## X-ray crystallographic data

Full crystallographic details have been deposited in cif-format with the Cambridge Crystallographic Data Centre, the CCDC deposition numbers are 284653 ($LCoNH^tBu$) and 299818 ($LCoN^tBu$). Copies of this information can be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge, CB21EZ, UK, Fax: +44-1223-336-033, e-mail: deposit@ccdc.cam.ac.uk, Web: http://www.ccdc.cam.ac.uk/conts/retrieving/html.

## $LCoNH^tBu$ Structure Determination.

Deep green crystals of **$LCoNH^tBu$** were grown from $Et_2O$/hexamethyldisiloxane by diffusion at -35°C, shipped over dry ice and kept at -70C for a few days. For the structure determination a prismatic crystal 0.30 x 0.15 x 0.10 mm in size was mounted on a standard Bruker X8 Apex2 CCD-based X-ray diffractometer equipped with an Oxford Cryostream 700 low temperature device. Intensities were measured at 203(2) K using graphite monochromatized Mo-$K_\alpha$ radiation ($\lambda$ = 0.71073 Å). A full sphere of data, 2662 frames each at 5.500 cm detector distance, was collected with scan width of 0.50° in $\omega$ and an exposure time of 15 s/frame. Analysis of the frames showed negligible decay during data collection. The data were integrated using the Bruker SAINT software package with a narrow frame algorithm[1] yielding a total of 32313 reflections of which 12109 independent. The SADABS program was used for the absorption correction.[2] The final cell constants were based on 6425 reflections with $I>10\sigma(I)$.

The structure was solved by direct methods and refined by full matrix least-squares techniques with the SHELX97 software package.[3] The observed reflection condition (oko: k = 2n) indicated $P2_1/m$ (#11) and $P2_1$ (#4) as possible space groups. Initial attempts to solve the structure within the higher symmetry $P2_1/m$ did not yield acceptable result, while solution in $P2_1$ resulted in starting R-factor of c.a. 19% and the refinement was consequently carried out in the latter space group. Initially all non-hydrogen atoms have been found and assigned from the Fourier maps and their thermal parameters refined anisotropically. Next, the hydrogen atoms have been added to the refinement as riding models and their thermal parameters refined isotropically. The amido hydrogen was located directly from the Fourier maps. Last, some positional disorder of a limited number of C- and N- atoms has been modeled and refined. After the refinement converged, a close examination of the solution as well as a test using the PLATON program confirmed the lack of possible higher symmetry.[4] The main crystallographic details are summarized in Table 1.

**Table 1.** Crystal data and structure refinement for **LCoNH$^t$Bu**

| | |
|---|---|
| Empirical formula | $C_{31}$ $H_{47}$ B Co $N_7$ |
| Formula weight | 587.54 |
| Temperature | 203(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Monoclinic, P $2_1$ (#4) |
| Unit cell dimensions | a = 15.777(3) Å alpha = 90 deg.<br>b = 11.349(2) Å beta = 105.160(10) deg.<br>c = 30.139(6) Å gamma = 90 deg. |
| Volume, Z | 5208.7(17) Å$^3$, 6 |
| Calculated density | 1.125 g/cm$^3$ |
| Absorption coefficient | 0.523 mm$^{-1}$ |
| F(000) | 1889 |
| Crystal size | 0.30 x 0.15 x 0.10 mm |
| Theta range for data collection | 0.70 to 22.00 deg. |
| Limiting indices | -16<=h<=16, -11<=k<=11, -31<=l<=31 |
| Reflections collected / unique | 32313 / 12109 [R(int) = 0.0352] |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / parameters | 12109 / 1127 |
| Goodness-of-fit on $F^2$ | 1.089 |
| Final R indices [I>2σ(I)] | [a]R1 = 0.0537, [b]Rw2 = 0.1563 |
| R indices (all data) | R1 = 0.0657, wR2 = 0.1664 |

[a] $R1 = \Sigma \| \|F_o\| - \|F_c\| / \Sigma |F_o|$ (based on reflections with $I > 2\sigma(I)$)

[b] $R_w2 = [\Sigma w(\|F_o\| - \|F_c\|)^2 / \Sigma w |F_o|2]^{1/2}$ ; $w = 1 / [\sigma^2(F_o^2) + (0.1181P)^2]$;
$P=[Max(F_o^2,0) + 2F_c^2]/3$ (all data)

**Table 2.** Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$ x $10^3$) for **LCoNH$^t$Bu**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| Co(1) | -4464(1) | 4319(1) | 7366(1) | 34(1) |
| B(1) | -4219(5) | 6490(7) | 8008(3) | 35(2) |
| N(1) | -4800(3) | 6837(5) | 7508(2) | 34(1) |
| N(2) | -5520(4) | 6614(5) | 6803(2) | 38(1) |
| C(1) | -4980(4) | 6024(6) | 7161(2) | 33(2) |
| C(2) | -5258(4) | 7858(6) | 7368(2) | 40(2) |
| C(3) | -5689(5) | 7728(6) | 6939(2) | 42(2) |
| C(4) | -5880(5) | 6105(7) | 6338(2) | 45(2) |
| C(5) | -6380(7) | 7077(9) | 6010(3) | 84(3) |
| C(6) | -5098(5) | 5683(7) | 6165(2) | 50(2) |
| C(7) | -6507(5) | 5130(8) | 6369(3) | 63(2) |
| N(3) | -3327(3) | 5943(5) | 7958(2) | 33(1) |
| N(4) | -2369(3) | 4873(5) | 7739(2) | 39(1) |
| C(8) | -3252(4) | 5012(6) | 7692(2) | 36(2) |
| C(9) | -2495(4) | 6401(6) | 8166(2) | 41(2) |
| C(10) | -1912(5) | 5761(7) | 8029(2) | 47(2) |
| C(11) | -1965(4) | 3972(6) | 7502(3) | 46(2) |
| C(12) | -2325(6) | 2817(8) | 7586(4) | 83(3) |
| C(13) | -2203(7) | 4294(11) | 6985(3) | 97(4) |
| C(14) | -975(5) | 3984(10) | 7683(4) | 88(3) |
| N(5) | -4798(3) | 5497(5) | 8157(2) | 32(1) |
| N(6) | -5498(3) | 3869(5) | 8167(2) | 32(1) |
| C(15) | -4930(4) | 4432(6) | 7956(2) | 31(2) |
| C(16) | -5318(4) | 5626(6) | 8463(2) | 33(2) |
| C(17) | -5737(4) | 4622(6) | 8475(2) | 33(2) |
| C(18) | -5739(4) | 2589(6) | 8105(2) | 41(2) |
| C(19) | -6223(5) | 2355(7) | 7606(2) | 49(2) |
| C(20) | -4890(5) | 1878(6) | 8239(3) | 51(2) |
| C(21) | -6342(5) | 2260(8) | 8405(3) | 62(2) |
| C(22) | -3955(4) | 7547(6) | 8381(2) | 37(2) |
| C(23) | -3740(5) | 8678(7) | 8268(3) | 52(2) |
| C(24) | -3338(5) | 9467(7) | 8594(4) | 63(2) |
| C(25) | -3132(5) | 9197(9) | 9040(3) | 63(2) |
| C(26) | -3331(5) | 8101(9) | 9161(3) | 64(3) |
| C(27) | -3728(4) | 7286(7) | 8843(2) | 43(2) |
| N(97) | -4771(5) | 3186(6) | 6894(2) | 68(2) |

