Table 5. Bond Angles(°)

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| N(1) | Sc(1) | N(2) | 94.00(16) | N(1) | Sc(1) | C(1) | 111.4(2) |
| N(1) | Sc(1) | C(2) | 109.2(2) | N(2) | Sc(1) | C(1) | 113.2(2) |
| N(2) | Sc(1) | C(2) | 108.9(2) | C(1) | Sc(1) | C(2) | 117.6(3) |
| Sc(1) | N(1) | C(4) | 105.1(3) | Sc(1) | N(1) | C(8) | 127.8(4) |
| C(4) | N(1) | C(8) | 125.6(5) | Sc(1) | N(2) | C(6) | 104.1(3) |
| Sc(1) | N(2) | C(20) | 126.1(4) | C(6) | N(2) | C(20) | 127.4(5) |
| Sc(1) | C(1) | C(38) | 119.4(5) | Sc(1) | C(2) | C(39) | 129.0(5) |
| C(4) | C(3) | C(35) | 107.4(5) | C(4) | C(3) | C(36) | 111.1(5) |
| C(4) | C(3) | C(37) | 117.4(5) | C(35) | C(3) | C(36) | 108.2(6) |
| C(35) | C(3) | C(37) | 106.0(5) | C(36) | C(3) | C(37) | 106.3(6) |
| N(1) | C(4) | C(3) | 126.8(5) | N(1) | C(4) | C(5) | 121.2(5) |
| C(3) | C(4) | C(5) | 111.9(5) | C(4) | C(5) | C(6) | 136.4(5) |
| N(2) | C(6) | C(5) | 120.5(5) | N(2) | C(6) | C(7) | 125.9(5) |
| C(5) | C(6) | C(7) | 113.4(5) | C(6) | C(7) | C(32) | 116.4(5) |
| C(6) | C(7) | C(33) | 111.7(5) | C(6) | C(7) | C(34) | 105.9(5) |
| C(32) | C(7) | C(33) | 105.2(5) | C(32) | C(7) | C(34) | 108.2(5) |
| C(33) | C(7) | C(34) | 109.4(6) | N(1) | C(8) | C(9) | 119.5(5) |
| N(1) | C(8) | C(13) | 119.9(5) | C(9) | C(8) | C(13) | 120.4(5) |
| C(8) | C(9) | C(10) | 117.9(6) | C(8) | C(9) | C(18) | 124.0(5) |
| C(10) | C(9) | C(18) | 118.1(6) | C(9) | C(10) | C(11) | 121.6(6) |
| C(10) | C(11) | C(12) | 120.1(5) | C(11) | C(12) | C(13) | 120.6(6) |
| C(8) | C(13) | C(12) | 119.1(5) | C(8) | C(13) | C(15) | 122.2(5) |
| C(12) | C(13) | C(15) | 118.7(5) | C(13) | C(15) | C(14) | 108.6(5) |
| C(13) | C(15) | C(16) | 113.2(5) | C(14) | C(15) | C(16) | 109.2(6) |

Table 5. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| C(9) | C(18) | C(17) | 111.1(6) | C(9) | C(18) | C(19) | 112.4(6) |
| C(17) | C(18) | C(19) | 109.7(6) | N(2) | C(20) | C(21) | 118.9(5) |
| N(2) | C(20) | C(25) | 119.5(5) | C(21) | C(20) | C(25) | 121.4(5) |
| C(20) | C(21) | C(22) | 118.1(5) | C(20) | C(21) | C(30) | 124.4(5) |
| C(22) | C(21) | C(30) | 117.4(6) | C(21) | C(22) | C(23) | 120.4(6) |
| C(22) | C(23) | C(24) | 120.5(6) | C(23) | C(24) | C(25) | 121.9(6) |
| C(20) | C(25) | C(24) | 117.6(6) | C(20) | C(25) | C(27) | 123.0(5) |
| C(24) | C(25) | C(27) | 119.3(6) | C(25) | C(27) | C(26) | 113.6(5) |
| C(25) | C(27) | C(28) | 113.3(5) | C(26) | C(27) | C(28) | 109.0(6) |
| C(21) | C(30) | C(29) | 113.6(5) | C(21) | C(30) | C(31) | 110.4(6) |
| C(29) | C(30) | C(31) | 109.8(6) | | | | |

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*Table 1. Crystal data and structure refinement*

A. Crystal Data

| | |
|---|---|
| Empirical Formula | $C_{49}H_{67}N_2Sc$ 4b |
| Formula Weight | 729.04 |
| Crystal Color, Habit | yellow, prism |
| Crystal Dimensions | 0.38 X 0.30 X 0.24 mm |
| Crystal System | monoclinic |
| No. of Reflections Used for Unit Cell Determination ($2\theta$ range) | 25 ( 13.4 - 19.3° ) |
| Omega Scan Peak Width at Half-height | 0.22° |
| Lattice Parameters | a = 12.653(4)Å<br>b = 12.096(3) Å<br>c = 28.069(4) Å<br>$\beta$ = 90.77(2)°<br><br>V = 4296(2) Å$^3$ |
| Space Group | $P2_1/c$ (#14) |
| Z value | 4 |
| $D_{calc}$ | 1.127 g/cm$^3$ |
| $F_{000}$ | 1584.00 |
| $\mu$(MoK$\alpha$) | 0.205 mm$^{-1}$ |

B. Intensity Measurements

| | |
|---|---|
| Diffractometer | Rigaku AFC6S |
| Radiation | MoK$\alpha$ ($\lambda$ = 0.71069 Å)<br>Zr-filter monochromatized |

| | |
|---|---|
| Temperature | -103.0°C |
| Scan Type | $\omega$-$2\theta$ |
| Scan Rate | 4.0°/min (in $\omega$) (up to 4 scans) |
| Scan Width | $(0.52 + 0.34 \tan \theta)°$ |
| $2\theta_{max}$ | 50.1° |
| No. of Reflections Measured | Total: 7977<br>Unique: 7607 ($R_{int} = 0.085$) |
| Corrections | Lorentz-polarization<br>Absorption<br>(trans. factors: 0.9261 - 0.9524)<br>Decay (0.39%) |

C. Structure Solution and Refinement

| | |
|---|---|
| Structure Solution | Direct Methods |
| Refinement | Full-matrix least-squares |
| Function Minimized | $\Sigma w(\lvert Fo\rvert - \lvert Fc\rvert)^2$ |
| Anomalous Dispersion | All non-hydrogen atoms |
| No. Observations (I>2.00$\sigma$(I)) | 2073 |
| No. Variables | 469 |
| Residuals: R; Rw | 0.063 ; 0.136 |
| Goodness of Fit Indicator | 1.02 |
| Max Shift/Error in Final Cycle | 0.00 |
| Maximum peak in Final Diff. Map | 0.25 $e^-/\mathring{A}^3$ |
| Minimum peak in Final Diff. Map | -0.31 $e^-/\mathring{A}^3$ |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters (Å$^2$x $10^3$) for [ArNC($^t$Bu)CHC($^t$Bu)NAr]Sc($CH_2C_6H_5$)$_2$. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Sc(1) | 1535(1) | 2255(1) | 1058(1) | 43(1) |
| N(1) | 671(4) | 3381(4) | 1463(2) | 34(1) |
| N(2) | 3026(4) | 2779(5) | 1326(2) | 39(1) |
| C(1) | 1033(5) | 2381(6) | 283(2) | 41(2) |
| C(2) | 1254(6) | 625(6) | 1383(3) | 59(2) |
| C(3) | 366(5) | 5420(6) | 1207(2) | 46(2) |
| C(4) | 1050(5) | 4368(6) | 1308(2) | 37(2) |
| C(5) | 2108(5) | 4471(6) | 1178(2) | 42(2) |
| C(6) | 3063(5) | 3863(6) | 1262(2) | 41(2) |
| C(7) | 4068(5) | 4609(6) | 1247(3) | 48(2) |
| C(8) | -250(5) | 3257(5) | 1753(2) | 39(2) |
| C(9) | -1181(5) | 2777(6) | 1569(2) | 49(2) |
| C(10) | -2053(5) | 2696(6) | 1864(3) | 52(2) |
| C(11) | -2010(6) | 3033(6) | 2330(3) | 58(2) |
| C(12) | -1077(6) | 3454(6) | 2512(3) | 57(2) |
| C(13) | -178(5) | 3543(6) | 2238(2) | 43(2) |
| C(14) | 1135(7) | 3278(8) | 2906(3) | 101(3) |
| C(15) | 850(6) | 3940(7) | 2465(3) | 56(2) |
| C(16) | 835(7) | 5150(7) | 2604(3) | 97(3) |
| C(17) | -1645(6) | 1191(7) | 1018(3) | 72(3) |
| C(18) | -1305(5) | 2407(6) | 1053(3) | 55(2) |
| C(19) | -2088(7) | 3117(7) | 774(3) | 92(3) |
| C(20) | 3905(5) | 2036(6) | 1425(3) | 41(2) |
| C(21) | 4431(5) | 1574(6) | 1034(3) | 45(2) |
| C(22) | 5247(5) | 823(6) | 1130(3) | 54(2) |
| C(23) | 5518(6) | 541(7) | 1589(3) | 64(2) |
| C(24) | 4965(6) | 969(7) | 1964(3) | 61(2) |
| C(25) | 4128(5) | 1705(6) | 1899(3) | 47(2) |
| C(26) | 4175(7) | 2904(7) | 2627(3) | 94(3) |
| C(27) | 3525(6) | 2120(7) | 2320(3) | 59(2) |

