| C(43) | C(44) | H(56) | 106.4 | C(43) | C(44) | H(57) | 106.4 |
| H(56) | C(44) | H(57) | 109.4 | C(45) | C(46) | H(58) | 109.4 |
| C(45) | C(46) | H(59) | 109.4 | C(45) | C(46) | H(60) | 109.5 |
| H(58) | C(46) | H(59) | 109.5 | H(58) | C(46) | H(60) | 109.5 |
| H(59) | C(46) | H(60) | 109.6 | C(45) | C(47) | H(61) | 109.5 |
| C(45) | C(47) | H(62) | 109.5 | C(45) | C(47) | H(63) | 109.5 |

Table 6. Bond Angles($^{\circ}$) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|-------|-------|-------|-------|-------|-------|-------|-------|
| H(61) | C(47) | H(62) | 109.5 | H(61) | C(47) | H(63) | 109.5 |
| H(62) | C(47) | H(63) | 109.4 | C(43) | C(48) | H(64) | 109.5 |
| C(43) | C(48) | H(65) | 109.5 | C(43) | C(48) | H(66) | 109.4 |
| H(64) | C(48) | H(65) | 109.5 | H(64) | C(48) | H(66) | 109.5 |
| H(65) | C(48) | H(66) | 109.5 | C(49) | C(50) | H(67) | 109.2 |
| C(49) | C(50) | H(68) | 109.5 | C(49) | C(50) | H(69) | 109.4 |
| H(67) | C(50) | H(68) | 109.6 | H(67) | C(50) | H(69) | 109.4 |
| H(68) | C(50) | H(69) | 109.8 | C(49) | C(51) | H(70) | 109.5 |
| C(49) | C(51) | H(71) | 109.4 | C(49) | C(51) | H(72) | 109.4 |
| H(70) | C(51) | H(71) | 109.5 | H(70) | C(51) | H(72) | 109.6 |
| H(71) | C(51) | H(72) | 109.4 | C(49) | C(52) | H(73) | 109.4 |
| C(49) | C(52) | H(74) | 109.6 | C(49) | C(52) | H(75) | 109.5 |
| H(73) | C(52) | H(74) | 109.5 | H(73) | C(52) | H(75) | 109.4 |
| H(74) | C(52) | H(75) | 109.5 | | | | |

Table 7. Torsion Angles(°) S15D

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|------------|-------|-------|-------|-------|---------|
| Lu(1) | Lu(2) | C(29) | Si(2) | -138.8(10) | Lu(1) | Lu(2) | C(29) | C(30) | 91(1) |
| Lu(1) | Lu(2) | C(29) | C(33) | -8(2) | Lu(1) | Lu(2) | C(30) | C(29) | -126(1) |
| Lu(1) | Lu(2) | C(30) | C(31) | 0(2) | Lu(1) | Lu(2) | C(31) | C(30) | 179(1) |
| Lu(1) | Lu(2) | C(31) | C(32) | -71(1) | Lu(1) | Lu(2) | C(31) | C(39) | 49(2) |
| Lu(1) | Lu(2) | C(32) | C(31) | 110(1) | Lu(1) | Lu(2) | C(32) | C(33) | -126(2) |
| Lu(1) | Lu(2) | C(33) | C(29) | 174(1) | Lu(1) | Lu(2) | C(33) | C(32) | 56(2) |
| Lu(1) | Lu(2) | C(34) | Si(2) | 135.6(10) | Lu(1) | Lu(2) | C(34) | C(35) | -102(2) |
| Lu(1) | Lu(2) | C(34) | C(38) | 3(2) | Lu(1) | Lu(2) | C(35) | C(34) | 122(1) |
| Lu(1) | Lu(2) | C(35) | C(36) | 4(2) | Lu(1) | Lu(2) | C(37) | C(36) | -116(1) |
| Lu(1) | Lu(2) | C(37) | C(38) | 128(2) | Lu(1) | Lu(2) | C(38) | C(34) | -177(1) |
| Lu(1) | Lu(2) | C(38) | C(37) | -58(2) | Lu(1) | C(3) | Si(1) | C(1) | -126(1) |
| Lu(1) | C(3) | Si(1) | C(2) | 108(1) | Lu(1) | C(3) | Si(1) | C(8) | -11(1) |
| Lu(1) | C(3) | C(4) | C(5) | -69(2) | Lu(1) | C(3) | C(7) | C(6) | 70(2) |
| Lu(1) | C(4) | C(3) | Si(1) | -89(2) | Lu(1) | C(4) | C(3) | C(7) | 69(1) |
| Lu(1) | C(4) | C(5) | C(6) | -66(2) | Lu(1) | C(4) | C(5) | C(13) | 116(3) |
| Lu(1) | C(5) | C(4) | C(3) | 65(2) | Lu(1) | C(5) | C(6) | C(7) | -61(2) |
| Lu(1) | C(5) | C(13) | C(14) | 173(1) | Lu(1) | C(5) | C(13) | C(18) | 43(3) |
| Lu(1) | C(6) | C(5) | C(4) | 63(2) | Lu(1) | C(6) | C(5) | C(13) | -119(2) |
| Lu(1) | C(6) | C(7) | C(3) | -66(2) | Lu(1) | C(7) | C(3) | Si(1) | 88(2) |
| Lu(1) | C(7) | C(3) | C(4) | -69(1) | Lu(1) | C(7) | C(6) | C(5) | 64(2) |
| Lu(1) | C(9) | C(10) | C(23) | -122(1) | Lu(1) | C(9) | C(10) | C(11) | 68(1) |
| Lu(1) | C(9) | C(8) | Si(1) | 89(1) | Lu(1) | C(9) | C(8) | C(12) | -73(1) |
| Lu(1) | C(10) | C(23) | C(24) | 87(2) | Lu(1) | C(10) | C(23) | C(25) | -22(4) |
| Lu(1) | C(10) | C(23) | C(26) | -171(2) | Lu(1) | C(10) | C(9) | C(8) | -68(1) |