| | | | | |
|---|---|---|---|---|
| C(28) | -4759(5) | 2014(6) | 6705(2) | 47(2) |
| C(29) | -4217(6) | 1953(8) | 6362(3) | 72(3) |
| C(30) | -5687(7) | 1661(11) | 6470(3) | 91(3) |
| C(31) | -4436(7) | 1141(8) | 7080(3) | 81(3) |
| Co(2) | -2021(1) | 5341(1) | 10642(1) | 32(1) |
| B(2) | -4033(4) | 5692(6) | 10290(2) | 30(2) |
| N(8) | -3811(3) | 4935(4) | 10734(2) | 28(1) |
| N(9) | -3018(3) | 4177(5) | 11375(2) | 33(1) |
| C(32) | -2948(4) | 4752(6) | 10991(2) | 34(2) |
| C(33) | -4394(4) | 4401(6) | 10954(2) | 35(2) |
| C(34) | -3894(4) | 3954(6) | 11355(2) | 39(2) |
| C(35) | -2283(5) | 3831(7) | 11765(2) | 50(2) |
| C(36) | -2627(6) | 3626(9) | 12189(3) | 74(3) |
| C(37) | -1594(5) | 4797(8) | 11867(3) | 61(2) |
| C(38) | -1903(6) | 2689(8) | 11642(3) | 78(3) |
| N(10) | -3502(3) | 6879(4) | 10401(2) | 29(1) |
| N(11) | -2444(3) | 8140(5) | 10642(2) | 35(1) |
| C(39) | -2615(4) | 6976(6) | 10576(2) | 33(2) |
| C(40) | -3867(4) | 8009(5) | 10342(2) | 30(2) |
| C(41) | -3218(4) | 8790(6) | 10484(2) | 39(2) |
| C(42) | -1552(5) | 8659(7) | 10824(3) | 56(2) |
| C(43) | -1017(7) | 8410(14) | 10499(5) | 131(5) |
| C(44) | -1128(7) | 8028(11) | 11259(4) | 127(5) |
| C(45) | -1612(7) | 9948(9) | 10915(7) | 183(9) |
| N(12) | -3657(3) | 5019(4) | 9932(2) | 31(1) |
| N(13) | -2704(3) | 4360(5) | 9582(2) | 33(1) |
| C(46) | -2772(4) | 4865(5) | 9986(2) | 32(2) |
| C(47) | -4119(4) | 4562(5) | 9511(2) | 33(2) |
| C(48) | -3518(4) | 4164(6) | 9293(2) | 37(2) |
| C(49) | -1836(4) | 4120(6) | 9472(2) | 42(2) |
| C(50) | -1310(4) | 3264(7) | 9824(3) | 49(2) |
| C(51) | -1353(5) | 5293(7) | 9495(3) | 59(2) |
| C(52) | -2055(6) | 3576(9) | 8979(3) | 70(3) |
| C(53) | -5065(4) | 6059(5) | 10094(2) | 27(1) |
| C(54) | -5647(4) | 6199(6) | 10372(2) | 33(2) |
| C(55) | -6495(4) | 6648(6) | 10205(2) | 38(2) |
| C(56) | -6782(4) | 6992(6) | 9756(2) | 40(2) |
| C(57) | -6216(4) | 6921(5) | 9473(2) | 35(2) |
| C(58) | -5369(4) | 6483(6) | 9646(2) | 34(2) |
| N(98) | -836(4) | 4964(12) | 10870(3) | 126(5) |
| C(59) | 49(5) | 4764(8) | 10986(3) | 63(2) |
| C(60A) | 412(18) | 3480(30) | 10900(20) | 80(20) |
| C(60B) | 10(20) | 3390(30) | 11071(9) | 86(12) |
| C(61) | 561(6) | 5330(13) | 11453(4) | 79(4) |
| C(62A) | 540(30) | 5210(60) | 10637(14) | 95(13) |
| C(62B) | 260(30) | 5190(70) | 10549(16) | 90(20) |

| | | | | |
|---|---|---|---|---|
| Co(3) | -1761(1) | 7248(1) | 5879(1) | 35(1) |
| B(3) | -16(5) | 6137(8) | 6449(3) | 37(2) |
| N(15) | 149(3) | 6929(5) | 6052(2) | 35(1) |
| N(16) | -109(4) | 8181(6) | 5479(2) | 45(2) |
| C(63) | -506(5) | 7628(6) | 5782(2) | 40(2) |
| C(64) | 894(4) | 6992(7) | 5895(3) | 47(2) |
| C(65) | 737(5) | 7752(7) | 5537(3) | 50(2) |
| C(66) | -517(5) | 9058(7) | 5129(2) | 51(2) |
| C(67) | 190(6) | 9753(11) | 4984(4) | 93(4) |
| C(68) | -1020(6) | 9907(9) | 5339(3) | 88(3) |
| C(69) | -1034(7) | 8463(11) | 4739(3) | 98(4) |
| N(17) | -500(3) | 6883(5) | 6747(2) | 30(1) |
| N(18) | -1463(3) | 7956(5) | 6964(2) | 35(1) |
| C(70) | -1289(4) | 7430(6) | 6587(2) | 35(2) |
| C(71) | -189(4) | 7085(7) | 7204(2) | 40(2) |
| C(72) | -803(5) | 7718(6) | 7338(2) | 46(2) |
| C(73) | -2282(5) | 8618(6) | 6963(2) | 47(2) |
| C(74) | -3076(5) | 7756(8) | 6842(3) | 64(2) |
| C(75) | -2387(6) | 9590(7) | 6599(3) | 63(2) |
| C(76) | -2234(5) | 9137(8) | 7426(3) | 61(2) |
| N(19) | -686(3) | 5155(5) | 6184(2) | 33(1) |
| N(20) | -1845(3) | 4398(6) | 5741(2) | 43(2) |
| C(77) | -1493(4) | 5438(6) | 5920(2) | 33(2) |
| C(78) | -533(5) | 3978(7) | 6147(2) | 46(2) |
| C(79) | -1251(5) | 3488(7) | 5884(2) | 46(2) |
| C(80) | -2752(4) | 4268(7) | 5424(2) | 48(2) |
| C(81) | -2778(5) | 4876(9) | 4973(3) | 68(3) |
| C(82) | -3406(5) | 4797(8) | 5647(3) | 67(2) |
| C(83) | -2946(5) | 2931(8) | 5353(4) | 82(3) |
| C(84) | 854(4) | 5620(6) | 6788(2) | 39(2) |
| C(85) | 1643(4) | 6227(7) | 6903(2) | 50(2) |
| C(86) | 2366(5) | 5878(10) | 7272(3) | 72(3) |
| C(87) | 2299(7) | 4926(11) | 7528(4) | 87(3) |
| C(88) | 1510(7) | 4278(9) | 7427(3) | 78(3) |
| C(89) | 788(5) | 4652(7) | 7054(3) | 56(2) |
| C(90) | -6442(4) | 3445(7) | 4729(3) | 52(2) |
| N(97) | -2890(11) | 7888(18) | 5625(6) | 57(5) |
| C(91A) | -3368(18) | 8160(20) | 4798(7) | 92(7) |
| C(91B) | -4010(12) | 8050(20) | 4783(7) | 77(7) |
| C(92) | -6433(8) | 4745(10) | 4754(4) | 75(4) |
| C(93A) | -5451(19) | 2900(40) | 4724(16) | 60(50) |
| C(93B) | -5805(11) | 3250(20) | 4419(7) | 73(6) |

**Table 3.** Bond lengths [Å] and angles [deg] for **LCoNH$^t$Bu**.

| | |
|---|---|
| Co(1)-N(97) | 1.886(7) |
| Co(1)-C(8) | 2.064(7) |
| Co(1)-C(15) | 2.099(6) |
| Co(1)-C(1) | 2.128(7) |
| B(1)-N(3) | 1.579(9) |
| B(1)-N(5) | 1.589(9) |
| B(1)-N(1) | 1.595(9) |
| B(1)-C(22) | 1.621(10) |
| N(1)-C(1) | 1.368(8) |
| N(1)-C(2) | 1.373(8) |
| N(2)-C(1) | 1.363(8) |
| N(2)-C(3) | 1.377(9) |
| N(2)-C(4) | 1.485(9) |
| C(2)-C(3) | 1.303(9) |
| C(4)-C(7) | 1.504(11) |
| C(4)-C(6) | 1.536(10) |
| C(4)-C(5) | 1.552(11) |
| N(3)-C(8) | 1.351(8) |
| N(3)-C(9) | 1.398(8) |
| N(4)-C(8) | 1.371(8) |
| N(4)-C(10) | 1.404(9) |
| N(4)-C(11) | 1.483(9) |
| C(9)-C(10) | 1.322(10) |
| C(11)-C(12) | 1.476(12) |
| C(11)-C(14) | 1.513(11) |
| C(11)-C(13) | 1.547(11) |
| N(5)-C(15) | 1.343(8) |
| N(5)-C(16) | 1.392(8) |
| N(6)-C(15) | 1.382(8) |
| N(6)-C(17) | 1.387(8) |
| N(6)-C(18) | 1.501(9) |
| C(16)-C(17) | 1.323(9) |
| C(18)-C(19) | 1.520(9) |
| C(18)-C(21) | 1.521(9) |
| C(18)-C(20) | 1.526(10) |
| C(22)-C(27) | 1.377(9) |
| C(22)-C(23) | 1.393(10) |
| C(23)-C(24) | 1.358(11) |
| C(24)-C(25) | 1.333(12) |
| C(25)-C(26) | 1.357(13) |
| C(26)-C(27) | 1.361(11) |
| N(97)-C(28) | 1.448(10) |
| C(28)-C(31) | 1.489(11) |