| | | | | |
|---|---|---|---|---|
| C(28) | 3129(6) | 1158(7) | 2621(3) | 77(3) |
| C(29) | 3717(5) | 791(6) | 271(2) | 62(2) |
| C(30) | 4170(5) | 1819(6) | 516(2) | 47(2) |
| C(31) | 5119(5) | 2244(7) | 233(2) | 67(2) |
| C(32) | 3915(6) | 5564(6) | 1602(3) | 73(3) |
| C(33) | 5121(5) | 4047(6) | 1382(3) | 61(2) |
| C(34) | 4175(5) | 5072(6) | 739(3) | 64(2) |
| C(35) | 236(6) | 5484(7) | 662(2) | 79(3) |
| C(36) | -739(5) | 5477(6) | 1434(2) | 53(2) |
| C(37) | 947(6) | 6476(6) | 1378(3) | 75(3) |
| C(38) | 1713(6) | 2589(7) | -124(3) | 54(2) |
| C(39) | 1845(6) | 1811(7) | -490(3) | 67(2) |
| C(40) | 2532(8) | 1987(9) | -863(3) | 86(3) |
| C(41) | 3098(7) | 2956(11) | -898(4) | 97(4) |
| C(42) | 2963(7) | 3731(9) | -547(3) | 85(3) |
| C(43) | 2302(6) | 3565(7) | -171(3) | 61(2) |
| C(44) | 1739(7) | -297(7) | 1143(3) | 58(2) |
| C(45) | 1231(6) | -752(7) | 737(3) | 69(3) |
| C(46) | 1687(9) | -1566(8) | 466(3) | 86(3) |
| C(47) | 2661(9) | -1996(8) | 590(4) | 89(3) |
| C(48) | 3197(7) | -1585(8) | 992(4) | 82(3) |
| C(49) | 2718(7) | -753(7) | 1267(3) | 66(2) |

Table 3. Bond lengths [Å] and angles [°] for [ArNC($^t$Bu)CHC($^t$Bu)NAr]Sc($CH_2C_6H_5$)$_2$.

| | |
|---|---|
| Sc(1)-N(1) | 2.091(5) |
| Sc(1)-N(2) | 2.118(5) |
| Sc(1)-C(2) | 2.203(7) |
| Sc(1)-C(1) | 2.265(6) |
| Sc(1)-C(4) | 2.722(7) |
| Sc(1)-C(5) | 2.796(7) |
| Sc(1)-C(6) | 2.796(7) |
| N(1)-C(4) | 1.361(8) |
| N(1)-C(8) | 1.438(7) |
| N(2)-C(6) | 1.325(8) |
| N(2)-C(20) | 1.454(8) |
| C(1)-C(38) | 1.460(8) |
| C(2)-C(44) | 1.443(10) |
| C(3)-C(4) | 1.562(9) |
| C(3)-C(35) | 1.539(9) |
| C(3)-C(36) | 1.545(8) |
| C(3)-C(37) | 1.548(9) |
| C(4)-C(5) | 1.399(8) |
| C(5)-C(6) | 1.431(9) |
| C(6)-C(7) | 1.560(9) |
| C(7)-C(33) | 1.539(9) |
| C(7)-C(34) | 1.540(9) |
| C(7)-C(32) | 1.540(9) |
| C(8)-C(13) | 1.406(8) |
| C(8)-C(9) | 1.406(9) |
| C(9)-C(10) | 1.391(8) |
| C(9)-C(18) | 1.523(9) |
| C(10)-C(11) | 1.370(9) |
| C(11)-C(12) | 1.378(9) |
| C(12)-C(13) | 1.388(9) |
| C(13)-C(15) | 1.518(9) |
| C(14)-C(15) | 1.515(10) |
| C(15)-C(16) | 1.514(10) |
| C(17)-C(18) | 1.535(9) |

| | |
|---|---|
| C(18)-C(19) | 1.519(9) |
| C(20)-C(21) | 1.406(9) |
| C(20)-C(25) | 1.413(9) |
| C(21)-C(22) | 1.398(9) |
| C(21)-C(30) | 1.517(9) |
| C(22)-C(23) | 1.374(9) |
| C(23)-C(24) | 1.372(9) |
| C(24)-C(25) | 1.393(9) |
| C(25)-C(27) | 1.502(9) |
| C(26)-C(27) | 1.516(9) |
| C(27)-C(28) | 1.527(9) |
| C(29)-C(30) | 1.530(9) |
| C(30)-C(31) | 1.536(8) |
| C(38)-C(39) | 1.405(9) |
| C(38)-C(43) | 1.403(10) |
| C(39)-C(40) | 1.386(11) |
| C(40)-C(41) | 1.378(12) |
| C(41)-C(42) | 1.373(12) |
| C(42)-C(43) | 1.370(10) |
| C(44)-C(49) | 1.395(10) |
| C(44)-C(45) | 1.412(10) |
| C(45)-C(46) | 1.375(11) |
| C(46)-C(47) | 1.379(11) |
| C(47)-C(48) | 1.398(12) |
| C(48)-C(49) | 1.410(11) |

| | |
|---|---|
| N(1)-Sc(1)-N(2) | 94.7(2) |
| N(1)-Sc(1)-C(2) | 105.7(3) |
| N(2)-Sc(1)-C(2) | 105.6(3) |
| N(1)-Sc(1)-C(1) | 109.7(2) |
| N(2)-Sc(1)-C(1) | 123.9(2) |
| C(2)-Sc(1)-C(1) | 114.4(3) |
| N(1)-Sc(1)-C(4) | 29.26(18) |
| N(2)-Sc(1)-C(4) | 80.3(2) |
| C(2)-Sc(1)-C(4) | 134.1(2) |
| C(1)-Sc(1)-C(4) | 97.1(2) |

| | |
|---|---|
| N(1)-Sc(1)-C(5) | 56.5(2) |
| N(2)-Sc(1)-C(5) | 56.1(2) |
| C(2)-Sc(1)-C(5) | 148.4(3) |
| C(1)-Sc(1)-C(5) | 96.9(2) |
| C(6)-Sc(1)-C(5) | 29.33(18) |
| N(2)-Sc(1)-C(6) | 78.5(2) |
| N(1)-Sc(1)-C(6) | 27.05(19) |
| C(1)-Sc(1)-C(6) | 130.8(3) |
| C(2)-Sc(1)-C(6) | 109.5(2) |
| C(4)-Sc(1)-C(6) | 56.8(2) |
| C(5)-Sc(1)-C(6) | 29.66(18) |
| C(6)-N(2)-C(20) | 127.5(5) |
| C(6)-N(2)-Sc(1) | 106.3(4) |
| C(20)-N(2)-Sc(1) | 123.9(4) |
| C(4)-N(1)-C(8) | 124.4(6) |
| C(4)-N(1)-Sc(1) | 102.0(4) |
| C(8)-N(1)-Sc(1) | 132.3(4) |
| C(44)-C(2)-Sc(1) | 115.3(5) |
| C(38)-C(1)-Sc(1) | 127.0(4) |
| C(33)-C(7)-C(34) | 107.6(6) |
| C(33)-C(7)-C(32) | 106.7(6) |
| C(34)-C(7)-C(32) | 109.8(6) |
| C(33)-C(7)-C(6) | 116.2(6) |
| C(34)-C(7)-C(6) | 108.5(6) |
| C(32)-C(7)-C(6) | 107.9(6) |
| N(2)-C(6)-C(5) | 120.0(6) |
| N(2)-C(6)-C(7) | 127.4(6) |
| C(5)-C(6)-C(7) | 112.6(6) |
| N(2)-C(6)-Sc(1) | 46.6(3) |
| C(5)-C(6)-Sc(1) | 75.2(4) |
| C(7)-C(6)-Sc(1) | 163.4(5) |
| C(4)-C(5)-C(6) | 136.1(7) |
| C(4)-C(5)-Sc(1) | 72.4(4) |
| C(6)-C(5)-Sc(1) | 75.2(4) |
| N(1)-C(4)-C(5) | 120.3(6) |
| N(1)-C(4)-C(3) | 125.2(6) |