Table 7. Torsion Angles($^{\circ}$) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|------------|-------|-------|-------|-------|------------|
| Lu(1) | C(10) | C(11) | C(12) | 61(1) | Lu(1) | C(11) | C(10) | C(23) | 133(3) |
| Lu(1) | C(11) | C(10) | C(9) | -61(1) | Lu(1) | C(11) | C(12) | C(8) | 62(1) |
| Lu(1) | C(12) | C(11) | C(10) | -62(1) | Lu(1) | C(12) | C(8) | Si(1) | -92(1) |
| Lu(1) | C(12) | C(8) | C(9) | 69(1) | Lu(1) | C(8) | Si(1) | C(1) | 128(1) |
| Lu(1) | C(8) | Si(1) | C(2) | -103(1) | Lu(1) | C(8) | Si(1) | C(3) | 11(1) |
| Lu(1) | C(8) | C(9) | C(10) | 73(1) | Lu(1) | C(8) | C(12) | C(11) | -69(1) |
| Lu(2) | Lu(1) | C(3) | Si(1) | -128.1(10) | Lu(2) | Lu(1) | C(3) | C(4) | 109(1) |
| Lu(2) | Lu(1) | C(3) | C(7) | -1(2) | Lu(2) | Lu(1) | C(4) | C(3) | -110(1) |
| Lu(2) | Lu(1) | C(4) | C(5) | 7(2) | Lu(2) | Lu(1) | C(5) | C(4) | -174(1) |
| Lu(2) | Lu(1) | C(5) | C(6) | -61(1) | Lu(2) | Lu(1) | C(5) | C(13) | 55(2) |
| Lu(2) | Lu(1) | C(6) | C(5) | 123(1) | Lu(2) | Lu(1) | C(6) | C(7) | -120(1) |
| Lu(2) | Lu(1) | C(7) | C(3) | 179(1) | Lu(2) | Lu(1) | C(7) | C(6) | 64(1) |
| Lu(2) | Lu(1) | C(9) | C(10) | -3(1) | Lu(2) | Lu(1) | C(9) | C(8) | 108.5(10) |
| Lu(2) | Lu(1) | C(10) | C(23) | -80(2) | Lu(2) | Lu(1) | C(10) | C(9) | 177.3(9) |
| Lu(2) | Lu(1) | C(10) | C(11) | 62(1) | Lu(2) | Lu(1) | C(11) | C(10) | -121.6(10) |
| Lu(2) | Lu(1) | C(11) | C(12) | 121(1) | Lu(2) | Lu(1) | C(12) | C(11) | -62(1) |
| Lu(2) | Lu(1) | C(12) | C(8) | -177.0(9) | Lu(2) | Lu(1) | C(8) | Si(1) | 131.4(6) |
| Lu(2) | Lu(1) | C(8) | C(9) | -107.7(10) | Lu(2) | Lu(1) | C(8) | C(12) | 4(1) |
| Lu(2) | C(29) | Si(2) | C(27) | -127(1) | Lu(2) | C(29) | Si(2) | C(28) | 104(1) |
| Lu(2) | C(29) | Si(2) | C(34) | -10(1) | Lu(2) | C(29) | C(30) | C(31) | -59(2) |
| Lu(2) | C(29) | C(33) | C(32) | 63(2) | Lu(2) | C(30) | C(29) | Si(2) | -98(2) |
| Lu(2) | C(30) | C(29) | C(33) | 74(1) | Lu(2) | C(30) | C(31) | C(32) | -72(2) |
| Lu(2) | C(30) | C(31) | C(39) | 128(3) | Lu(2) | C(31) | C(30) | C(29) | 57(2) |
| Lu(2) | C(31) | C(32) | C(33) | -62(2) | Lu(2) | C(31) | C(39) | C(40) | -176(2) |

Table 7. Torsion Angles(°) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|-----------|-------|-------|-------|-------|----------|
| Lu(2) | C(31) | C(39) | C(44) | 55(3) | Lu(2) | C(32) | C(31) | C(30) | 70(2) |
| Lu(2) | C(32) | C(31) | C(39) | -128(3) | Lu(2) | C(32) | C(33) | C(29) | -57(2) |
| Lu(2) | C(33) | C(29) | Si(2) | 100(2) | Lu(2) | C(33) | C(29) | C(30) | -72(1) |
| Lu(2) | C(33) | C(32) | C(31) | 58(2) | Lu(2) | C(34) | Si(2) | C(27) | 124(1) |
| Lu(2) | C(34) | Si(2) | C(28) | -107(1) | Lu(2) | C(34) | Si(2) | C(29) | 9(1) |
| Lu(2) | C(34) | C(35) | C(36) | 76(2) | Lu(2) | C(34) | C(38) | C(37) | -67(2) |
| Lu(2) | C(35) | C(34) | Si(2) | 89(2) | Lu(2) | C(35) | C(34) | C(38) | -70(2) |
| Lu(2) | C(35) | C(36) | C(37) | 58(2) | Lu(2) | C(35) | C(36) | C(49) | -120(3) |
| Lu(2) | C(37) | C(36) | C(35) | -56(2) | Lu(2) | C(37) | C(36) | C(49) | 121(3) |
| Lu(2) | C(37) | C(38) | C(34) | 65(2) | Lu(2) | C(38) | C(34) | Si(2) | -87(3) |
| Lu(2) | C(38) | C(34) | C(35) | 69(2) | Lu(2) | C(38) | C(37) | C(36) | -75(2) |
| Si(1) | C(3) | Lu(1) | C(4) | 122(2) | Si(1) | C(3) | Lu(1) | C(5) | 156(1) |
| Si(1) | C(3) | Lu(1) | C(6) | -163(1) | Si(1) | C(3) | Lu(1) | C(7) | -126(2) |
| Si(1) | C(3) | Lu(1) | C(9) | 39(1) | Si(1) | C(3) | Lu(1) | C(10) | 35(1) |
| Si(1) | C(3) | Lu(1) | C(11) | 2(1) | Si(1) | C(3) | Lu(1) | C(12) | -11(1) |
| Si(1) | C(3) | Lu(1) | C(8) | 9(1) | Si(1) | C(3) | C(4) | C(5) | -159(2) |
| Si(1) | C(3) | C(7) | C(6) | 159(2) | Si(1) | C(8) | Lu(1) | C(3) | -9.1(10) |
| Si(1) | C(8) | Lu(1) | C(4) | -39.0(10) | Si(1) | C(8) | Lu(1) | C(5) | -37(1) |
| Si(1) | C(8) | Lu(1) | C(6) | -2(1) | Si(1) | C(8) | Lu(1) | C(7) | 12.9(10) |
| Si(1) | C(8) | Lu(1) | C(9) | -120(1) | Si(1) | C(8) | Lu(1) | C(10) | -158(1) |
| Si(1) | C(8) | Lu(1) | C(11) | 163(1) | Si(1) | C(8) | Lu(1) | C(12) | 127(1) |
| Si(1) | C(8) | C(9) | C(10) | 163(1) | Si(1) | C(8) | C(12) | C(11) | -162(1) |
| Si(2) | C(29) | Lu(2) | C(30) | 129(2) | Si(2) | C(29) | Lu(2) | C(31) | 158(2) |
| Si(2) | C(29) | Lu(2) | C(32) | -161(2) | Si(2) | C(29) | Lu(2) | C(33) | -130(2) |