| | |
|---|---|
| C(28)-C(30) | 1.505(12) |
| C(28)-C(29) | 1.505(11) |
| Co(2)-N(98) | 1.865(6) |
| Co(2)-C(39) | 2.066(7) |
| Co(2)-C(46) | 2.093(6) |
| Co(2)-C(32) | 2.120(7) |
| B(2)-N(8) | 1.551(9) |
| B(2)-N(12) | 1.560(9) |
| B(2)-N(10) | 1.575(9) |
| B(2)-C(53) | 1.635(9) |
| N(8)-C(32) | 1.394(8) |
| N(8)-C(33) | 1.404(8) |
| N(9)-C(32) | 1.359(8) |
| N(9)-C(34) | 1.390(8) |
| N(9)-C(35) | 1.472(9) |
| C(33)-C(34) | 1.356(9) |
| C(35)-C(38) | 1.514(11) |
| C(35)-C(37) | 1.517(11) |
| C(35)-C(36) | 1.534(11) |
| N(10)-C(39) | 1.365(8) |
| N(10)-C(40) | 1.398(8) |
| N(11)-C(39) | 1.352(9) |
| N(11)-C(41) | 1.399(8) |
| N(11)-C(42) | 1.491(9) |
| C(40)-C(41) | 1.337(9) |
| C(42)-C(43) | 1.480(14) |
| C(42)-C(44) | 1.490(14) |
| C(42)-C(45) | 1.496(13) |
| N(12)-C(46) | 1.373(8) |
| N(12)-C(47) | 1.388(8) |
| N(13)-C(48) | 1.368(8) |
| N(13)-C(46) | 1.377(8) |
| N(13)-C(49) | 1.515(8) |
| C(47)-C(48) | 1.364(9) |
| C(49)-C(50) | 1.514(10) |
| C(49)-C(51) | 1.527(11) |
| C(49)-C(52) | 1.562(11) |
| C(53)-C(58) | 1.395(8) |
| C(53)-C(54) | 1.406(8) |
| C(54)-C(55) | 1.397(9) |
| C(55)-C(56) | 1.367(10) |
| C(56)-C(57) | 1.389(9) |
| C(57)-C(58) | 1.393(9) |
| N(98)-C(59) | 1.367(10) |
| C(59)-C(62B) | 1.52(5) |
| C(59)-C(62A) | 1.54(4) |

| | |
|---|---|
| C(59)-C(61) | 1.566(13) |
| C(59)-C(60B) | 1.59(3) |
| C(59)-C(60A) | 1.61(4) |
| C(60A)-C(60B) | 0.92(4) |
| Co(3)-N(99B) | 1.87(2) |
| Co(3)-N(99A) | 1.891(18) |
| Co(3)-C(70) | 2.080(6) |
| Co(3)-C(77) | 2.095(7) |
| Co(3)-C(63) | 2.119(7) |
| B(3)-N(15) | 1.571(10) |
| B(3)-N(17) | 1.570(9) |
| B(3)-C(84) | 1.592(10) |
| B(3)-N(19) | 1.600(9) |
| N(15)-C(64) | 1.379(8) |
| N(15)-C(63) | 1.385(9) |
| N(16)-C(65) | 1.387(9) |
| N(16)-C(63) | 1.387(9) |
| N(16)-C(66) | 1.470(9) |
| C(64)-C(65) | 1.354(10) |
| C(66)-C(69) | 1.414(13) |
| C(66)-C(68) | 1.491(12) |
| C(66)-C(67) | 1.520(12) |
| N(17)-C(71) | 1.356(8) |
| N(17)-C(70) | 1.361(8) |
| N(18)-C(72) | 1.346(8) |
| N(18)-C(70) | 1.373(8) |
| N(18)-C(73) | 1.494(8) |
| C(71)-C(72) | 1.349(10) |
| C(73)-C(76) | 1.499(10) |
| C(73)-C(75) | 1.533(11) |
| C(73)-C(74) | 1.556(11) |
| N(19)-C(77) | 1.351(8) |
| N(19)-C(78) | 1.367(9) |
| N(20)-C(77) | 1.355(9) |
| N(20)-C(79) | 1.386(9) |
| N(20)-C(80) | 1.506(8) |
| C(78)-C(79) | 1.323(10) |
| C(80)-C(82) | 1.497(10) |
| C(80)-C(81) | 1.515(11) |
| C(80)-C(83) | 1.551(12) |
| C(84)-C(89) | 1.380(10) |
| C(84)-C(85) | 1.385(10) |
| C(85)-C(86) | 1.427(12) |
| C(86)-C(87) | 1.347(15) |
| C(87)-C(88) | 1.410(15) |
| C(88)-C(89) | 1.439(11) |

| | |
|---|---|
| C(90)-N(99A)#1 | 1.434(19) |
| C(90)-N(99B)#1 | 1.47(2) |
| C(90)-C(92) | 1.477(14) |
| C(90)-C(91B)#1 | 1.526(19) |
| C(90)-C(93B) | 1.557(18) |
| C(90)-C(91A)#1 | 1.57(3) |
| C(90)-C(93A) | 1.69(3) |
| N(99A)-N(99B) | 0.744(16) |
| N(99A)-C(90)#2 | 1.434(19) |
| N(99B)-C(90)#2 | 1.47(2) |
| C(91A)-C(91B) | 1.01(3) |
| C(91A)-C(90)#2 | 1.57(3) |
| C(91B)-C(90)#2 | 1.526(19) |
| C(91B)-C(93A)#2 | 1.90(5) |
| C(93A)-C(93B) | 1.02(5) |
| C(93A)-C(91B)#1 | 1.90(5) |

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|---|---|
| N(97)-Co(1)-C(8) | 130.0(3) |
| N(97)-Co(1)-C(15) | 127.1(3) |
| C(8)-Co(1)-C(15) | 93.4(2) |
| N(97)-Co(1)-C(1) | 113.4(3) |
| C(8)-Co(1)-C(1) | 91.6(2) |
| C(15)-Co(1)-C(1) | 89.9(2) |
| N(3)-B(1)-N(5) | 109.9(5) |
| N(3)-B(1)-N(1) | 108.3(5) |
| N(5)-B(1)-N(1) | 102.2(5) |
| N(3)-B(1)-C(22) | 106.4(5) |
| N(5)-B(1)-C(22) | 113.0(5) |
| N(1)-B(1)-C(22) | 116.9(6) |
| C(1)-N(1)-C(2) | 110.2(5) |
| C(1)-N(1)-B(1) | 120.6(5) |
| C(2)-N(1)-B(1) | 128.7(5) |
| C(1)-N(2)-C(3) | 110.2(5) |
| C(1)-N(2)-C(4) | 124.2(6) |
| C(3)-N(2)-C(4) | 125.6(5) |
| N(2)-C(1)-N(1) | 103.7(5) |
| N(2)-C(1)-Co(1) | 142.1(5) |
| N(1)-C(1)-Co(1) | 113.8(4) |
| C(3)-C(2)-N(1) | 107.9(6) |
| C(2)-C(3)-N(2) | 107.9(6) |
| N(2)-C(4)-C(7) | 108.9(6) |
| N(2)-C(4)-C(6) | 107.4(5) |
| C(7)-C(4)-C(6) | 113.1(6) |
| N(2)-C(4)-C(5) | 109.3(6) |
| C(7)-C(4)-C(5) | 109.2(7) |
| C(6)-C(4)-C(5) | 109.0(6) |