| | |
|---|---|
| C(5)-C(4)-C(3) | 114.2(6) |
| N(1)-C(4)-Sc(1) | 48.7(3) |
| C(5)-C(4)-Sc(1) | 78.3(4) |
| C(3)-C(4)-Sc(1) | 147.5(5) |
| C(35)-C(3)-C(36) | 108.8(6) |
| C(35)-C(3)-C(37) | 108.1(6) |
| C(36)-C(3)-C(37) | 105.3(6) |
| C(35)-C(3)-C(4) | 105.9(6) |
| C(36)-C(3)-C(4) | 117.6(6) |
| C(37)-C(3)-C(4) | 110.9(6) |
| C(21)-C(20)-C(25) | 122.0(7) |
| C(21)-C(20)-N(2) | 117.7(6) |
| C(25)-C(20)-N(2) | 119.8(6) |
| C(22)-C(21)-C(20) | 117.7(7) |
| C(2)-C(21)-C(30) | 117.4(7) |
| C(20)-C(21)-C(30) | 124.9(7) |
| C(23)-C(22)-C(21) | 121.0(7) |
| C(24)-C(23)-C(22) | 120.2(8) |
| C(23)-C(24)-C(25) | 122.3(7) |
| C(24)-C(25)-C(20) | 116.5(7) |
| C(24)-C(25)-C(27) | 120.2(7) |
| C(20)-C(25)-C(27) | 123.2(7) |
| C(25)-C(27)-C(26) | 112.2(6) |
| C(25)-C(27)-C(28) | 110.8(7) |
| C(26)-C(27)-C(28) | 110.0(6) |
| C(21)-C(30)-C(29) | 110.4(6) |
| C(21)-C(30)-C(31) | 113.6(6) |
| C(29)-C(30)-C(31) | 109.3(6) |
| C(13)-C(8)-C(9) | 120.0(6) |
| C(13)-C(8)-N(1) | 118.6(6) |
| C(9)-C(8)-N(1) | 121.1(6) |
| C(10)-C(9)-C(8) | 118.5(7) |
| C(10)-C(9)-C(18) | 118.3(7) |
| C(8)-C(9)-C(18) | 123.1(6) |
| C(11)-C(10)-C(9) | 121.7(7) |
| C(10)-C(11)-C(12) | 119.1(7) |

| | |
|---|---|
| C(11)-C(12)-C(13) | 121.8(7) |
| C(12)-C(13)-C(8) | 118.4(7) |
| C(12)-C(13)-C(15) | 119.7(7) |
| C(8)-C(13)-C(15) | 121.9(6) |
| C(14)-C(15)-C(16) | 107.7(7) |
| C(14)-C(15)-C(13) | 111.7(6) |
| C(16)-C(15)-C(13) | 113.6(7) |
| C(9)-C(18)-C(19) | 112.5(6) |
| C(9)-C(18)-C(17) | 111.6(7) |
| C(19)-C(18)-C(17) | 109.2(6) |
| C(49)-C(44)-C(45) | 116.0(8) |
| C(49)-C(44)-C(2) | 124.8(8) |
| C(45)-C(44)-C(2) | 119.0(8) |
| C(46)-C(45)-C(44) | 122.4(9) |
| C(45)-C(46)-C(47) | 120.7(10) |
| C(46)-C(47)-C(48) | 119.5(10) |
| C(47)-C(48)-C(49) | 119.1(9) |
| C(44)-C(49)-C(48) | 122.2(9) |
| C(39)-C(38)-C(43) | 115.1(7) |
| C(39)-C(38)-C(1) | 122.2(8) |
| C(43)-C(38)-C(1) | 122.6(7) |
| C(40)-C(39)-C(38) | 122.1(9) |
| C(39)-C(40)-C(41) | 121.2(10) |
| C(42)-C(41)-C(40) | 117.4(9) |
| C(43)-C(42)-C(41) | 122.3(10) |
| C(42)-C(43)-C(38) | 121.9(9) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for $[ArNC(^tBu)CHC(^tBu)NAr]Sc(CH_2C_6H_5)_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12} ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Sc(1) | 36(1) | 46(1) | 45(1) | -6(1) | 0(1) | 0(1) |
| N(1) | 28(3) | 40(4) | 33(3) | 2(3) | 6(3) | -2(3) |
| N(2) | 37(3) | 37(4) | 43(4) | 0(3) | 3(3) | 5(3) |
| C(1) | 38(4) | 49(5) | 35(4) | -2(4) | 6(3) | 2(4) |
| C(2) | 43(5) | 49(5) | 85(7) | 0(5) | 2(4) | -2(4) |
| C(3) | 55(5) | 38(5) | 46(5) | 0(4) | 10(4) | 11(4) |
| C(4) | 44(5) | 43(5) | 23(4) | 0(4) | 1(3) | -1(4) |
| C(5) | 46(5) | 37(5) | 43(5) | 5(4) | -1(4) | -3(4) |
| C(6) | 44(5) | 45(5) | 35(4) | -1(4) | -2(4) | -1(4) |
| C(7) | 41(5) | 53(5) | 50(5) | 5(4) | -3(4) | -9(4) |
| C(8) | 35(4) | 38(4) | 45(5) | -3(4) | 10(4) | 3(3) |
| C(9) | 43(5) | 50(5) | 54(5) | -3(5) | 6(4) | 9(4) |
| C(10) | 35(4) | 51(5) | 70(6) | -8(5) | 10(4) | 1(4) |
| C(11) | 50(5) | 68(6) | 56(6) | 4(5) | 28(4) | 3(5) |
| C(12) | 64(6) | 57(6) | 51(5) | -7(4) | 20(5) | 2(5) |
| C(13) | 52(5) | 41(5) | 38(5) | 5(4) | 19(4) | 2(4) |
| C(14) | 98(8) | 104(8) | 100(8) | 28(7) | -33(6) | -6(6) |
| C(15) | 57(5) | 73(6) | 38(5) | -15(5) | 13(4) | -13(5) |
| C(16) | 118(8) | 83(8) | 91(8) | 0(6) | -10(6) | -39(6) |
| C(17) | 60(5) | 86(7) | 69(6) | -20(5) | 4(5) | -3(5) |
| C(18) | 41(4) | 61(6) | 62(5) | -16(5) | -6(4) | -3(4) |
| C(19) | 94(7) | 96(8) | 85(7) | -13(6) | -41(6) | 4(6) |
| C(20) | 30(4) | 38(5) | 55(5) | 10(4) | -3(4) | -7(4) |
| C(21) | 30(4) | 57(5) | 47(5) | 10(4) | -3(4) | -1(4) |
| C(22) | 41(5) | 59(6) | 62(6) | 3(5) | 6(4) | 9(4) |
| C(23) | 45(5) | 70(6) | 78(7) | 18(6) | -1(5) | 14(5) |
| C(24) | 56(5) | 71(6) | 56(6) | 16(5) | -14(4) | 8(5) |
| C(25) | 38(5) | 53(5) | 49(5) | 8(4) | -13(4) | -1(4) |
| C(26) | 139(9) | 73(7) | 72(6) | -7(6) | 5(6) | -23(7) |
| C(27) | 65(5) | 63(6) | 49(5) | 3(5) | 0(4) | 5(5) |
| C(28) | 80(6) | 88(7) | 65(6) | 11(6) | 9(5) | -2(6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(29) | 59(5) | 78(6) | 50(5) | 0(5) | 4(4) | 1(5) |
| C(30) | 38(4) | 52(5) | 51(5) | 3(4) | 3(4) | 10(4) |
| C(31) | 53(5) | 82(6) | 67(6) | 20(5) | 17(4) | 4(5) |
| C(32) | 67(6) | 66(6) | 87(7) | -9(5) | -19(5) | -14(5) |
| C(33) | 36(5) | 63(6) | 83(6) | 3(5) | -7(4) | -14(4) |
| C(34) | 48(5) | 67(6) | 78(6) | 18(5) | 8(4) | -12(4) |
| C(35) | 91(7) | 99(7) | 48(6) | 16(5) | 0(5) | 48(6) |
| C(36) | 42(5) | 49(5) | 69(6) | -1(4) | 11(4) | 11(4) |
| C(37) | 78(6) | 47(6) | 100(7) | 4(5) | 41(5) | 16(5) |
| C(38) | 50(5) | 68(7) | 42(5) | 6(5) | -11(4) | 7(5) |
| C(39) | 69(6) | 81(7) | 51(6) | -12(5) | -5(5) | 8(5) |
| C(40) | 87(8) | 125(10) | 46(6) | -18(6) | -4(5) | 36(7) |
| C(41) | 68(7) | 159(13) | 63(7) | 26(8) | 20(5) | 17(8) |
| C(42) | 61(6) | 129(10) | 65(7) | 19(7) | 6(5) | -5(6) |
| C(43) | 54(5) | 70(7) | 58(6) | 6(5) | -7(4) | 1(5) |
| C(44) | 73(7) | 48(6) | 53(6) | 10(5) | 1(5) | -25(5) |
| C(45) | 57(6) | 62(6) | 90(7) | -4(6) | 12(5) | 0(5) |
| C(46) | 99(8) | 78(8) | 82(8) | 2(6) | 18(6) | -14(6) |
| C(47) | 103(9) | 67(8) | 99(9) | 9(7) | 30(7) | 0(7) |
| C(48) | 71(7) | 62(7) | 114(9) | 22(6) | 19(7) | 1(6) |
| C(49) | 65(6) | 60(6) | 71(6) | 15(6) | 0(5) | -7(5) |