Table 7. Torsion Angles($^{\circ}$) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|---------|-------|-------|-------|-------|---------|
| Si(2) | C(29) | Lu(2) | C(34) | 8(1) | Si(2) | C(29) | Lu(2) | C(35) | 38(1) |
| Si(2) | C(29) | Lu(2) | C(37) | 2(1) | Si(2) | C(29) | Lu(2) | C(38) | -11(1) |
| Si(2) | C(29) | C(30) | C(31) | -157(2) | Si(2) | C(29) | C(33) | C(32) | 164(2) |
| Si(2) | C(34) | Lu(2) | C(29) | -7(1) | Si(2) | C(34) | Lu(2) | C(30) | -38(1) |
| Si(2) | C(34) | Lu(2) | C(31) | -35(1) | Si(2) | C(34) | Lu(2) | C(32) | 1(1) |
| Si(2) | C(34) | Lu(2) | C(33) | 15(1) | Si(2) | C(34) | Lu(2) | C(35) | -121(2) |
| Si(2) | C(34) | Lu(2) | C(37) | 165(2) | Si(2) | C(34) | Lu(2) | C(38) | 131(2) |
| Si(2) | C(34) | C(35) | C(36) | 166(2) | Si(2) | C(34) | C(38) | C(37) | -155(2) |
| C(1) | Si(1) | C(3) | C(4) | -48(2) | C(1) | Si(1) | C(3) | C(7) | 156(2) |
| C(1) | Si(1) | C(8) | C(9) | 51(2) | C(1) | Si(1) | C(8) | C(12) | -148(1) |
| C(2) | Si(1) | C(3) | C(4) | -174(2) | C(2) | Si(1) | C(3) | C(7) | 31(3) |
| C(2) | Si(1) | C(8) | C(9) | 179(1) | C(2) | Si(1) | C(8) | C(12) | -20(2) |
| C(3) | Lu(1) | Lu(2) | C(29) | -65(1) | C(3) | Lu(1) | Lu(2) | C(30) | -14(1) |
| C(3) | Lu(1) | Lu(2) | C(31) | -14(1) | C(3) | Lu(1) | Lu(2) | C(32) | -46(1) |
| C(3) | Lu(1) | Lu(2) | C(33) | -70(1) | C(3) | Lu(1) | Lu(2) | C(34) | 173(1) |
| C(3) | Lu(1) | Lu(2) | C(35) | 119(1) | C(3) | Lu(1) | Lu(2) | C(37) | 150(1) |
| C(3) | Lu(1) | Lu(2) | C(38) | 175(1) | C(3) | Lu(1) | C(4) | C(5) | 118(2) |
| C(3) | Lu(1) | C(5) | C(4) | -36(1) | C(3) | Lu(1) | C(5) | C(6) | 77(1) |
| C(3) | Lu(1) | C(5) | C(13) | -165(2) | C(3) | Lu(1) | C(6) | C(5) | -79(1) |
| C(3) | Lu(1) | C(6) | C(7) | 37(1) | C(3) | Lu(1) | C(7) | C(6) | -114(2) |
| C(3) | Lu(1) | C(9) | C(10) | -172(1) | C(3) | Lu(1) | C(9) | C(8) | -60(1) |
| C(3) | Lu(1) | C(10) | C(23) | 110(2) | C(3) | Lu(1) | C(10) | C(9) | 8(1) |
| C(3) | Lu(1) | C(10) | C(11) | -107(1) | C(3) | Lu(1) | C(11) | C(10) | 87(1) |
| C(3) | Lu(1) | C(11) | C(12) | -29(1) | C(3) | Lu(1) | C(12) | C(11) | 154(1) |

Table 7. Torsion Angles($^{\circ}$) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|------|-------|-------|-------|---------|------|-------|-------|-------|---------|
| C(3) | Lu(1) | C(12) | C(8) | 39(1) | C(3) | Lu(1) | C(8) | C(9) | 111(1) |
| C(3) | Lu(1) | C(8) | C(12) | -136(1) | C(3) | Si(1) | C(8) | C(9) | -65(1) |
| C(3) | Si(1) | C(8) | C(12) | 94(1) | C(3) | C(4) | Lu(1) | C(5) | -118(2) |
| C(3) | C(4) | Lu(1) | C(6) | -80(2) | C(3) | C(4) | Lu(1) | C(7) | -39(1) |
| C(3) | C(4) | Lu(1) | C(9) | 91(1) | C(3) | C(4) | Lu(1) | C(10) | 105(1) |
| C(3) | C(4) | Lu(1) | C(11) | 81(1) | C(3) | C(4) | Lu(1) | C(12) | 51(1) |
| C(3) | C(4) | Lu(1) | C(8) | 59(1) | C(3) | C(4) | C(5) | C(6) | -1(3) |
| C(3) | C(4) | C(5) | C(13) | -177(3) | C(3) | C(7) | Lu(1) | C(4) | 39(1) |
| C(3) | C(7) | Lu(1) | C(5) | 78(1) | C(3) | C(7) | Lu(1) | C(6) | 114(2) |
| C(3) | C(7) | Lu(1) | C(9) | -14(1) | C(3) | C(7) | Lu(1) | C(10) | -28(2) |
| C(3) | C(7) | Lu(1) | C(11) | -73(1) | C(3) | C(7) | Lu(1) | C(12) | -69(1) |
| C(3) | C(7) | Lu(1) | C(8) | -40(1) | C(3) | C(7) | C(6) | C(5) | -2(3) |
| C(4) | Lu(1) | Lu(2) | C(29) | -13(1) | C(4) | Lu(1) | Lu(2) | C(30) | 37(1) |
| C(4) | Lu(1) | Lu(2) | C(31) | 36(1) | C(4) | Lu(1) | Lu(2) | C(32) | 5(1) |
| C(4) | Lu(1) | Lu(2) | C(33) | -19(1) | C(4) | Lu(1) | Lu(2) | C(34) | -135(1) |
| C(4) | Lu(1) | Lu(2) | C(35) | 170(1) | C(4) | Lu(1) | Lu(2) | C(37) | -158(1) |
| C(4) | Lu(1) | Lu(2) | C(38) | -132(1) | C(4) | Lu(1) | C(3) | C(7) | -110(2) |
| C(4) | Lu(1) | C(5) | C(6) | 113(2) | C(4) | Lu(1) | C(5) | C(13) | -129(3) |
| C(4) | Lu(1) | C(6) | C(5) | -37(1) | C(4) | Lu(1) | C(6) | C(7) | 79(1) |
| C(4) | Lu(1) | C(7) | C(6) | -74(1) | C(4) | Lu(1) | C(9) | C(10) | 154(1) |
| C(4) | Lu(1) | C(9) | C(8) | -93(1) | C(4) | Lu(1) | C(10) | C(23) | 76(2) |
| C(4) | Lu(1) | C(10) | C(9) | -26(1) | C(4) | Lu(1) | C(10) | C(11) | -141(1) |
| C(4) | Lu(1) | C(11) | C(10) | 50(1) | C(4) | Lu(1) | C(11) | C(12) | -66(1) |
| C(4) | Lu(1) | C(12) | C(11) | 129(1) | C(4) | Lu(1) | C(12) | C(8) | 15(1) |