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| C(8)-N(3)-C(9) | 109.8(5) |
| C(8)-N(3)-B(1) | 125.6(5) |
| C(9)-N(3)-B(1) | 124.5(5) |
| C(8)-N(4)-C(10) | 108.9(6) |
| C(8)-N(4)-C(11) | 125.7(6) |
| C(10)-N(4)-C(11) | 125.3(5) |
| N(3)-C(8)-N(4) | 105.9(6) |
| N(3)-C(8)-Co(1) | 111.5(4) |
| N(4)-C(8)-Co(1) | 142.6(5) |
| C(10)-C(9)-N(3) | 107.7(6) |
| C(9)-C(10)-N(4) | 107.6(6) |
| C(12)-C(11)-N(4) | 107.2(6) |
| C(12)-C(11)-C(14) | 110.7(7) |
| N(4)-C(11)-C(14) | 110.7(6) |
| C(12)-C(11)-C(13) | 112.3(8) |
| N(4)-C(11)-C(13) | 107.4(6) |
| C(14)-C(11)-C(13) | 108.5(7) |
| C(15)-N(5)-C(16) | 110.1(5) |
| C(15)-N(5)-B(1) | 123.0(5) |
| C(16)-N(5)-B(1) | 126.5(5) |
| C(15)-N(6)-C(17) | 110.3(5) |
| C(15)-N(6)-C(18) | 124.4(5) |
| C(17)-N(6)-C(18) | 125.1(5) |
| N(5)-C(15)-N(6) | 104.6(5) |
| N(5)-C(15)-Co(1) | 112.9(4) |
| N(6)-C(15)-Co(1) | 140.7(5) |
| C(17)-C(16)-N(5) | 108.3(6) |
| C(16)-C(17)-N(6) | 106.5(5) |
| N(6)-C(18)-C(19) | 109.7(5) |
| N(6)-C(18)-C(21) | 110.0(6) |
| C(19)-C(18)-C(21) | 108.4(6) |
| N(6)-C(18)-C(20) | 107.6(5) |
| C(19)-C(18)-C(20) | 110.4(6) |
| C(21)-C(18)-C(20) | 110.8(6) |
| C(27)-C(22)-C(23) | 115.5(7) |
| C(27)-C(22)-B(1) | 119.6(6) |
| C(23)-C(22)-B(1) | 123.2(6) |
| C(24)-C(23)-C(22) | 121.8(8) |
| C(25)-C(24)-C(23) | 121.6(8) |
| C(24)-C(25)-C(26) | 118.0(8) |
| C(25)-C(26)-C(27) | 121.9(9) |
| C(26)-C(27)-C(22) | 121.1(8) |
| C(28)-N(97)-Co(1) | 153.5(6) |
| N(97)-C(28)-C(31) | 110.5(7) |
| N(97)-C(28)-C(30) | 108.5(7) |
| C(31)-C(28)-C(30) | 106.1(8) |

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| N(97)-C(28)-C(29) | 112.3(7) |
| C(31)-C(28)-C(29) | 110.3(7) |
| C(30)-C(28)-C(29) | 108.8(7) |
| N(98)-Co(2)-C(39) | 128.9(4) |
| N(98)-Co(2)-C(46) | 123.6(3) |
| C(39)-Co(2)-C(46) | 90.5(2) |
| N(98)-Co(2)-C(32) | 120.1(4) |
| C(39)-Co(2)-C(32) | 88.7(2) |
| C(46)-Co(2)-C(32) | 95.3(2) |
| N(8)-B(2)-N(12) | 106.6(5) |
| N(8)-B(2)-N(10) | 107.6(5) |
| N(12)-B(2)-N(10) | 106.7(5) |
| N(8)-B(2)-C(53) | 115.5(5) |
| N(12)-B(2)-C(53) | 113.4(5) |
| N(10)-B(2)-C(53) | 106.4(5) |
| C(32)-N(8)-C(33) | 109.7(5) |
| C(32)-N(8)-B(2) | 121.9(5) |
| C(33)-N(8)-B(2) | 128.3(5) |
| C(32)-N(9)-C(34) | 110.5(5) |
| C(32)-N(9)-C(35) | 125.8(5) |
| C(34)-N(9)-C(35) | 123.6(5) |
| N(9)-C(32)-N(8) | 105.0(5) |
| N(9)-C(32)-Co(2) | 142.5(5) |
| N(8)-C(32)-Co(2) | 112.2(4) |
| C(34)-C(33)-N(8) | 106.4(5) |
| C(33)-C(34)-N(9) | 108.1(6) |
| N(9)-C(35)-C(38) | 108.3(6) |
| N(9)-C(35)-C(37) | 110.0(6) |
| C(38)-C(35)-C(37) | 111.1(7) |
| N(9)-C(35)-C(36) | 109.2(6) |
| C(38)-C(35)-C(36) | 108.8(7) |
| C(37)-C(35)-C(36) | 109.4(7) |
| C(39)-N(10)-C(40) | 108.7(5) |
| C(39)-N(10)-B(2) | 125.9(5) |
| C(40)-N(10)-B(2) | 125.4(5) |
| C(39)-N(11)-C(41) | 110.0(5) |
| C(39)-N(11)-C(42) | 124.9(6) |
| C(41)-N(11)-C(42) | 124.9(6) |
| N(11)-C(39)-N(10) | 106.3(5) |
| N(11)-C(39)-Co(2) | 142.7(5) |
| N(10)-C(39)-Co(2) | 111.0(4) |
| C(41)-C(40)-N(10) | 108.2(5) |
| C(40)-C(41)-N(11) | 106.6(6) |
| C(43)-C(42)-N(11) | 109.1(7) |
| C(43)-C(42)-C(44) | 106.8(10) |
| N(11)-C(42)-C(44) | 107.3(7) |

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| C(43)-C(42)-C(45) | 112.5(12) |
| N(11)-C(42)-C(45) | 110.8(7) |
| C(44)-C(42)-C(45) | 110.1(11) |
| C(46)-N(12)-C(47) | 109.7(5) |
| C(46)-N(12)-B(2) | 122.5(5) |
| C(47)-N(12)-B(2) | 127.7(5) |
| C(48)-N(13)-C(46) | 110.7(5) |
| C(48)-N(13)-C(49) | 125.7(5) |
| C(46)-N(13)-C(49) | 123.5(5) |
| N(12)-C(46)-N(13) | 105.0(5) |
| N(12)-C(46)-Co(2) | 112.8(4) |
| N(13)-C(46)-Co(2) | 142.0(4) |
| C(48)-C(47)-N(12) | 107.4(5) |
| C(47)-C(48)-N(13) | 107.1(5) |
| C(50)-C(49)-N(13) | 108.9(5) |
| C(50)-C(49)-C(51) | 110.7(6) |
| N(13)-C(49)-C(51) | 107.5(6) |
| C(50)-C(49)-C(52) | 110.9(6) |
| N(13)-C(49)-C(52) | 106.9(5) |
| C(51)-C(49)-C(52) | 111.7(6) |
| C(58)-C(53)-C(54) | 115.3(5) |
| C(58)-C(53)-B(2) | 119.7(5) |
| C(54)-C(53)-B(2) | 123.9(5) |
| C(55)-C(54)-C(53) | 122.6(6) |
| C(56)-C(55)-C(54) | 120.0(6) |
| C(55)-C(56)-C(57) | 119.4(6) |
| C(56)-C(57)-C(58) | 120.0(6) |
| C(57)-C(58)-C(53) | 122.5(6) |
| C(59)-N(98)-Co(2) | 172.4(9) |
| N(98)-C(59)-C(62B) | 99.6(19) |
| N(98)-C(59)-C(62A) | 115(2) |
| C(62B)-C(59)-C(62A) | 17(3) |
| N(98)-C(59)-C(61) | 114.5(8) |
| C(62B)-C(59)-C(61) | 117.9(19) |
| C(62A)-C(59)-C(61) | 104.4(17) |
| N(98)-C(59)-C(60B) | 97.0(14) |
| C(62B)-C(59)-C(60B) | 119(3) |
| C(62A)-C(59)-C(60B) | 119(3) |
| C(61)-C(59)-C(60B) | 107.0(13) |
| N(98)-C(59)-C(60A) | 119.4(14) |
| C(62B)-C(59)-C(60A) | 89(3) |
| C(62A)-C(59)-C(60A) | 86(3) |
| C(61)-C(59)-C(60A) | 113(2) |
| C(60B)-C(59)-C(60A) | 33.4(14) |
| C(60B)-C(60A)-C(59) | 72(3) |
| C(60A)-C(60B)-C(59) | 75(4) |