Table 1. Crystal data and structure refinement for [ArNC(Me)CHC(Me)NAr]Sc($CH_2SiMe_3$)$_2$. 6a

| | | |
|---|---|---|
| Empirical formula | C37 H63 N2 Sc Si2 | |
| Formula weight | 637.03 | |
| Temperature | 160(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P-1 | |
| Unit cell dimensions | a = 10.4634(6) Å | $\alpha$= 80.055(2)°. |
| | b = 11.1017(6) Å | $\beta$= 79.994(2)°. |
| | c = 18.0333(10) Å | $\gamma$ = 72.406(2)°. |
| Volume | 1950.23(19) Å$^3$ | |
| Z | 2 | |
| Density (calculated) | 1.085 Mg/m$^3$ | |
| Absorption coefficient | 0.275 mm$^{-1}$ | |
| F(000) | 696 | |
| Crystal size | 0.70 x 0.60 x 0.40 mm$^3$ | |
| Theta range for data collection | 2.06 to 29.01°. | |
| Index ranges | -14<=h<=14, -13<=k<=14, -24<=l<=21 | |
| Reflections collected | 16280 | |
| Independent reflections | 9288 [R(int) = 0.0126] | |
| Completeness to theta = 26.00° | 98.7 % | |
| Absorption correction | Empirical | |
| Max. and min. transmission | 0.898 and 0.831 | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 9288 / 0 / 408 | |
| Goodness-of-fit on F$^2$ | 1.051 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0351, wR2 = 0.0915 | |
| R indices (all data) | R1 = 0.0418, wR2 = 0.0933 | |
| Extinction coefficient | 0.0024(8) | |
| Largest diff. peak and hole | 0.309 and -0.233 e.Å$^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for [ArNC(Me)CHC(Me)NAr]Sc($CH_2SiMe_3$)$_2$. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Sc(1) | 7645(1) | 1685(1) | 2581(1) | 18(1) |
| N(1) | 6929(1) | 61(1) | 2726(1) | 19(1) |
| N(2) | 6283(1) | 2637(1) | 1773(1) | 19(1) |
| Si(1) | 10844(1) | 622(1) | 1300(1) | 25(1) |
| Si(2) | 7495(1) | 3845(1) | 3921(1) | 25(1) |
| C(1) | 9822(1) | 1448(1) | 2102(1) | 25(1) |
| C(2) | 7017(1) | 2537(1) | 3644(1) | 27(1) |
| C(3) | 7158(2) | -1690(1) | 1988(1) | 30(1) |
| C(4) | 6943(1) | -300(1) | 2051(1) | 21(1) |
| C(5) | 6753(1) | 554(1) | 1380(1) | 23(1) |
| C(6) | 6273(1) | 1903(1) | 1266(1) | 21(1) |
| C(7) | 5746(2) | 2470(1) | 517(1) | 31(1) |
| C(8) | 6719(1) | -772(1) | 3418(1) | 20(1) |
| C(9) | 7790(1) | -1380(1) | 3851(1) | 25(1) |
| C(10) | 7528(2) | -2109(1) | 4542(1) | 32(1) |
| C(11) | 6248(2) | -2236(2) | 4804(1) | 34(1) |
| C(12) | 5205(1) | -1641(1) | 4373(1) | 28(1) |
| C(13) | 5413(1) | -912(1) | 3676(1) | 22(1) |
| C(14) | 3122(2) | 669(2) | 3686(1) | 40(1) |
| C(15) | 4207(1) | -298(1) | 3240(1) | 26(1) |
| C(16) | 3601(2) | -1305(2) | 3070(1) | 37(1) |
| C(17) | 9741(2) | -734(2) | 4157(1) | 42(1) |
| C(18) | 9231(1) | -1308(1) | 3593(1) | 28(1) |
| C(19) | 10187(2) | -2626(2) | 3469(1) | 39(1) |
| C(20) | 5662(1) | 4000(1) | 1657(1) | 20(1) |
| C(21) | 6380(1) | 4810(1) | 1203(1) | 24(1) |
| C(22) | 5761(1) | 6124(1) | 1127(1) | 27(1) |
| C(23) | 4478(1) | 6624(1) | 1480(1) | 29(1) |
| C(24) | 3788(1) | 5821(1) | 1932(1) | 29(1) |
| C(25) | 4363(1) | 4502(1) | 2036(1) | 23(1) |

| | | | | |
|---|---|---|---|---|
| C(26) | 2530(2) | 3485(2) | 2080(1) | 58(1) |
| C(27) | 3561(1) | 3659(1) | 2525(1) | 27(1) |
| C(28) | 2863(2) | 4176(2) | 3265(1) | 35(1) |
| C(29) | 7835(2) | 4701(2) | -66(1) | 50(1) |
| C(30) | 7793(1) | 4328(1) | 798(1) | 33(1) |
| C(31) | 8802(2) | 4802(2) | 1104(1) | 50(1) |
| C(32) | 12665(2) | 666(2) | 1109(1) | 41(1) |
| C(33) | 10178(2) | 1356(2) | 373(1) | 36(1) |
| C(34) | 10874(2) | -1100(1) | 1473(1) | 33(1) |
| C(35) | 6632(2) | 5381(2) | 3370(1) | 50(1) |
| C(36) | 9367(2) | 3580(2) | 3728(1) | 56(1) |
| C(37) | 7034(2) | 4009(2) | 4959(1) | 37(1) |

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Table 3. Bond lengths [Å] and angles [°] for [ArNC(Me)CHC(Me)NAr]Sc($CH_2SiMe_3$)$_2$.