Table 7. Torsion Angles($^{\circ}$) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|------|-------|-------|-------|---------|------|-------|-------|-------|---------|
| C(4) | Lu(1) | C(8) | C(9) | 81(1) | C(4) | Lu(1) | C(8) | C(12) | -166(1) |
| C(4) | C(3) | Lu(1) | C(5) | 34(1) | C(4) | C(3) | Lu(1) | C(6) | 73(1) |
| C(4) | C(3) | Lu(1) | C(7) | 110(2) | C(4) | C(3) | Lu(1) | C(9) | -82(1) |
| C(4) | C(3) | Lu(1) | C(10) | -87(1) | C(4) | C(3) | Lu(1) | C(11) | -120(1) |
| C(4) | C(3) | Lu(1) | C(12) | -134(1) | C(4) | C(3) | Lu(1) | C(8) | -113(1) |
| C(4) | C(3) | Si(1) | C(8) | 66(2) | C(4) | C(3) | C(7) | C(6) | 1(3) |
| C(4) | C(5) | Lu(1) | C(6) | -113(2) | C(4) | C(5) | Lu(1) | C(7) | -76(1) |
| C(4) | C(5) | Lu(1) | C(9) | 31(1) | C(4) | C(5) | Lu(1) | C(10) | 57(1) |
| C(4) | C(5) | Lu(1) | C(11) | 42(2) | C(4) | C(5) | Lu(1) | C(12) | -16(2) |
| C(4) | C(5) | Lu(1) | C(8) | -2(1) | C(4) | C(5) | C(6) | C(7) | 1(3) |
| C(4) | C(5) | C(13) | C(14) | 80(4) | C(4) | C(5) | C(13) | C(18) | -49(4) |
| C(5) | Lu(1) | Lu(2) | C(29) | -9(1) | C(5) | Lu(1) | Lu(2) | C(30) | 41(1) |
| C(5) | Lu(1) | Lu(2) | C(31) | 40(1) | C(5) | Lu(1) | Lu(2) | C(32) | 9.0(10) |
| C(5) | Lu(1) | Lu(2) | C(33) | -15(1) | C(5) | Lu(1) | Lu(2) | C(34) | -131(1) |
| C(5) | Lu(1) | Lu(2) | C(35) | 174(1) | C(5) | Lu(1) | Lu(2) | C(37) | -154(1) |
| C(5) | Lu(1) | Lu(2) | C(38) | -128(1) | C(5) | Lu(1) | C(3) | C(7) | -76(1) |
| C(5) | Lu(1) | C(6) | C(7) | 116(2) | C(5) | Lu(1) | C(7) | C(6) | -35(1) |
| C(5) | Lu(1) | C(9) | C(10) | 138(1) | C(5) | Lu(1) | C(9) | C(8) | -108(1) |
| C(5) | Lu(1) | C(10) | C(23) | 49(2) | C(5) | Lu(1) | C(10) | C(9) | -53(1) |
| C(5) | Lu(1) | C(10) | C(11) | -168(1) | C(5) | Lu(1) | C(11) | C(10) | 23(2) |
| C(5) | Lu(1) | C(11) | C(12) | -94(2) | C(5) | Lu(1) | C(12) | C(11) | 139(1) |
| C(5) | Lu(1) | C(12) | C(8) | 24(1) | C(5) | Lu(1) | C(8) | C(9) | 83(1) |
| C(5) | Lu(1) | C(8) | C(12) | -164(1) | C(5) | C(4) | Lu(1) | C(6) | 37(1) |
| C(5) | C(4) | Lu(1) | C(7) | 78(1) | C(5) | C(4) | Lu(1) | C(9) | -149(1) |

Table 7. Torsion Angles($^{\circ}$) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|------|-------|-------|-------|---------|------|-------|-------|-------|-----------|
| C(5) | C(4) | Lu(1) | C(10) | -136(1) | C(5) | C(4) | Lu(1) | C(11) | -160(1) |
| C(5) | C(4) | Lu(1) | C(12) | 169(1) | C(5) | C(4) | Lu(1) | C(8) | 177(1) |
| C(5) | C(4) | C(3) | C(7) | 0(3) | C(5) | C(6) | Lu(1) | C(7) | -116(2) |
| C(5) | C(6) | Lu(1) | C(9) | -47(2) | C(5) | C(6) | Lu(1) | C(10) | -22(3) |
| C(5) | C(6) | Lu(1) | C(11) | -139(2) | C(5) | C(6) | Lu(1) | C(12) | -122(1) |
| C(5) | C(6) | Lu(1) | C(8) | -86(1) | C(5) | C(13) | C(14) | C(15) | -73(3) |
| C(5) | C(13) | C(14) | C(19) | 51(3) | C(5) | C(13) | C(18) | C(17) | 81(3) |
| C(6) | Lu(1) | Lu(2) | C(29) | -37(1) | C(6) | Lu(1) | Lu(2) | C(30) | 13(1) |
| C(6) | Lu(1) | Lu(2) | C(31) | 13(1) | C(6) | Lu(1) | Lu(2) | C(32) | -18.4(10) |
| C(6) | Lu(1) | Lu(2) | C(33) | -42(1) | C(6) | Lu(1) | Lu(2) | C(34) | -158(1) |
| C(6) | Lu(1) | Lu(2) | C(35) | 147(1) | C(6) | Lu(1) | Lu(2) | C(37) | 178(1) |
| C(6) | Lu(1) | Lu(2) | C(38) | -156(1) | C(6) | Lu(1) | C(3) | C(7) | -36(1) |
| C(6) | Lu(1) | C(5) | C(13) | 117(3) | C(6) | Lu(1) | C(9) | C(10) | 162(1) |
| C(6) | Lu(1) | C(9) | C(8) | -85(1) | C(6) | Lu(1) | C(10) | C(23) | 63(3) |
| C(6) | Lu(1) | C(10) | C(9) | -39(2) | C(6) | Lu(1) | C(10) | C(11) | -154(2) |
| C(6) | Lu(1) | C(11) | C(10) | 140(3) | C(6) | Lu(1) | C(11) | C(12) | 22(3) |
| C(6) | Lu(1) | C(12) | C(11) | -172(1) | C(6) | Lu(1) | C(12) | C(8) | 73(1) |
| C(6) | Lu(1) | C(8) | C(9) | 118(1) | C(6) | Lu(1) | C(8) | C(12) | -129(1) |
| C(6) | C(5) | Lu(1) | C(7) | 36(1) | C(6) | C(5) | Lu(1) | C(9) | 144(1) |
| C(6) | C(5) | Lu(1) | C(10) | 170(1) | C(6) | C(5) | Lu(1) | C(11) | 155(1) |
| C(6) | C(5) | Lu(1) | C(12) | 96(2) | C(6) | C(5) | Lu(1) | C(8) | 110(1) |
| C(6) | C(5) | C(13) | C(14) | -95(3) | C(6) | C(5) | C(13) | C(18) | 134(2) |
| C(6) | C(7) | Lu(1) | C(9) | -128(1) | C(6) | C(7) | Lu(1) | C(10) | -142(1) |
| C(6) | C(7) | Lu(1) | C(11) | 172(1) | C(6) | C(7) | Lu(1) | C(12) | 176(1) |