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| N(99B)-Co(3)-N(99A) | 22.8(5) |
| N(99B)-Co(3)-C(70) | 130.8(6) |
| N(99A)-Co(3)-C(70) | 115.1(6) |
| N(99B)-Co(3)-C(77) | 129.0(7) |
| N(99A)-Co(3)-C(77) | 123.7(7) |
| C(70)-Co(3)-C(77) | 91.4(3) |
| N(99B)-Co(3)-C(63) | 111.2(7) |
| N(99A)-Co(3)-C(63) | 133.0(5) |
| C(70)-Co(3)-C(63) | 91.4(2) |
| C(77)-Co(3)-C(63) | 91.5(3) |
| N(15)-B(3)-N(17) | 109.2(6) |
| N(15)-B(3)-C(84) | 114.3(5) |
| N(17)-B(3)-C(84) | 107.5(5) |
| N(15)-B(3)-N(19) | 103.6(5) |
| N(17)-B(3)-N(19) | 107.8(5) |
| C(84)-B(3)-N(19) | 114.2(6) |
| C(64)-N(15)-C(63) | 109.9(6) |
| C(64)-N(15)-B(3) | 128.1(6) |
| C(63)-N(15)-B(3) | 121.9(5) |
| C(65)-N(16)-C(63) | 110.1(6) |
| C(65)-N(16)-C(66) | 123.6(6) |
| C(63)-N(16)-C(66) | 126.2(6) |
| N(15)-C(63)-N(16) | 104.5(6) |
| N(15)-C(63)-Co(3) | 112.5(4) |
| N(16)-C(63)-Co(3) | 141.5(5) |
| C(65)-C(64)-N(15) | 108.2(6) |
| C(64)-C(65)-N(16) | 107.0(6) |
| C(69)-C(66)-N(16) | 108.8(8) |
| C(69)-C(66)-C(68) | 113.9(8) |
| N(16)-C(66)-C(68) | 108.3(6) |
| C(69)-C(66)-C(67) | 108.5(8) |
| N(16)-C(66)-C(67) | 109.9(6) |
| C(68)-C(66)-C(67) | 107.4(8) |
| C(71)-N(17)-C(70) | 109.8(5) |
| C(71)-N(17)-B(3) | 124.8(5) |
| C(70)-N(17)-B(3) | 125.4(5) |
| C(72)-N(18)-C(70) | 109.1(5) |
| C(72)-N(18)-C(73) | 125.6(6) |
| C(70)-N(18)-C(73) | 125.2(5) |
| N(17)-C(70)-N(18) | 105.5(5) |
| N(17)-C(70)-Co(3) | 111.6(4) |
| N(18)-C(70)-Co(3) | 142.9(5) |
| C(72)-C(71)-N(17) | 107.1(5) |
| N(18)-C(72)-C(71) | 108.5(6) |
| N(18)-C(73)-C(76) | 111.2(6) |
| N(18)-C(73)-C(75) | 107.2(6) |

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| C(76)-C(73)-C(75) | 110.6(7) |
| N(18)-C(73)-C(74) | 109.2(6) |
| C(76)-C(73)-C(74) | 107.9(7) |
| C(75)-C(73)-C(74) | 110.8(6) |
| C(77)-N(19)-C(78) | 110.2(6) |
| C(77)-N(19)-B(3) | 121.7(6) |
| C(78)-N(19)-B(3) | 127.8(6) |
| C(77)-N(20)-C(79) | 110.6(5) |
| C(77)-N(20)-C(80) | 124.1(6) |
| C(79)-N(20)-C(80) | 125.3(6) |
| N(19)-C(77)-N(20) | 104.6(6) |
| N(19)-C(77)-Co(3) | 114.4(4) |
| N(20)-C(77)-Co(3) | 140.8(5) |
| C(79)-C(78)-N(19) | 108.5(6) |
| C(78)-C(79)-N(20) | 106.1(7) |
| C(82)-C(80)-N(20) | 109.1(6) |
| C(82)-C(80)-C(81) | 111.2(7) |
| N(20)-C(80)-C(81) | 108.8(6) |
| C(82)-C(80)-C(83) | 108.6(7) |
| N(20)-C(80)-C(83) | 107.7(6) |
| C(81)-C(80)-C(83) | 111.4(7) |
| C(89)-C(84)-C(85) | 116.7(7) |
| C(89)-C(84)-B(3) | 118.8(6) |
| C(85)-C(84)-B(3) | 123.0(7) |
| C(84)-C(85)-C(86) | 122.7(9) |
| C(87)-C(86)-C(85) | 120.3(9) |
| C(86)-C(87)-C(88) | 119.4(9) |
| C(87)-C(88)-C(89) | 119.2(9) |
| C(84)-C(89)-C(88) | 121.7(8) |
| N(99A)#1-C(90)-N(99B)#1 | 29.7(6) |
| N(99A)#1-C(90)-C(92) | 118.3(11) |
| N(99B)#1-C(90)-C(92) | 107.9(12) |
| N(99A)#1-C(90)-C(91B)#1 | 130.8(14) |
| N(99B)#1-C(90)-C(91B)#1 | 116.4(13) |
| C(92)-C(90)-C(91B)#1 | 104.4(11) |
| N(99A)#1-C(90)-C(93B) | 87.5(11) |
| N(99B)#1-C(90)-C(93B) | 117.1(12) |
| C(92)-C(90)-C(93B) | 100.0(11) |
| C(91B)#1-C(90)-C(93B) | 108.9(11) |
| N(99A)#1-C(90)-C(91A)#1 | 107.8(12) |
| N(99B)#1-C(90)-C(91A)#1 | 83.2(12) |
| C(92)-C(90)-C(91A)#1 | 99.4(11) |
| C(91B)#1-C(90)-C(91A)#1 | 38.1(9) |
| C(93B)-C(90)-C(91A)#1 | 145.5(13) |
| N(99A)#1-C(90)-C(93A) | 109.6(13) |
| N(99B)#1-C(90)-C(93A) | 135.3(16) |

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|---|---|
| C(92)-C(90)-C(93A) | 112(2) |
| C(91B)#1-C(90)-C(93A) | 72.5(18) |
| C(93B)-C(90)-C(93A) | 36.5(19) |
| C(91A)#1-C(90)-C(93A) | 109(2) |
| N(99B)-N(99A)-C(90)#2 | 78(3) |
| N(99B)-N(99A)-Co(3) | 77(3) |
| C(90)#2-N(99A)-Co(3) | 154.3(12) |
| N(99A)-N(99B)-C(90)#2 | 73(3) |
| N(99A)-N(99B)-Co(3) | 80(3) |
| C(90)#2-N(99B)-Co(3) | 152.5(14) |
| C(91B)-C(91A)-C(90)#2 | 69(2) |
| C(91A)-C(91B)-C(90)#2 | 73.1(17) |
| C(91A)-C(91B)-C(93A)#2 | 129(2) |
| C(90)#2-C(91B)-C(93A)#2 | 57.6(11) |
| C(93B)-C(93A)-C(90) | 64.9(15) |
| C(93B)-C(93A)-C(91B)#1 | 115(2) |
| C(90)-C(93A)-C(91B)#1 | 49.9(13) |
| C(93A)-C(93B)-C(90) | 79(3) |

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Symmetry transformations used to generate equivalent atoms:
#1 -x-1,y-1/2,-z+1  #2 -x-1,y+1/2,-z+1