| | |
|---|---|
| Sc(1)-N(1) | 2.1130(10) |
| Sc(1)-N(2) | 2.1320(10) |
| Sc(1)-C(2) | 2.1954(14) |
| Sc(1)-C(1) | 2.2446(13) |
| Sc(1)-C(4) | 2.8732(12) |
| N(2)-C(6) | 1.3288(16) |
| N(2)-C(20) | 1.4493(15) |
| N(1)-C(4) | 1.3417(16) |
| N(1)-C(8) | 1.4461(15) |
| C(1)-Si(1) | 1.8448(14) |
| C(2)-Si(2) | 1.8390(14) |
| C(3)-C(4) | 1.5127(17) |
| C(4)-C(5) | 1.4049(17) |
| C(5)-C(6) | 1.4188(17) |
| C(6)-C(7) | 1.5100(17) |
| C(8)-C(9) | 1.4092(17) |
| C(8)-C(13) | 1.4107(17) |
| C(9)-C(10) | 1.3961(19) |
| C(9)-C(18) | 1.5209(18) |
| C(10)-C(11) | 1.381(2) |
| C(11)-C(12) | 1.384(2) |
| C(12)-C(13) | 1.3932(18) |
| C(13)-C(15) | 1.5224(17) |
| C(14)-C(15) | 1.526(2) |
| C(15)-C(16) | 1.536(2) |
| C(17)-C(18) | 1.531(2) |
| C(18)-C(19) | 1.530(2) |
| C(20)-C(25) | 1.4062(17) |
| C(20)-C(21) | 1.4075(17) |
| C(21)-C(22) | 1.3981(18) |
| C(21)-C(30) | 1.5132(18) |
| C(22)-C(23) | 1.375(2) |
| C(23)-C(24) | 1.383(2) |
| C(24)-C(25) | 1.3979(18) |

| | |
|---|---|
| C(25)-C(27) | 1.5138(18) |
| C(26)-C(27) | 1.525(2) |
| C(27)-C(28) | 1.5211(19) |
| C(29)-C(30) | 1.538(2) |
| C(30)-C(31) | 1.528(2) |
| Si(1)-C(34) | 1.8748(15) |
| Si(1)-C(33) | 1.8788(15) |
| Si(1)-C(32) | 1.8906(15) |
| Si(2)-C(36) | 1.8694(18) |
| Si(2)-C(35) | 1.8731(17) |
| Si(2)-C(37) | 1.8759(15) |
| | |
| N(1)-Sc(1)-N(2) | 90.71(4) |
| N(1)-Sc(1)-C(2) | 107.58(5) |
| N(2)-Sc(1)-C(2) | 110.91(5) |
| N(1)-Sc(1)-C(1) | 117.18(5) |
| N(2)-Sc(1)-C(1) | 113.12(5) |
| C(2)-Sc(1)-C(1) | 114.84(5) |
| N(1)-Sc(1)-C(4) | 25.93(4) |
| N(2)-Sc(1)-C(4) | 74.61(4) |
| C(2)-Sc(1)-C(4) | 132.09(4) |
| C(1)-Sc(1)-C(4) | 104.58(4) |
| C(6)-N(2)-C(20) | 120.73(10) |
| C(6)-N(2)-Sc(1) | 112.86(8) |
| C(20)-N(2)-Sc(1) | 124.94(8) |
| C(4)-N(1)-C(8) | 120.06(10) |
| C(4)-N(1)-Sc(1) | 110.55(8) |
| C(8)-N(1)-Sc(1) | 128.10(8) |
| N(2)-C(6)-C(5) | 123.28(11) |
| N(2)-C(6)-C(7) | 121.33(11) |
| C(5)-C(6)-C(7) | 115.39(11) |
| C(4)-C(5)-C(6) | 130.74(12) |
| N(1)-C(4)-C(5) | 123.53(11) |
| N(1)-C(4)-C(3) | 119.86(11) |
| C(5)-C(4)-C(3) | 116.61(11) |
| N(1)-C(4)-Sc(1) | 43.52(6) |

| | |
|---|---|
| C(5)-C(4)-Sc(1) | 84.69(7) |
| C(3)-C(4)-Sc(1) | 151.32(9) |
| C(25)-C(20)-C(21) | 120.75(11) |
| C(25)-C(20)-N(2) | 118.80(11) |
| C(21)-C(20)-N(2) | 120.37(11) |
| C(24)-C(25)-C(20) | 118.23(12) |
| C(24)-C(25)-C(27) | 119.57(12) |
| C(20)-C(25)-C(27) | 122.17(11) |
| C(23)-C(24)-C(25) | 121.45(13) |
| C(22)-C(23)-C(24) | 119.73(12) |
| C(23)-C(22)-C(21) | 121.29(13) |
| C(22)-C(21)-C(20) | 118.53(12) |
| C(22)-C(21)-C(30) | 118.38(12) |
| C(20)-C(21)-C(30) | 123.09(11) |
| C(25)-C(27)-C(28) | 112.43(12) |
| C(25)-C(27)-C(26) | 109.86(12) |
| C(28)-C(27)-C(26) | 110.43(13) |
| C(21)-C(30)-C(31) | 111.07(14) |
| C(21)-C(30)-C(29) | 111.32(12) |
| C(31)-C(30)-C(29) | 110.94(14) |
| C(9)-C(8)-C(13) | 120.42(11) |
| C(9)-C(8)-N(1) | 120.26(11) |
| C(13)-C(8)-N(1) | 119.23(11) |
| C(10)-C(9)-C(8) | 118.65(12) |
| C(10)-C(9)-C(18) | 118.22(12) |
| C(8)-C(9)-C(18) | 123.11(12) |
| C(11)-C(10)-C(9) | 121.33(13) |
| C(10)-C(11)-C(12) | 119.58(13) |
| C(11)-C(12)-C(13) | 121.48(13) |
| C(12)-C(13)-C(8) | 118.53(11) |
| C(12)-C(13)-C(15) | 117.80(11) |
| C(8)-C(13)-C(15) | 123.66(11) |
| C(13)-C(15)-C(14) | 110.58(12) |
| C(13)-C(15)-C(16) | 111.14(11) |
| C(14)-C(15)-C(16) | 109.67(12) |
| C(9)-C(18)-C(19) | 110.82(12) |