Table 7. Torsion Angles($^{\circ}$) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|-----------|-------|-------|-------|-------|---------|
| C(6) | C(7) | Lu(1) | C(8) | -154(1) | C(7) | Lu(1) | Lu(2) | C(29) | -65(1) |
| C(7) | Lu(1) | Lu(2) | C(30) | -14(1) | C(7) | Lu(1) | Lu(2) | C(31) | -15(1) |
| C(7) | Lu(1) | Lu(2) | C(32) | -47.0(10) | C(7) | Lu(1) | Lu(2) | C(33) | -71(1) |
| C(7) | Lu(1) | Lu(2) | C(34) | 172(1) | C(7) | Lu(1) | Lu(2) | C(35) | 118(1) |
| C(7) | Lu(1) | Lu(2) | C(37) | 149(1) | C(7) | Lu(1) | Lu(2) | C(38) | 175(1) |
| C(7) | Lu(1) | C(5) | C(13) | 153(2) | C(7) | Lu(1) | C(9) | C(10) | -164(1) |
| C(7) | Lu(1) | C(9) | C(8) | -52(1) | C(7) | Lu(1) | C(10) | C(23) | 126(2) |
| C(7) | Lu(1) | C(10) | C(9) | 24(1) | C(7) | Lu(1) | C(10) | C(11) | -90(1) |
| C(7) | Lu(1) | C(11) | C(10) | 123(1) | C(7) | Lu(1) | C(11) | C(12) | 6(1) |
| C(7) | Lu(1) | C(12) | C(11) | -175(1) | C(7) | Lu(1) | C(12) | C(8) | 70(1) |
| C(7) | Lu(1) | C(8) | C(9) | 133(1) | C(7) | Lu(1) | C(8) | C(12) | -114(1) |
| C(7) | C(3) | Lu(1) | C(9) | 166(1) | C(7) | C(3) | Lu(1) | C(10) | 162(1) |
| C(7) | C(3) | Lu(1) | C(11) | 129(1) | C(7) | C(3) | Lu(1) | C(12) | 114(1) |
| C(7) | C(3) | Lu(1) | C(8) | 136(1) | C(7) | C(3) | Si(1) | C(8) | -88(2) |
| C(7) | C(6) | Lu(1) | C(9) | 69(1) | C(7) | C(6) | Lu(1) | C(10) | 94(2) |
| C(7) | C(6) | Lu(1) | C(11) | -22(4) | C(7) | C(6) | Lu(1) | C(12) | -5(2) |
| C(7) | C(6) | Lu(1) | C(8) | 30(2) | C(7) | C(6) | C(5) | C(13) | 179(2) |
| C(13) | C(5) | Lu(1) | C(9) | -98(2) | C(13) | C(5) | Lu(1) | C(10) | -72(2) |
| C(13) | C(5) | Lu(1) | C(11) | -86(3) | C(13) | C(5) | Lu(1) | C(12) | -145(2) |
| C(13) | C(5) | Lu(1) | C(8) | -132(2) | C(13) | C(14) | C(15) | C(16) | -59(3) |
| C(13) | C(14) | C(19) | C(20) | 69(3) | C(13) | C(14) | C(19) | C(21) | -174(2) |
| C(13) | C(18) | C(17) | C(16) | 51(3) | C(13) | C(18) | C(17) | C(22) | 172(2) |
| C(14) | C(13) | C(18) | C(17) | -49(3) | C(14) | C(15) | C(16) | C(17) | 58(3) |
| C(15) | C(14) | C(13) | C(18) | 56(3) | C(15) | C(14) | C(19) | C(20) | -164(2) |