**Table 4.** Anisotropic displacement parameters ($Å^2$ x $10^3$) for **LCoNH$^t$Bu**.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [ $h^2 a^{*2}$ U11 + ... + 2 h k a* b* U12 ]

| Atom | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Co(1) | 40(1) | 33(1) | 31(1) | 1(1) | 13(1) | 5(1) |
| B(1) | 43(5) | 31(4) | 34(4) | 1(3) | 14(4) | 1(4) |
| N(1) | 43(3) | 32(3) | 29(3) | 3(2) | 14(3) | 7(3) |
| N(2) | 44(3) | 48(4) | 23(3) | 10(3) | 7(3) | 12(3) |
| C(1) | 31(3) | 42(4) | 29(4) | 7(3) | 10(3) | 7(3) |
| C(2) | 48(4) | 23(4) | 50(5) | -4(3) | 16(4) | 8(3) |
| C(3) | 57(5) | 30(4) | 35(4) | 9(3) | 8(4) | 19(3) |
| C(4) | 47(4) | 53(5) | 31(4) | 8(3) | 5(3) | 7(4) |
| C(5) | 112(8) | 79(7) | 42(5) | 9(5) | -10(5) | 32(6) |
| C(6) | 51(4) | 66(6) | 35(4) | -3(4) | 16(3) | 0(4) |
| C(7) | 49(5) | 85(7) | 55(5) | -19(5) | 15(4) | 5(5) |
| N(3) | 35(3) | 31(3) | 32(3) | 5(3) | 8(2) | 3(3) |
| N(4) | 34(3) | 48(4) | 39(3) | 4(3) | 16(3) | 6(3) |
| C(8) | 44(4) | 35(4) | 31(4) | 11(3) | 15(3) | 10(3) |
| C(9) | 40(4) | 41(4) | 41(4) | 2(3) | 11(3) | 1(4) |
| C(10) | 37(4) | 56(5) | 47(4) | 1(4) | 9(3) | -3(4) |
| C(11) | 42(4) | 45(5) | 55(5) | -4(4) | 20(4) | 12(3) |
| C(12) | 75(6) | 59(6) | 123(9) | -2(6) | 43(6) | 19(5) |
| C(13) | 121(8) | 119(9) | 64(6) | 3(6) | 47(6) | 58(8) |
| C(14) | 48(5) | 92(8) | 131(9) | -25(6) | 35(5) | 21(5) |
| N(5) | 35(3) | 34(3) | 30(3) | 2(2) | 12(2) | 5(3) |
| N(6) | 33(3) | 35(3) | 26(3) | 4(2) | 8(2) | 1(2) |
| C(15) | 31(3) | 29(4) | 34(3) | 4(3) | 10(3) | 2(3) |
| C(16) | 34(3) | 41(4) | 24(3) | -2(3) | 7(3) | 7(3) |
| C(17) | 33(3) | 39(5) | 29(4) | 7(3) | 11(3) | 5(3) |
| C(18) | 40(4) | 43(5) | 41(4) | 10(3) | 12(3) | -2(3) |
| C(19) | 55(4) | 42(4) | 41(4) | -1(4) | 0(3) | -3(4) |
| C(20) | 58(5) | 39(4) | 54(5) | 14(4) | 13(4) | 11(4) |
| C(21) | 82(6) | 50(5) | 63(5) | 9(4) | 38(4) | -10(5) |
| C(22) | 38(4) | 33(4) | 45(4) | 0(3) | 19(3) | 2(3) |
| C(23) | 45(4) | 45(5) | 68(5) | 3(4) | 19(4) | 5(4) |
| C(24) | 40(4) | 38(5) | 106(8) | -18(5) | 11(5) | -10(4) |
| C(25) | 48(5) | 61(6) | 82(7) | -37(5) | 20(5) | 2(5) |
| C(26) | 45(5) | 93(8) | 62(5) | -32(5) | 30(4) | -11(5) |
| C(27) | 46(4) | 53(4) | 36(4) | -15(4) | 21(3) | -1(4) |
| N(97) | 95(5) | 52(4) | 59(4) | -12(4) | 26(4) | 4(4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(28) | 54(5) | 36(4) | 49(4) | -6(3) | 12(4) | 7(4) |
| C(29) | 96(7) | 63(6) | 66(6) | -6(5) | 34(5) | 14(5) |
| C(30) | 95(8) | 101(8) | 79(7) | -20(6) | 25(6) | 0(6) |
| C(31) | 99(7) | 51(6) | 101(8) | 7(5) | 39(6) | 10(5) |
| Co(2) | 28(1) | 33(1) | 33(1) | 2(1) | 5(1) | 3(1) |
| B(2) | 25(4) | 35(5) | 29(4) | -1(3) | 8(3) | 0(3) |
| N(8) | 25(3) | 30(3) | 29(3) | 1(2) | 8(2) | -1(2) |
| N(9) | 39(3) | 28(3) | 30(3) | 6(2) | 7(2) | 2(3) |
| C(32) | 39(4) | 33(4) | 28(4) | -4(3) | 7(3) | 2(3) |
| C(33) | 40(4) | 32(4) | 39(4) | 2(3) | 21(3) | 0(3) |
| C(34) | 51(4) | 28(4) | 40(4) | 4(3) | 20(4) | 0(3) |
| C(35) | 61(5) | 54(5) | 27(4) | 3(3) | -3(4) | -1(4) |
| C(36) | 92(7) | 89(7) | 36(5) | 24(4) | 7(4) | 3(5) |
| C(37) | 51(5) | 68(6) | 55(5) | 13(4) | -2(4) | -9(4) |
| C(38) | 79(6) | 61(6) | 77(6) | 1(5) | -10(5) | 33(5) |
| N(10) | 31(3) | 29(3) | 25(3) | 3(2) | 7(2) | -2(2) |
| N(11) | 33(3) | 25(3) | 48(3) | -4(3) | 11(3) | -6(3) |
| C(39) | 34(4) | 37(4) | 25(3) | 6(3) | 5(3) | -1(3) |
| C(40) | 25(3) | 29(4) | 36(4) | 1(3) | 10(3) | 5(3) |
| C(41) | 41(4) | 25(4) | 52(4) | 0(3) | 18(3) | 5(3) |
| C(42) | 34(4) | 44(5) | 81(6) | -13(4) | 1(4) | -5(4) |
| C(43) | 76(7) | 173(14) | 168(12) | -37(11) | 75(8) | -61(8) |
| C(44) | 81(7) | 106(9) | 147(12) | 9(8) | -56(8) | -41(7) |
| C(45) | 71(7) | 47(7) | 370(20) | -59(10) | -63(11) | -10(6) |
| N(12) | 33(3) | 29(3) | 28(3) | -1(2) | 5(2) | 2(2) |
| N(13) | 31(3) | 37(3) | 33(3) | 0(3) | 12(2) | 8(3) |
| C(46) | 31(4) | 29(4) | 36(4) | 4(3) | 9(3) | 2(3) |
| C(47) | 34(4) | 30(4) | 33(4) | 5(3) | 3(3) | 1(3) |
| C(48) | 50(4) | 34(4) | 29(4) | -1(3) | 14(3) | 3(3) |
| C(49) | 43(4) | 49(5) | 40(4) | -7(4) | 22(3) | 1(4) |
| C(50) | 37(4) | 55(5) | 60(5) | 4(4) | 24(4) | 14(4) |
| C(51) | 52(4) | 60(5) | 76(5) | 6(5) | 35(4) | -7(4) |
| C(52) | 68(5) | 92(7) | 64(6) | -10(5) | 40(5) | 12(5) |
| C(53) | 29(3) | 23(4) | 29(4) | 0(3) | 6(3) | -2(3) |
| C(54) | 35(4) | 31(4) | 32(4) | 8(3) | 7(3) | 8(3) |
| C(55) | 32(4) | 35(4) | 52(5) | -2(3) | 19(3) | 4(3) |
| C(56) | 29(4) | 30(4) | 57(5) | -5(3) | 3(3) | 1(3) |
| C(57) | 37(4) | 27(4) | 39(4) | 1(3) | 6(3) | 3(3) |
| C(58) | 34(4) | 31(4) | 38(4) | 6(3) | 12(3) | 3(3) |
| N(98) | 39(4) | 257(14) | 71(5) | -47(7) | -8(4) | 52(6) |
| C(59) | 34(4) | 86(7) | 69(6) | 18(5) | 15(4) | 8(4) |
| C(60A) | 67(16) | 80(20) | 400(70) | 10(30) | 100(30) | 4(14) |
| C(60B) | 200(40) | 66(17) | 91(17) | 27(13) | 0(20) | 40(20) |
| C(61) | 64(6) | 149(11) | 94(8) | -19(8) | -16(6) | -5(7) |
| C(62A) | 90(30) | 210(40) | 44(13) | -15(18) | 23(19) | -70(30) |
| C(62B) | 49(19) | 380(70) | 130(40) | 70(40) | -2(18) | -120(30) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Co(3) | 31(1) | 41(1) | 30(1) | 4(1) | 3(1) | 2(1) |
| B(3) | 26(4) | 51(5) | 34(4) | 0(4) | 5(3) | 3(4) |
| N(15) | 30(3) | 39(3) | 36(3) | 0(3) | 12(3) | 1(3) |
| N(16) | 45(3) | 57(4) | 38(3) | 7(3) | 19(3) | 0(3) |
| C(63) | 52(4) | 43(4) | 28(4) | -6(3) | 13(3) | -2(4) |
| C(64) | 35(4) | 55(5) | 54(5) | -9(4) | 16(4) | 1(3) |
| C(65) | 47(5) | 63(5) | 47(5) | 6(4) | 25(4) | -3(4) |
| C(66) | 48(4) | 71(6) | 34(4) | 17(4) | 12(4) | 2(4) |
| C(67) | 78(7) | 120(9) | 86(7) | 51(6) | 32(5) | 8(6) |
| C(68) | 93(7) | 94(8) | 86(7) | 55(6) | 38(6) | 29(6) |
| C(69) | 83(7) | 128(10) | 70(7) | 28(7) | -2(6) | -2(7) |
| N(17) | 24(3) | 39(3) | 26(3) | -1(2) | 2(2) | 5(2) |
| N(18) | 33(3) | 42(3) | 28(3) | 2(3) | 5(3) | 6(3) |
| C(70) | 39(4) | 36(4) | 32(4) | 1(3) | 14(3) | -1(3) |
| C(71) | 29(3) | 58(5) | 29(4) | -8(3) | -1(3) | 11(4) |
| C(72) | 56(5) | 49(4) | 27(4) | -5(3) | 3(4) | 4(4) |
| C(73) | 56(5) | 44(5) | 40(4) | 5(3) | 13(4) | 25(4) |
| C(74) | 42(4) | 65(6) | 92(6) | 3(5) | 31(4) | 2(4) |
| C(75) | 73(5) | 45(5) | 77(6) | 5(4) | 30(5) | 20(4) |
| C(76) | 65(5) | 72(6) | 48(5) | -2(4) | 17(4) | 21(5) |
| N(19) | 37(3) | 31(3) | 31(3) | 1(2) | 10(3) | 4(3) |
| N(20) | 38(3) | 53(4) | 38(3) | -6(3) | 8(3) | 0(3) |
| C(77) | 25(3) | 40(4) | 30(4) | -5(3) | 2(3) | -6(3) |
| C(78) | 39(4) | 53(5) | 43(4) | -2(4) | 4(4) | 8(4) |
| C(79) | 46(4) | 43(5) | 46(4) | -7(4) | 4(4) | 3(4) |
| C(80) | 28(4) | 65(5) | 49(4) | -14(4) | 6(3) | -6(4) |
| C(81) | 53(5) | 96(7) | 50(5) | -15(5) | 3(4) | -7(5) |
| C(82) | 41(4) | 87(7) | 70(6) | -26(5) | 13(4) | -8(4) |
| C(83) | 50(5) | 79(7) | 104(8) | -46(6) | -4(5) | -30(5) |
| C(84) | 25(4) | 51(5) | 37(4) | -8(3) | 3(3) | 5(3) |
| C(85) | 45(5) | 58(5) | 47(4) | -16(4) | 9(4) | 9(4) |
| C(86) | 40(5) | 92(8) | 72(6) | -45(6) | -5(5) | 14(5) |
| C(87) | 67(7) | 89(8) | 78(7) | -25(7) | -27(6) | 37(6) |
| C(88) | 106(8) | 60(6) | 53(5) | 11(5) | -7(5) | 36(6) |
| C(89) | 64(5) | 48(5) | 49(5) | 0(4) | 2(4) | 8(4) |
| C(90) | 35(4) | 57(5) | 53(5) | -22(4) | -6(4) | -5(4) |
| N(99A) | 40(10) | 81(11) | 51(12) | 38(10) | 15(8) | 6(8) |
| N(99B) | 67(13) | 88(15) | 49(12) | 11(10) | 19(9) | 23(11) |
| C(91A) | 108(18) | 100(17) | 43(12) | 22(11) | -23(14) | 16(16) |
| C(91B) | 55(12) | 103(17) | 51(12) | -23(10) | -24(11) | -16(13) |
| C(92) | 138(10) | 93(9) | 75(7) | -4(6) | 15(7) | -41(7) |
| C(93A) | 120(30) | 390(70) | 450(80) | -320(60) | -160(40) | 200(40) |
| C(93B) | 40(10) | 109(16) | 75(13) | -1(12) | 22(10) | 34(11) |