| | |
|---|---|
| C(9)-C(18)-C(17) | 111.94(12) |
| C(19)-C(18)-C(17) | 109.82(12) |
| Si(1)-C(1)-Sc(1) | 130.32(7) |
| C(1)-Si(1)-C(34) | 110.06(7) |
| C(1)-Si(1)-C(33) | 112.13(6) |
| C(34)-Si(1)-C(33) | 108.93(7) |
| C(1)-Si(1)-C(32) | 115.08(7) |
| C(34)-Si(1)-C(32) | 106.77(7) |
| C(33)-Si(1)-C(32) | 103.48(8) |
| Si(2)-C(2)-Sc(1) | 128.79(7) |
| C(2)-Si(2)-C(36) | 110.80(8) |
| C(2)-Si(2)-C(35) | 109.01(8) |
| C(36)-Si(2)-C(35) | 109.50(10) |
| C(2)-Si(2)-C(37) | 113.57(7) |
| C(36)-Si(2)-C(37) | 105.52(8) |
| C(35)-Si(2)-C(37) | 108.32(8) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x $10^3$) for [ArNC(Me)CHC(Me)NAr]Sc($CH_2SiMe_3$)$_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Sc(1) | 17(1) | 17(1) | 20(1) | -2(1) | -2(1) | -5(1) |
| N(1) | 20(1) | 17(1) | 21(1) | -1(1) | -3(1) | -5(1) |
| N(2) | 18(1) | 17(1) | 20(1) | 0(1) | 0(1) | -4(1) |
| Si(1) | 21(1) | 28(1) | 26(1) | -6(1) | 0(1) | -5(1) |
| Si(2) | 28(1) | 25(1) | 24(1) | -6(1) | -1(1) | -9(1) |
| C(1) | 22(1) | 26(1) | 26(1) | -5(1) | -2(1) | -7(1) |
| C(2) | 28(1) | 26(1) | 27(1) | -5(1) | -1(1) | -9(1) |
| C(3) | 42(1) | 21(1) | 29(1) | -6(1) | -1(1) | -11(1) |
| C(4) | 19(1) | 19(1) | 24(1) | -4(1) | 0(1) | -5(1) |
| C(5) | 26(1) | 22(1) | 20(1) | -5(1) | 0(1) | -6(1) |
| C(6) | 19(1) | 23(1) | 19(1) | -1(1) | 0(1) | -6(1) |
| C(7) | 38(1) | 30(1) | 22(1) | -1(1) | -9(1) | -7(1) |
| C(8) | 25(1) | 17(1) | 19(1) | -2(1) | -2(1) | -7(1) |
| C(9) | 25(1) | 25(1) | 25(1) | -2(1) | -4(1) | -7(1) |
| C(10) | 33(1) | 36(1) | 26(1) | 5(1) | -10(1) | -11(1) |
| C(11) | 40(1) | 38(1) | 22(1) | 7(1) | -6(1) | -17(1) |
| C(12) | 28(1) | 33(1) | 25(1) | 0(1) | -1(1) | -14(1) |
| C(13) | 24(1) | 22(1) | 22(1) | -3(1) | -3(1) | -8(1) |
| C(14) | 32(1) | 34(1) | 50(1) | -6(1) | -2(1) | -4(1) |
| C(15) | 22(1) | 30(1) | 26(1) | 2(1) | -3(1) | -9(1) |
| C(16) | 33(1) | 43(1) | 39(1) | -7(1) | -11(1) | -14(1) |
| C(17) | 31(1) | 45(1) | 54(1) | -9(1) | -11(1) | -13(1) |
| C(18) | 22(1) | 29(1) | 32(1) | 2(1) | -6(1) | -5(1) |
| C(19) | 31(1) | 36(1) | 44(1) | -4(1) | -3(1) | -2(1) |
| C(20) | 21(1) | 18(1) | 20(1) | -1(1) | -4(1) | -3(1) |
| C(21) | 23(1) | 22(1) | 24(1) | 1(1) | -3(1) | -6(1) |
| C(22) | 32(1) | 21(1) | 28(1) | 2(1) | -5(1) | -9(1) |
| C(23) | 35(1) | 19(1) | 30(1) | -2(1) | -7(1) | -2(1) |
| C(24) | 25(1) | 24(1) | 31(1) | -5(1) | -1(1) | 1(1) |
| C(25) | 23(1) | 22(1) | 22(1) | -3(1) | -2(1) | -4(1) |
| C(26) | 69(1) | 91(2) | 38(1) | -12(1) | 3(1) | -59(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(27) | 23(1) | 25(1) | 30(1) | -3(1) | 4(1) | -6(1) |
| C(28) | 37(1) | 34(1) | 28(1) | -3(1) | 4(1) | -7(1) |
| C(29) | 47(1) | 44(1) | 42(1) | 6(1) | 18(1) | -8(1) |
| C(30) | 26(1) | 25(1) | 41(1) | 4(1) | 6(1) | -7(1) |
| C(31) | 27(1) | 36(1) | 85(1) | 2(1) | -4(1) | -12(1) |
| C(32) | 28(1) | 51(1) | 44(1) | -13(1) | 6(1) | -13(1) |
| C(33) | 39(1) | 34(1) | 28(1) | -6(1) | -2(1) | -3(1) |
| C(34) | 33(1) | 30(1) | 34(1) | -7(1) | -3(1) | -4(1) |
| C(35) | 85(1) | 28(1) | 35(1) | -1(1) | -11(1) | -12(1) |
| C(36) | 37(1) | 82(2) | 63(1) | -34(1) | 8(1) | -30(1) |
| C(37) | 47(1) | 37(1) | 29(1) | -8(1) | -3(1) | -12(1) |

*EXPERIMENTAL DETAILS*

A. Crystal Data

| | | |
|---|---|---|
| Empirical Formula | $C_{43}H_{75}N_2Si_2Sc$ | 6b |
| Formula Weight | 721.21 | |
| Crystal Color, Habit | pale, block | |
| Crystal Dimensions | 0.48 X 0.45 X 0.44 mm | |
| Crystal System | monoclinic | |
| No. of Reflections Used for Unit Cell Determination ($2\theta$ range) | 25 ( 18.1 - 21.1° ) | |
| Omega Scan Peak Width at Half-height | 0.23° | |
| Lattice Parameters | a = 13.469(6) Å<br>b = 17.939(6) Å<br>c = 19.132(5) Å<br>$\beta$ = 90.93(3)°<br><br>V = 4622(3) Å$^3$ | |
| Space Group | $P2_1/c$ (#14) | |
| Z value | 4 | |
| $D_{calc}$ | 1.036 g/cm$^3$ | |
| $F_{000}$ | 1584.00 | |
| $\mu$(MoK$\alpha$) | 2.36 cm$^{-1}$ | |

B. Intensity Measurements

| | |
|---|---|
| Diffractometer | Rigaku AFC6S |
| Radiation | MoK$\alpha$ ($\lambda$ = 0.71069 Å)<br>graphite monochromated |

| | |
|---|---|
| Temperature | -103.0°C |
| Scan Type | $\omega$-$2\theta$ |
| Scan Rate | 8.0°/min (in $\omega$) (up to 4 scans) |
| Scan Width | $(1.26 + 0.34 \tan\theta)^\circ$ |
| $2\theta_{max}$ | 55.1° |
| No. of Reflections Measured | Total: 11468<br>Unique: 11016 ($R_{int} = 0.087$) |
| Corrections | Lorentz-polarization<br>Absorption<br>(trans. factors: 0.8940 - 0.9022)<br>Decay (3.08%)<br>Secondary Extinction<br>(coefficient: 1.14299e-07) |

C. Structure Solution and Refinement

| | |
|---|---|
| Structure Solution | Direct Methods |
| Refinement | Full-matrix least-squares |
| Function Minimized | $\Sigma w(\lvert Fo\rvert - \lvert Fc\rvert)^2$ |
| Least Squares Weights | $w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$ |
| p-factor | 0.0150 |
| Anomalous Dispersion | All non-hydrogen atoms |
| No. Observations (I>3.00$\sigma$(I)) | 3339 |
| No. Variables | 434 |
| Reflection/Parameter Ratio | 7.69 |
| Residuals: R; Rw | 0.060 ; 0.059 |
| Goodness of Fit Indicator | 2.18 |
| Max Shift/Error in Final Cycle | 0.01 |
| Maximum peak in Final Diff. Map | 0.31 $e^-/\AA^3$ |
| Minimum peak in Final Diff. Map | -0.32 $e^-/\AA^3$ |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| Sc(1) | 0.20847(9) | 0.00063(8) | 0.22998(7) | 2.14(3) |
| Si(1) | -0.06914(17) | 0.02676(14) | 0.25261(13) | 4.16(6) |
| Si(2) | 0.2481(2) | -0.15563(15) | 0.10699(13) | 5.48(8) |
| N(1) | 0.2793(3) | 0.0093(3) | 0.3277(3) | 1.92(12) |
| N(2) | 0.2692(4) | 0.1035(3) | 0.1929(3) | 1.88(13) |
| C(1) | 0.0452(5) | -0.0192(4) | 0.2245(4) | 3.6(2) |
| C(2) | 0.2855(6) | -0.0904(4) | 0.1758(4) | 3.8(2) |
| C(3) | 0.2327(5) | 0.0899(4) | 0.4339(4) | 3.2(2) |
| C(4) | 0.2544(5) | 0.0759(4) | 0.3550(3) | 2.04(16) |
| C(5) | 0.2364(5) | 0.1376(4) | 0.3118(4) | 2.78(18) |
| C(6) | 0.2604(5) | 0.1566(4) | 0.2405(3) | 2.19(17) |
| C(7) | 0.2693(6) | 0.2425(4) | 0.2299(4) | 3.5(2) |
| C(8) | 0.3297(5) | -0.0502(4) | 0.3649(3) | 2.15(17) |
| C(9) | 0.2795(5) | -0.1140(4) | 0.3860(3) | 2.35(18) |
| C(10) | 0.3331(6) | -0.1709(4) | 0.4192(4) | 3.3(2) |
| C(11) | 0.4330(6) | -0.1651(4) | 0.4311(4) | 3.5(2) |
| C(12) | 0.4833(5) | -0.1039(5) | 0.4060(4) | 3.1(2) |
| C(13) | 0.4348(5) | -0.0465(4) | 0.3722(3) | 2.15(16) |
| C(14) | 0.5888(6) | -0.0074(5) | 0.3108(4) | 5.3(2) |
| C(15) | 0.4933(5) | 0.0183(4) | 0.3438(3) | 2.87(18) |
| C(16) | 0.5176(7) | 0.0779(5) | 0.3977(5) | 6.2(3) |
| C(17) | 0.1434(6) | -0.1881(5) | 0.3264(4) | 5.1(3) |
| C(18) | 0.1673(6) | -0.1239(4) | 0.3764(4) | 3.6(2) |
| C(19) | 0.1144(6) | -0.1384(5) | 0.4450(4) | 5.1(3) |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| C(20) | 0.2969(5) | 0.1138(4) | 0.1208(4) | 2.62(18) |
| C(21) | 0.2209(6) | 0.1249(4) | 0.0700(4) | 2.76(19) |
| C(22) | 0.2477(6) | 0.1332(4) | 0.0012(4) | 3.5(2) |
| C(23) | 0.3457(7) | 0.1290(5) | -0.0191(4) | 4.4(2) |
| C(24) | 0.4185(6) | 0.1157(5) | 0.0307(4) | 4.5(2) |
| C(25) | 0.3962(5) | 0.1063(4) | 0.1010(4) | 2.94(19) |
| C(26) | 0.5518(6) | 0.1501(5) | 0.1643(5) | 6.6(3) |
| C(27) | 0.4790(5) | 0.0854(5) | 0.1522(4) | 3.7(2) |
| C(28) | 0.5374(6) | 0.0181(5) | 0.1256(4) | 5.3(3) |
| C(29) | 0.0616(6) | 0.2016(5) | 0.0652(4) | 4.5(2) |
| C(30) | 0.1120(5) | 0.1285(4) | 0.0869(4) | 2.99(19) |
| C(31) | 0.0573(6) | 0.0647(5) | 0.0499(4) | 4.8(3) |
| C(32) | 0.3019(6) | 0.2695(4) | 0.1587(4) | 4.3(2) |
| C(33) | 0.3486(7) | 0.2720(5) | 0.2829(4) | 6.5(3) |
| C(34) | 0.1686(7) | 0.2789(4) | 0.2443(5) | 5.9(3) |
| C(35) | 0.1194(6) | 0.0858(5) | 0.4407(4) | 5.4(3) |
| C(36) | 0.2659(7) | 0.1678(5) | 0.4578(4) | 5.4(3) |
| C(37) | 0.2781(5) | 0.0353(4) | 0.4867(3) | 3.11(19) |
| C(38) | -0.0578(6) | 0.1313(5) | 0.2572(5) | 6.4(3) |
| C(39) | -0.1754(6) | 0.0064(6) | 0.1894(4) | 7.4(3) |
| C(40) | -0.1063(6) | -0.0064(6) | 0.3406(4) | 5.8(3) |
| C(41) | 0.2578(7) | -0.1085(6) | 0.0212(5) | 7.8(3) |
| C(42) | 0.1165(8) | -0.1900(5) | 0.1150(5) | 8.4(4) |
| C(43) | 0.3281(10) | -0.2390(6) | 0.1087(6) | 13.7(5) |