Table 7. Torsion Angles($^{\circ}$) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|---------|-------|-------|-------|-------|---------|
| C(15) | C(14) | C(19) | C(21) | -48(3) | C(15) | C(16) | C(17) | C(18) | -55(3) |
| C(15) | C(16) | C(17) | C(22) | -173(2) | C(16) | C(15) | C(14) | C(19) | 175(2) |
| C(18) | C(13) | C(14) | C(19) | -178(2) | C(23) | C(10) | Lu(1) | C(9) | 102(2) |
| C(23) | C(10) | Lu(1) | C(11) | -142(2) | C(23) | C(10) | Lu(1) | C(12) | -177(2) |
| C(23) | C(10) | Lu(1) | C(8) | 141(2) | C(23) | C(10) | C(9) | C(8) | 168(2) |
| C(23) | C(10) | C(11) | C(12) | -164(2) | C(24) | C(23) | C(10) | C(9) | 166(1) |
| C(24) | C(23) | C(10) | C(11) | -29(3) | C(25) | C(23) | C(10) | C(9) | 56(3) |
| C(25) | C(23) | C(10) | C(11) | -139(2) | C(26) | C(23) | C(10) | C(9) | -92(3) |
| C(26) | C(23) | C(10) | C(11) | 72(4) | C(27) | Si(2) | C(29) | C(30) | -44(3) |
| C(27) | Si(2) | C(29) | C(33) | 144(2) | C(27) | Si(2) | C(34) | C(35) | 48(3) |
| C(27) | Si(2) | C(34) | C(38) | -159(3) | C(28) | Si(2) | C(29) | C(30) | -171(2) |
| C(28) | Si(2) | C(29) | C(33) | 17(3) | C(28) | Si(2) | C(34) | C(35) | 176(2) |
| C(28) | Si(2) | C(34) | C(38) | -30(3) | C(29) | Lu(2) | Lu(1) | C(9) | 132(1) |
| C(29) | Lu(2) | Lu(1) | C(10) | 130(1) | C(29) | Lu(2) | Lu(1) | C(11) | 156(1) |
| C(29) | Lu(2) | Lu(1) | C(12) | -176(1) | C(29) | Lu(2) | Lu(1) | C(8) | -179(1) |
| C(29) | Lu(2) | C(30) | C(31) | 125(2) | C(29) | Lu(2) | C(31) | C(30) | -34(1) |
| C(29) | Lu(2) | C(31) | C(32) | 74(1) | C(29) | Lu(2) | C(31) | C(39) | -163(3) |
| C(29) | Lu(2) | C(32) | C(31) | -83(2) | C(29) | Lu(2) | C(32) | C(33) | 39(2) |
| C(29) | Lu(2) | C(33) | C(32) | -118(2) | C(29) | Lu(2) | C(34) | C(35) | 114(2) |
| C(29) | Lu(2) | C(34) | C(38) | -139(2) | C(29) | Lu(2) | C(35) | C(34) | -55(2) |
| C(29) | Lu(2) | C(35) | C(36) | -172(2) | C(29) | Lu(2) | C(37) | C(36) | 86(2) |
| C(29) | Lu(2) | C(37) | C(38) | -28(2) | C(29) | Lu(2) | C(38) | C(34) | 34(2) |
| C(29) | Lu(2) | C(38) | C(37) | 153(2) | C(29) | Si(2) | C(34) | C(35) | -66(3) |
| C(29) | Si(2) | C(34) | C(38) | 86(3) | C(29) | C(30) | Lu(2) | C(31) | -125(2) |

Table 7. Torsion Angles($^{\circ}$) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|-----------|-------|-------|-------|-------|-----------|
| C(29) | C(30) | Lu(2) | C(32) | -83(1) | C(29) | C(30) | Lu(2) | C(33) | -46(1) |
| C(29) | C(30) | Lu(2) | C(34) | 49(1) | C(29) | C(30) | Lu(2) | C(35) | 81(1) |
| C(29) | C(30) | Lu(2) | C(37) | 73(1) | C(29) | C(30) | Lu(2) | C(38) | 43(1) |
| C(29) | C(30) | C(31) | C(32) | -15(3) | C(29) | C(30) | C(31) | C(39) | -174(3) |
| C(29) | C(33) | Lu(2) | C(30) | 45(1) | C(29) | C(33) | Lu(2) | C(31) | 83(1) |
| C(29) | C(33) | Lu(2) | C(32) | 118(2) | C(29) | C(33) | Lu(2) | C(34) | -35(1) |
| C(29) | C(33) | Lu(2) | C(35) | -12(1) | C(29) | C(33) | Lu(2) | C(37) | -69(2) |
| C(29) | C(33) | Lu(2) | C(38) | -64(1) | C(29) | C(33) | C(32) | C(31) | 0(3) |
| C(30) | Lu(2) | Lu(1) | C(9) | -176(1) | C(30) | Lu(2) | Lu(1) | C(10) | -178.6(9) |
| C(30) | Lu(2) | Lu(1) | C(11) | -152.3(9) | C(30) | Lu(2) | Lu(1) | C(12) | -125.8(9) |
| C(30) | Lu(2) | Lu(1) | C(8) | -128(1) | C(30) | Lu(2) | C(29) | C(33) | -100(2) |
| C(30) | Lu(2) | C(31) | C(32) | 108(2) | C(30) | Lu(2) | C(31) | C(39) | -129(3) |
| C(30) | Lu(2) | C(32) | C(31) | -38(1) | C(30) | Lu(2) | C(32) | C(33) | 84(2) |
| C(30) | Lu(2) | C(33) | C(32) | -72(2) | C(30) | Lu(2) | C(34) | C(35) | 83(2) |
| C(30) | Lu(2) | C(34) | C(38) | -170(2) | C(30) | Lu(2) | C(35) | C(34) | -92(2) |
| C(30) | Lu(2) | C(35) | C(36) | 150(2) | C(30) | Lu(2) | C(37) | C(36) | 47(2) |
| C(30) | Lu(2) | C(37) | C(38) | -67(2) | C(30) | Lu(2) | C(38) | C(34) | 10(2) |
| C(30) | Lu(2) | C(38) | C(37) | 129(2) | C(30) | C(29) | Lu(2) | C(31) | 28(1) |
| C(30) | C(29) | Lu(2) | C(32) | 68(1) | C(30) | C(29) | Lu(2) | C(33) | 100(2) |
| C(30) | C(29) | Lu(2) | C(34) | -120(1) | C(30) | C(29) | Lu(2) | C(35) | -91(1) |
| C(30) | C(29) | Lu(2) | C(37) | -127(1) | C(30) | C(29) | Lu(2) | C(38) | -141(1) |
| C(30) | C(29) | Si(2) | C(34) | 72(3) | C(30) | C(29) | C(33) | C(32) | -8(3) |
| C(30) | C(31) | Lu(2) | C(32) | -108(2) | C(30) | C(31) | Lu(2) | C(33) | -78(2) |
| C(30) | C(31) | Lu(2) | C(34) | -5(2) | C(30) | C(31) | Lu(2) | C(35) | 28(2) |