**Table 5.** Hydrogen coordinates ( x $10^4$) and equivalent isotropic displacement parameters (Å$^2$ x $10^3$) for **LCoNH$^t$Bu**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2) | -5260 | 8524 | 7547 | 47 |
| H(3) | -6049 | 8289 | 6756 | 50 |
| H(5A) | -5981 | 7698 | 5987 | 125 |
| H(5B) | -6843 | 7388 | 6128 | 125 |
| H(5C) | -6626 | 6746 | 5711 | 125 |
| H(6A) | -4724 | 6341 | 6149 | 75 |
| H(6B) | -5310 | 5343 | 5864 | 75 |
| H(6C) | -4772 | 5104 | 6372 | 75 |
| H(7A) | -6983 | 5444 | 6476 | 94 |
| H(7B) | -6205 | 4540 | 6579 | 94 |
| H(7C) | -6734 | 4784 | 6070 | 94 |
| H(9) | -2375 | 7041 | 8366 | 49 |
| H(10) | -1307 | 5877 | 8110 | 56 |
| H(12A) | -2950 | 2817 | 7459 | 124 |
| H(12B) | -2193 | 2676 | 7911 | 124 |
| H(12C) | -2066 | 2208 | 7443 | 124 |
| H(13A) | -1960 | 5051 | 6947 | 146 |
| H(13B) | -2830 | 4321 | 6868 | 146 |
| H(13C) | -1967 | 3711 | 6820 | 146 |
| H(14A) | -753 | 4739 | 7623 | 132 |
| H(14B) | -726 | 3381 | 7532 | 132 |
| H(14C) | -818 | 3840 | 8008 | 132 |
| H(16) | -5363 | 6302 | 8629 | 40 |
| H(17) | -6118 | 4454 | 8656 | 40 |
| H(19A) | -5849 | 2550 | 7412 | 73 |
| H(19B) | -6744 | 2830 | 7523 | 73 |
| H(19C) | -6381 | 1537 | 7569 | 73 |
| H(20A) | -4522 | 2093 | 8043 | 76 |
| H(20B) | -5024 | 1052 | 8204 | 76 |
| H(20C) | -4588 | 2041 | 8553 | 76 |
| H(21A) | -6045 | 2397 | 8722 | 92 |
| H(21B) | -6497 | 1442 | 8362 | 92 |
| H(21C) | -6864 | 2732 | 8321 | 92 |
| H(23) | -3875 | 8900 | 7960 | 62 |
| H(24) | -3204 | 10213 | 8504 | 75 |
| H(25) | -2859 | 9744 | 9261 | 76 |
| H(26) | -3192 | 7900 | 9471 | 77 |
| H(27) | -3848 | 6540 | 8939 | 52 |