Table 2. Anisotropic Displacement Parameters

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| Sc(1) | 0.0269(7) | 0.0269(7) | 0.0274(7) | 0.0005(8) | -0.0028(5) | -0.0010(8) |
| Si(1) | 0.0310(13) | 0.0643(19) | 0.0628(16) | 0.0023(12) | 0.0053(11) | 0.0113(14) |
| Si(2) | 0.122(3) | 0.0501(18) | 0.0366(15) | 0.0318(18) | 0.0015(16) | -0.0088(14) |
| N(1) | 0.022(3) | 0.023(4) | 0.028(3) | -0.001(3) | -0.002(2) | -0.002(3) |
| N(2) | 0.019(3) | 0.028(4) | 0.025(3) | -0.002(3) | 0.003(3) | -0.003(3) |
| C(1) | 0.035(5) | 0.042(6) | 0.060(5) | -0.005(4) | -0.015(4) | 0.006(4) |
| C(2) | 0.051(6) | 0.038(5) | 0.055(6) | -0.012(4) | 0.019(4) | -0.003(4) |
| C(3) | 0.042(5) | 0.041(5) | 0.039(5) | 0.006(4) | 0.004(4) | -0.010(4) |
| C(4) | 0.021(4) | 0.033(5) | 0.023(4) | -0.002(3) | -0.006(3) | -0.003(4) |
| C(5) | 0.041(5) | 0.032(5) | 0.032(4) | 0.010(4) | 0.003(4) | -0.002(4) |
| C(6) | 0.031(4) | 0.026(4) | 0.025(4) | -0.001(4) | -0.003(3) | 0.006(4) |
| C(7) | 0.064(6) | 0.025(5) | 0.042(5) | -0.011(4) | -0.004(4) | 0.002(4) |
| C(8) | 0.029(4) | 0.027(4) | 0.025(4) | -0.002(4) | 0.000(3) | 0.000(3) |
| C(9) | 0.031(5) | 0.031(5) | 0.028(4) | -0.001(4) | -0.001(4) | -0.004(4) |
| C(10) | 0.059(6) | 0.028(5) | 0.039(5) | -0.005(4) | 0.000(4) | 0.013(4) |
| C(11) | 0.055(6) | 0.037(5) | 0.042(5) | 0.009(5) | -0.011(4) | 0.006(4) |
| C(12) | 0.035(5) | 0.052(6) | 0.031(5) | 0.005(4) | -0.002(4) | 0.005(4) |
| C(13) | 0.031(4) | 0.024(4) | 0.027(4) | 0.001(4) | -0.002(3) | -0.001(3) |
| C(14) | 0.046(5) | 0.087(7) | 0.070(6) | -0.002(6) | 0.019(4) | 0.017(6) |
| C(15) | 0.029(4) | 0.047(6) | 0.033(4) | -0.002(4) | -0.004(3) | 0.013(4) |
| C(16) | 0.102(8) | 0.062(7) | 0.072(7) | -0.049(6) | 0.008(6) | -0.006(6) |
| C(17) | 0.064(6) | 0.070(7) | 0.060(6) | -0.034(5) | -0.016(5) | -0.004(5) |
| C(18) | 0.045(5) | 0.048(6) | 0.045(5) | -0.016(4) | -0.004(4) | 0.014(4) |
| C(19) | 0.058(6) | 0.065(7) | 0.071(6) | -0.021(5) | 0.014(5) | 0.008(5) |

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Table 2. Anisotropic Displacement Parameters (continued)

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| C(20) | 0.043(5) | 0.026(5) | 0.030(4) | 0.008(4) | 0.000(4) | 0.006(4) |
| C(21) | 0.049(5) | 0.028(5) | 0.028(4) | 0.003(4) | 0.003(4) | 0.000(4) |
| C(22) | 0.055(6) | 0.055(6) | 0.023(4) | 0.022(5) | -0.001(4) | 0.015(4) |
| C(23) | 0.067(6) | 0.069(7) | 0.032(5) | 0.029(5) | 0.012(5) | 0.010(5) |
| C(24) | 0.051(6) | 0.077(7) | 0.044(5) | 0.016(5) | 0.018(5) | 0.015(5) |
| C(25) | 0.026(4) | 0.054(6) | 0.032(4) | 0.004(4) | 0.007(4) | 0.010(4) |
| C(26) | 0.064(7) | 0.071(7) | 0.114(9) | -0.002(6) | -0.031(6) | 0.019(7) |
| C(27) | 0.025(5) | 0.060(6) | 0.054(5) | 0.007(4) | 0.006(4) | 0.016(5) |
| C(28) | 0.039(5) | 0.079(8) | 0.082(7) | 0.014(5) | 0.005(5) | 0.015(6) |
| C(29) | 0.046(5) | 0.058(6) | 0.067(6) | 0.013(5) | -0.011(4) | -0.001(5) |
| C(30) | 0.037(5) | 0.030(5) | 0.046(5) | 0.007(4) | -0.007(4) | 0.000(4) |
| C(31) | 0.059(6) | 0.065(7) | 0.059(6) | -0.005(5) | -0.011(5) | -0.004(5) |
| C(32) | 0.074(6) | 0.034(5) | 0.054(6) | -0.014(5) | -0.001(5) | 0.012(4) |
| C(33) | 0.147(10) | 0.051(6) | 0.047(6) | -0.043(7) | -0.023(6) | 0.008(5) |
| C(34) | 0.114(8) | 0.032(5) | 0.081(7) | 0.040(6) | 0.028(6) | 0.017(5) |
| C(35) | 0.051(6) | 0.119(9) | 0.036(5) | 0.023(6) | 0.015(4) | 0.012(6) |
| C(36) | 0.119(9) | 0.058(6) | 0.027(5) | 0.013(6) | -0.002(5) | -0.017(5) |
| C(37) | 0.057(5) | 0.045(5) | 0.016(4) | 0.004(4) | 0.003(4) | -0.002(4) |
| C(38) | 0.075(7) | 0.076(8) | 0.093(7) | 0.026(6) | 0.031(6) | 0.012(6) |
| C(39) | 0.038(5) | 0.178(11) | 0.064(6) | 0.007(7) | -0.005(4) | 0.039(8) |
| C(40) | 0.045(5) | 0.110(8) | 0.067(6) | -0.010(6) | 0.014(4) | 0.016(7) |
| C(41) | 0.109(9) | 0.133(10) | 0.054(7) | 0.041(8) | 0.002(6) | -0.006(7) |
| C(42) | 0.160(11) | 0.066(8) | 0.092(8) | -0.050(8) | -0.020(8) | -0.008(7) |
| C(43) | 0.278(17) | 0.123(11) | 0.116(10) | 0.129(11) | -0.101(10) | -0.079(9) |