Table 7. Torsion Angles($^{\circ}$) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|-----------|-------|-------|-------|-------|------------|
| C(30) | C(31) | Lu(2) | C(37) | 42(3) | C(30) | C(31) | Lu(2) | C(38) | -16(2) |
| C(30) | C(31) | C(32) | C(33) | 8(3) | C(30) | C(31) | C(39) | C(40) | 79(4) |
| C(30) | C(31) | C(39) | C(44) | -48(4) | C(31) | Lu(2) | Lu(1) | C(9) | -176.8(9) |
| C(31) | Lu(2) | Lu(1) | C(10) | -178.9(8) | C(31) | Lu(2) | Lu(1) | C(11) | -152.6(9) |
| C(31) | Lu(2) | Lu(1) | C(12) | -126.1(9) | C(31) | Lu(2) | Lu(1) | C(8) | -128.4(10) |
| C(31) | Lu(2) | C(29) | C(33) | -71(1) | C(31) | Lu(2) | C(32) | C(33) | 123(3) |
| C(31) | Lu(2) | C(33) | C(32) | -34(2) | C(31) | Lu(2) | C(34) | C(35) | 85(2) |
| C(31) | Lu(2) | C(34) | C(38) | -167(1) | C(31) | Lu(2) | C(35) | C(34) | -106(2) |
| C(31) | Lu(2) | C(35) | C(36) | 135(1) | C(31) | Lu(2) | C(37) | C(36) | 20(3) |
| C(31) | Lu(2) | C(37) | C(38) | -94(3) | C(31) | Lu(2) | C(38) | C(34) | 19(3) |
| C(31) | Lu(2) | C(38) | C(37) | 138(2) | C(31) | C(30) | Lu(2) | C(32) | 42(1) |
| C(31) | C(30) | Lu(2) | C(33) | 79(2) | C(31) | C(30) | Lu(2) | C(34) | 175(2) |
| C(31) | C(30) | Lu(2) | C(35) | -152(2) | C(31) | C(30) | Lu(2) | C(37) | -160(1) |
| C(31) | C(30) | Lu(2) | C(38) | 169(1) | C(31) | C(30) | C(29) | C(33) | 15(3) |
| C(31) | C(32) | Lu(2) | C(33) | -123(3) | C(31) | C(32) | Lu(2) | C(34) | -93(1) |
| C(31) | C(32) | Lu(2) | C(35) | -57(2) | C(31) | C(32) | Lu(2) | C(37) | -141(3) |
| C(31) | C(32) | Lu(2) | C(38) | -126(1) | C(31) | C(39) | C(40) | C(41) | -75(3) |
| C(31) | C(39) | C(40) | C(45) | 56(3) | C(31) | C(39) | C(44) | C(43) | 83(3) |
| C(32) | Lu(2) | Lu(1) | C(9) | 151.3(9) | C(32) | Lu(2) | Lu(1) | C(10) | 149.3(8) |
| C(32) | Lu(2) | Lu(1) | C(11) | 175.6(8) | C(32) | Lu(2) | Lu(1) | C(12) | -157.9(8) |
| C(32) | Lu(2) | Lu(1) | C(8) | -160.3(9) | C(32) | Lu(2) | C(29) | C(33) | -31(1) |
| C(32) | Lu(2) | C(31) | C(39) | 121(3) | C(32) | Lu(2) | C(34) | C(35) | 123(2) |
| C(32) | Lu(2) | C(34) | C(38) | -130(2) | C(32) | Lu(2) | C(35) | C(34) | -76(2) |
| C(32) | Lu(2) | C(35) | C(36) | 165(1) | C(32) | Lu(2) | C(37) | C(36) | 136(3) |

Table 7. Torsion Angles(°) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|-----------|-------|-------|-------|-------|----------|
| C(32) | Lu(2) | C(37) | C(38) | 21(4) | C(32) | Lu(2) | C(38) | C(34) | 69(2) |
| C(32) | Lu(2) | C(38) | C(37) | -171(2) | C(32) | C(31) | Lu(2) | C(33) | 30(1) |
| C(32) | C(31) | Lu(2) | C(34) | 103(1) | C(32) | C(31) | Lu(2) | C(35) | 136(1) |
| C(32) | C(31) | Lu(2) | C(37) | 151(2) | C(32) | C(31) | Lu(2) | C(38) | 92(2) |
| C(32) | C(31) | C(39) | C(40) | -76(4) | C(32) | C(31) | C(39) | C(44) | 156(2) |
| C(32) | C(33) | Lu(2) | C(34) | -153(2) | C(32) | C(33) | Lu(2) | C(35) | -130(2) |
| C(32) | C(33) | Lu(2) | C(37) | 172(2) | C(32) | C(33) | Lu(2) | C(38) | 177(2) |
| C(33) | Lu(2) | Lu(1) | C(9) | 127.1(9) | C(33) | Lu(2) | Lu(1) | C(10) | 125.1(8) |
| C(33) | Lu(2) | Lu(1) | C(11) | 151.4(9) | C(33) | Lu(2) | Lu(1) | C(12) | 177.9(9) |
| C(33) | Lu(2) | Lu(1) | C(8) | 175.6(10) | C(33) | Lu(2) | C(31) | C(39) | 151(3) |
| C(33) | Lu(2) | C(34) | C(35) | 137(2) | C(33) | Lu(2) | C(34) | C(38) | -116(2) |
| C(33) | Lu(2) | C(35) | C(34) | -47(2) | C(33) | Lu(2) | C(35) | C(36) | -165(1) |
| C(33) | Lu(2) | C(37) | C(36) | 124(2) | C(33) | Lu(2) | C(37) | C(38) | 9(2) |
| C(33) | Lu(2) | C(38) | C(34) | 67(2) | C(33) | Lu(2) | C(38) | C(37) | -173(2) |
| C(33) | C(29) | Lu(2) | C(34) | 138(1) | C(33) | C(29) | Lu(2) | C(35) | 168(1) |
| C(33) | C(29) | Lu(2) | C(37) | 132(1) | C(33) | C(29) | Lu(2) | C(38) | 118(1) |
| C(33) | C(29) | Si(2) | C(34) | -97(3) | C(33) | C(32) | Lu(2) | C(34) | 30(2) |
| C(33) | C(32) | Lu(2) | C(35) | 65(2) | C(33) | C(32) | Lu(2) | C(37) | -18(4) |
| C(33) | C(32) | Lu(2) | C(38) | -3(2) | C(33) | C(32) | C(31) | C(39) | 169(3) |
| C(34) | Lu(2) | Lu(1) | C(9) | 11(1) | C(34) | Lu(2) | Lu(1) | C(10) | 9(1) |
| C(34) | Lu(2) | Lu(1) | C(11) | 35(1) | C(34) | Lu(2) | Lu(1) | C(12) | 61(1) |
| C(34) | Lu(2) | Lu(1) | C(8) | 59(1) | C(34) | Lu(2) | C(31) | C(39) | -135(2) |
| C(34) | Lu(2) | C(35) | C(36) | -117(2) | C(34) | Lu(2) | C(37) | C(36) | 79(2) |
| C(34) | Lu(2) | C(37) | C(38) | -35(2) | C(34) | Lu(2) | C(38) | C(37) | 118(3) |