Table 2. Anisotropic Displacement Parameters (continued)

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|

The general temperature factor expression:

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

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Table 3. Bond Lengths(Å)

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| Sc(1) | N(1) | 2.091(5) | Sc(1) | N(2) | 2.144(5) |
| Sc(1) | C(1) | 2.229(7) | Sc(1) | C(2) | 2.202(7) |
| Si(1) | C(1) | 1.835(7) | Si(1) | C(38) | 1.884(9) |
| Si(1) | C(39) | 1.894(8) | Si(1) | C(40) | 1.861(8) |
| Si(2) | C(2) | 1.827(8) | Si(2) | C(41) | 1.853(9) |
| Si(2) | C(42) | 1.886(10) | Si(2) | C(43) | 1.844(10) |
| N(1) | C(4) | 1.349(8) | N(1) | C(8) | 1.446(8) |
| N(2) | C(6) | 1.325(7) | N(2) | C(20) | 1.446(8) |
| C(3) | C(4) | 1.562(8) | C(3) | C(35) | 1.536(10) |
| C(3) | C(36) | 1.535(10) | C(3) | C(37) | 1.528(9) |
| C(4) | C(5) | 1.400(9) | C(5) | C(6) | 1.447(8) |
| C(6) | C(7) | 1.561(9) | C(7) | C(32) | 1.518(9) |
| C(7) | C(33) | 1.555(10) | C(7) | C(34) | 1.534(10) |
| C(8) | C(9) | 1.392(8) | C(8) | C(13) | 1.422(8) |
| C(9) | C(10) | 1.398(9) | C(9) | C(18) | 1.530(9) |
| C(10) | C(11) | 1.365(9) | C(11) | C(12) | 1.382(10) |
| C(12) | C(13) | 1.376(9) | C(13) | C(15) | 1.511(9) |
| C(14) | C(15) | 1.514(9) | C(15) | C(16) | 1.516(10) |
| C(17) | C(18) | 1.530(10) | C(18) | C(19) | 1.526(10) |
| C(20) | C(21) | 1.413(9) | C(20) | C(25) | 1.403(8) |
| C(21) | C(22) | 1.379(9) | C(21) | C(30) | 1.508(9) |
| C(22) | C(23) | 1.384(9) | C(23) | C(24) | 1.378(10) |
| C(24) | C(25) | 1.393(9) | C(25) | C(27) | 1.518(9) |
| C(26) | C(27) | 1.534(11) | C(27) | C(28) | 1.532(10) |

Table 3. Bond Lengths(Å) (continued)

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| C(29) | C(30) | 1.531(10) | C(30) | C(31) | 1.529(10) |

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Table 5. Bond Angles(°)

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| N(1) | Sc(1) | N(2) | 93.5(2) | N(1) | Sc(1) | C(1) | 119.3(2) |
| N(1) | Sc(1) | C(2) | 105.3(3) | N(2) | Sc(1) | C(1) | 120.2(2) |
| N(2) | Sc(1) | C(2) | 107.3(2) | C(1) | Sc(1) | C(2) | 109.4(3) |
| C(1) | Si(1) | C(38) | 113.2(4) | C(1) | Si(1) | C(39) | 110.8(4) |
| C(1) | Si(1) | C(40) | 111.1(4) | C(38) | Si(1) | C(39) | 106.4(5) |
| C(38) | Si(1) | C(40) | 107.4(4) | C(39) | Si(1) | C(40) | 107.7(4) |
| C(2) | Si(2) | C(41) | 108.9(4) | C(2) | Si(2) | C(42) | 113.5(4) |
| C(2) | Si(2) | C(43) | 110.7(4) | C(41) | Si(2) | C(42) | 107.5(5) |
| C(41) | Si(2) | C(43) | 109.7(5) | C(42) | Si(2) | C(43) | 106.4(6) |
| Sc(1) | N(1) | C(4) | 107.4(4) | Sc(1) | N(1) | C(8) | 126.1(4) |
| C(4) | N(1) | C(8) | 125.5(5) | Sc(1) | N(2) | C(6) | 110.6(4) |
| Sc(1) | N(2) | C(20) | 122.1(4) | C(6) | N(2) | C(20) | 126.3(6) |
| Sc(1) | C(1) | Si(1) | 138.3(4) | Sc(1) | C(2) | Si(2) | 133.5(4) |
| C(4) | C(3) | C(35) | 106.0(6) | C(4) | C(3) | C(36) | 112.1(6) |
| C(4) | C(3) | C(37) | 117.2(6) | C(35) | C(3) | C(36) | 107.7(7) |
| C(35) | C(3) | C(37) | 107.5(6) | C(36) | C(3) | C(37) | 106.0(6) |
| N(1) | C(4) | C(3) | 124.6(6) | N(1) | C(4) | C(5) | 120.9(6) |
| C(3) | C(4) | C(5) | 114.2(6) | C(4) | C(5) | C(6) | 134.7(6) |
| N(2) | C(6) | C(5) | 120.2(6) | N(2) | C(6) | C(7) | 127.8(6) |
| C(5) | C(6) | C(7) | 112.0(6) | C(6) | C(7) | C(32) | 117.1(6) |
| C(6) | C(7) | C(33) | 107.7(6) | C(6) | C(7) | C(34) | 109.1(6) |
| C(32) | C(7) | C(33) | 105.7(6) | C(32) | C(7) | C(34) | 107.3(7) |
| C(33) | C(7) | C(34) | 109.8(7) | N(1) | C(8) | C(9) | 121.5(6) |
| N(1) | C(8) | C(13) | 118.2(6) | C(9) | C(8) | C(13) | 119.9(6) |

Table 5. Bond Angles(°) (continued)

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| C(8) | C(9) | C(10) | 118.8(6) | C(8) | C(9) | C(18) | 123.0(7) |
| C(10) | C(9) | C(18) | 118.1(7) | C(9) | C(10) | C(11) | 121.4(7) |
| C(10) | C(11) | C(12) | 119.4(7) | C(11) | C(12) | C(13) | 121.8(7) |
| C(8) | C(13) | C(12) | 118.4(6) | C(8) | C(13) | C(15) | 121.7(6) |
| C(12) | C(13) | C(15) | 119.9(6) | C(13) | C(15) | C(14) | 111.5(6) |
| C(13) | C(15) | C(16) | 113.9(6) | C(14) | C(15) | C(16) | 108.8(7) |
| C(9) | C(18) | C(17) | 111.1(7) | C(9) | C(18) | C(19) | 113.1(6) |
| C(17) | C(18) | C(19) | 108.3(6) | N(2) | C(20) | C(21) | 118.6(6) |
| N(2) | C(20) | C(25) | 120.4(6) | C(21) | C(20) | C(25) | 120.8(7) |
| C(20) | C(21) | C(22) | 118.2(7) | C(20) | C(21) | C(30) | 123.7(6) |
| C(22) | C(21) | C(30) | 118.0(7) | C(21) | C(22) | C(23) | 121.9(7) |
| C(22) | C(23) | C(24) | 119.1(7) | C(23) | C(24) | C(25) | 121.8(7) |
| C(20) | C(25) | C(24) | 118.1(7) | C(20) | C(25) | C(27) | 122.9(6) |
| C(24) | C(25) | C(27) | 119.0(7) | C(25) | C(27) | C(26) | 111.8(7) |
| C(25) | C(27) | C(28) | 110.9(7) | C(26) | C(27) | C(28) | 108.4(6) |
| C(21) | C(30) | C(29) | 114.0(6) | C(21) | C(30) | C(31) | 109.4(6) |
| C(29) | C(30) | C(31) | 107.9(6) | | | | |