Table 7. Torsion Angles(°) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|----------|-------|-------|-------|-------|----------|
| C(34) | C(35) | Lu(2) | C(37) | 80(2) | C(34) | C(35) | Lu(2) | C(38) | 41(2) |
| C(34) | C(35) | C(36) | C(37) | -11(3) | C(34) | C(35) | C(36) | C(49) | 169(3) |
| C(34) | C(38) | Lu(2) | C(35) | -41(1) | C(34) | C(38) | Lu(2) | C(37) | -118(3) |
| C(34) | C(38) | C(37) | C(36) | -9(4) | C(35) | Lu(2) | Lu(1) | C(9) | -43(1) |
| C(35) | Lu(2) | Lu(1) | C(10) | -45(1) | C(35) | Lu(2) | Lu(1) | C(11) | -18(1) |
| C(35) | Lu(2) | Lu(1) | C(12) | 7(1) | C(35) | Lu(2) | Lu(1) | C(8) | 5(1) |
| C(35) | Lu(2) | C(31) | C(39) | -101(2) | C(35) | Lu(2) | C(34) | C(38) | 106(2) |
| C(35) | Lu(2) | C(37) | C(36) | 38(1) | C(35) | Lu(2) | C(37) | C(38) | -76(2) |
| C(35) | Lu(2) | C(38) | C(37) | 77(2) | C(35) | C(34) | Lu(2) | C(37) | -73(2) |
| C(35) | C(34) | Lu(2) | C(38) | -106(2) | C(35) | C(34) | C(38) | C(37) | 2(3) |
| C(35) | C(36) | C(37) | C(38) | 12(3) | C(35) | C(36) | C(49) | C(50) | 40(4) |
| C(35) | C(36) | C(49) | C(51) | -91(4) | C(35) | C(36) | C(49) | C(52) | 154(3) |
| C(36) | C(35) | Lu(2) | C(37) | -37(1) | C(36) | C(35) | Lu(2) | C(38) | -76(2) |
| C(36) | C(35) | C(34) | C(38) | 6(3) | C(36) | C(37) | Lu(2) | C(38) | 115(3) |
| C(37) | Lu(2) | Lu(1) | C(9) | -12.1(9) | C(37) | Lu(2) | Lu(1) | C(10) | -14.1(9) |
| C(37) | Lu(2) | Lu(1) | C(11) | 12.1(9) | C(37) | Lu(2) | Lu(1) | C(12) | 38.6(9) |
| C(37) | Lu(2) | Lu(1) | C(8) | 36.3(10) | C(37) | Lu(2) | C(31) | C(39) | -87(3) |
| C(37) | Lu(2) | C(34) | C(38) | 33(1) | C(37) | C(36) | C(49) | C(50) | -137(4) |
| C(37) | C(36) | C(49) | C(51) | 90(4) | C(37) | C(36) | C(49) | C(52) | -23(5) |
| C(38) | Lu(2) | Lu(1) | C(9) | 13(1) | C(38) | Lu(2) | Lu(1) | C(10) | 11.3(9) |
| C(38) | Lu(2) | Lu(1) | C(11) | 37.6(10) | C(38) | Lu(2) | Lu(1) | C(12) | 64.1(10) |
| C(38) | Lu(2) | Lu(1) | C(8) | 61(1) | C(38) | Lu(2) | C(31) | C(39) | -146(2) |
| C(38) | C(37) | C(36) | C(49) | -169(3) | C(39) | C(40) | C(41) | C(42) | -61(3) |
| C(39) | C(40) | C(45) | C(46) | -95(3) | C(39) | C(40) | C(45) | C(47) | 149(2) |

Table 7. Torsion Angles($^{\circ}$) (continued)

| atom | atom | atom | atom | angle | atom | atom | atom | atom | angle |
|-------|-------|-------|-------|----------|-------|-------|-------|-------|-----------|
| C(39) | C(44) | C(43) | C(42) | 52(3) | C(39) | C(44) | C(43) | C(48) | 166(3) |
| C(40) | C(39) | C(44) | C(43) | -47(3) | C(40) | C(41) | C(42) | C(43) | 64(3) |
| C(41) | C(40) | C(39) | C(44) | 50(3) | C(41) | C(40) | C(45) | C(46) | 38(3) |
| C(41) | C(40) | C(45) | C(47) | -77(3) | C(41) | C(42) | C(43) | C(44) | -57(3) |
| C(41) | C(42) | C(43) | C(48) | -179(2) | C(42) | C(41) | C(40) | C(45) | 166(2) |
| C(44) | C(39) | C(40) | C(45) | -177(2) | C(9) | Lu(1) | C(10) | C(11) | -115(1) |
| C(9) | Lu(1) | C(11) | C(10) | 37.2(10) | C(9) | Lu(1) | C(11) | C(12) | -80(1) |
| C(9) | Lu(1) | C(12) | C(11) | 75(1) | C(9) | Lu(1) | C(12) | C(8) | -39(1) |
| C(9) | Lu(1) | C(8) | C(12) | 111(1) | C(9) | C(10) | Lu(1) | C(11) | 115(1) |
| C(9) | C(10) | Lu(1) | C(12) | 80(1) | C(9) | C(10) | Lu(1) | C(8) | 39.2(10) |
| C(9) | C(10) | C(11) | C(12) | 0(2) | C(9) | C(8) | Lu(1) | C(10) | -37.5(10) |
| C(9) | C(8) | Lu(1) | C(11) | -76(1) | C(9) | C(8) | Lu(1) | C(12) | -111(1) |
| C(9) | C(8) | C(12) | C(11) | 0(2) | C(10) | Lu(1) | C(9) | C(8) | 112(1) |
| C(10) | Lu(1) | C(11) | C(12) | -117(1) | C(10) | Lu(1) | C(12) | C(11) | 35(1) |
| C(10) | Lu(1) | C(12) | C(8) | -79(1) | C(10) | Lu(1) | C(8) | C(12) | 74(1) |
| C(10) | C(9) | Lu(1) | C(11) | -35.6(9) | C(10) | C(9) | Lu(1) | C(12) | -74(1) |
| C(10) | C(9) | Lu(1) | C(8) | -112(1) | C(10) | C(9) | C(8) | C(12) | 0(2) |
| C(10) | C(11) | Lu(1) | C(12) | 117(1) | C(10) | C(11) | Lu(1) | C(8) | 79(1) |
| C(10) | C(11) | C(12) | C(8) | 0(2) | C(11) | Lu(1) | C(9) | C(8) | 76(1) |
| C(11) | Lu(1) | C(12) | C(8) | -114(1) | C(11) | Lu(1) | C(8) | C(12) | 35(1) |
| C(11) | C(10) | Lu(1) | C(12) | -35(1) | C(11) | C(10) | Lu(1) | C(8) | -76(1) |
| C(11) | C(10) | C(9) | C(8) | 0(2) | C(11) | C(12) | Lu(1) | C(8) | 114(1) |
| C(12) | Lu(1) | C(9) | C(8) | 37(1) | C(12) | C(11) | Lu(1) | C(8) | -37(1) |