| | | | | |
|---|---|---|---|---|
| H(97) | -5093 | 3577 | 6667 | 81 |
| H(29A) | -4439 | 2509 | 6120 | 109 |
| H(29B) | -4250 | 1172 | 6236 | 109 |
| H(29C) | -3617 | 2138 | 6512 | 109 |
| H(30A) | -5929 | 2202 | 6225 | 137 |
| H(30B) | -6035 | 1676 | 6688 | 137 |
| H(30C) | -5690 | 880 | 6348 | 137 |
| H(31A) | -3846 | 1337 | 7246 | 122 |
| H(31B) | -4445 | 367 | 6950 | 122 |
| H(31C) | -4808 | 1156 | 7286 | 122 |
| H(33) | -5002 | 4361 | 10846 | 42 |
| H(34) | -4101 | 3566 | 11577 | 46 |
| H(36A) | -3056 | 3006 | 12127 | 111 |
| H(36B) | -2893 | 4336 | 12262 | 111 |
| H(36C) | -2149 | 3407 | 12445 | 111 |
| H(37A) | -1378 | 4926 | 11601 | 91 |
| H(37B) | -1117 | 4564 | 12121 | 91 |
| H(37C) | -1851 | 5510 | 11943 | 91 |
| H(38A) | -2349 | 2090 | 11584 | 117 |
| H(38B) | -1422 | 2448 | 11893 | 117 |
| H(38C) | -1699 | 2803 | 11372 | 117 |
| H(40) | -4459 | 8186 | 10225 | 36 |
| H(41) | -3271 | 9606 | 10478 | 46 |
| H(43A) | -995 | 7575 | 10452 | 196 |
| H(43B) | -433 | 8705 | 10622 | 196 |
| H(43C) | -1276 | 8788 | 10210 | 196 |
| H(44A) | -1458 | 8166 | 11481 | 191 |
| H(44B) | -540 | 8315 | 11378 | 191 |
| H(44C) | -1113 | 7199 | 11200 | 191 |
| H(45A) | -1834 | 10356 | 10630 | 275 |
| H(45B) | -1039 | 10245 | 11066 | 275 |
| H(45C) | -2001 | 10070 | 11109 | 275 |
| H(47) | -4726 | 4532 | 9398 | 40 |
| H(48) | -3638 | 3824 | 9002 | 44 |
| H(50A) | -1621 | 2530 | 9803 | 73 |
| H(50B) | -1228 | 3587 | 10127 | 73 |
| H(50C) | -748 | 3133 | 9765 | 73 |
| H(51A) | -1694 | 5822 | 9269 | 88 |
| H(51B) | -792 | 5166 | 9434 | 88 |
| H(51C) | -1270 | 5631 | 9795 | 88 |
| H(52A) | -2378 | 4138 | 8762 | 105 |
| H(52B) | -2402 | 2878 | 8971 | 105 |
| H(52C) | -1519 | 3379 | 8902 | 105 |
| H(54) | -5460 | 5984 | 10680 | 39 |
| H(55) | -6865 | 6713 | 10399 | 45 |
| H(56) | -7352 | 7271 | 9641 | 48 |

| | | | | |
|---|---|---|---|---|
| H(57) | -6403 | 7165 | 9168 | 42 |
| H(58) | -4991 | 6473 | 9455 | 41 |
| H(98) | -914 | 4606 | 11107 | 112 |
| H(60A) | 188 | 2759 | 11289 | 118 |
| H(60B) | -555 | 3203 | 10868 | 118 |
| H(60C) | -35 | 4106 | 11232 | 118 |
| H(61A) | 467 | 6166 | 11441 | 164 |
| H(61B) | 1177 | 5169 | 11507 | 164 |
| H(61C) | 352 | 5001 | 11699 | 164 |
| H(62A) | 377 | 6026 | 10571 | 127 |
| H(62B) | -227 | 5041 | 10289 | 127 |
| H(62C) | 771 | 4788 | 10509 | 127 |
| H(64) | 1414 | 6582 | 6015 | 57 |
| H(65) | 1123 | 7950 | 5362 | 60 |
| H(67A) | 548 | 10161 | 5245 | 139 |
| H(67B) | -80 | 10313 | 4751 | 139 |
| H(67C) | 550 | 9223 | 4864 | 139 |
| H(68A) | -632 | 10274 | 5601 | 132 |
| H(68B) | -1475 | 9494 | 5434 | 132 |
| H(68C) | -1279 | 10498 | 5117 | 132 |
| H(69A) | -671 | 7928 | 4624 | 146 |
| H(69B) | -1291 | 9027 | 4505 | 146 |
| H(69C) | -1491 | 8031 | 4824 | 146 |
| H(71) | 348 | 6835 | 7391 | 48 |
| H(72) | -775 | 7950 | 7637 | 55 |
| H(74A) | -3122 | 7411 | 6545 | 96 |
| H(74B) | -3606 | 8179 | 6836 | 96 |
| H(74C) | -2991 | 7145 | 7069 | 96 |
| H(75A) | -2412 | 9243 | 6306 | 94 |
| H(75B) | -1896 | 10119 | 6683 | 94 |
| H(75C) | -2920 | 10018 | 6582 | 94 |
| H(76A) | -2171 | 8516 | 7648 | 92 |
| H(76B) | -2762 | 9571 | 7413 | 92 |
| H(76C) | -1737 | 9656 | 7512 | 92 |
| H(78) | -12 | 3587 | 6285 | 55 |
| H(79) | -1338 | 2694 | 5810 | 56 |
| H(81A) | -2348 | 4528 | 4839 | 102 |
| H(81B) | -2650 | 5699 | 5028 | 102 |
| H(81C) | -3351 | 4788 | 4766 | 102 |
| H(82A) | -3373 | 4401 | 5933 | 100 |
| H(82B) | -3986 | 4711 | 5448 | 100 |
| H(82C) | -3277 | 5618 | 5705 | 100 |
| H(83A) | -2925 | 2571 | 5644 | 123 |
| H(83B) | -2514 | 2574 | 5224 | 123 |
| H(83C) | -3519 | 2822 | 5149 | 123 |
| H(85) | 1703 | 6890 | 6732 | 60 |

| | | | | |
|---|---|---|---|---|
| H(86) | 2885 | 6308 | 7337 | 86 |
| H(87) | 2770 | 4699 | 7770 | 104 |
| H(88) | 1456 | 3616 | 7599 | 94 |
| H(89) | 265 | 4231 | 6991 | 67 |
| H(99A) | -2816 | 7542 | 5886 | 68 |
| H(91A) | -4215 | 7323 | 4628 | 115 |
| H(91B) | -4341 | 8694 | 4618 | 115 |
| H(91C) | -4084 | 8023 | 5089 | 115 |
| H(92A) | -6912 | 5009 | 4870 | 157 |
| H(92B) | -6494 | 5066 | 4453 | 157 |
| H(92C) | -5888 | 5003 | 4956 | 157 |
| H(93A) | -5022 | 2362 | 4668 | 144 |
| H(93B) | -5839 | 2489 | 4868 | 144 |
| H(93C) | -5160 | 3522 | 4922 | 144 |
| H(97) | -2645 | 8070 | 5456 | 67 |

**LCoN$^t$Bu**

**Structure Determination.**

Violet / magenta crystals were shipped over dry ice and kept at -70C for a few days. For the structure determination a prismatic crystal 0.15 x 0.14 x 0.10 mm in size was mounted on a standard Bruker X8 Apex2 CCD-based X-ray diffractometer equipped with an Oxford Cryostream 700 low temperature device. Intensities were measured at 223(2) K using graphite monochromatized Mo-$K_\alpha$ radiation ($\lambda$ = 0.71073 Å). A full sphere of data, 3537 frames each at 5.000 cm detector distance, was collected with scan width of 0.50° in $\omega$ and phi and an exposure time of 15 s/frame. Analysis of the frames showed negligible decay during data collection. The data were integrated using the Bruker SAINT software package with a narrow frame algorithm[1] yielding a total of 42722 reflections of which 4150 independent. The SADABS program was used for the absorption correction.[2]

The structure was solved by direct methods and refined by full matrix least-squares techniques with the SHELX97 software package.[3] The reflection conditions indicated $P2_1/n$ (#14) as the only possible space group. The initial solution resulted in R-factor of c.a. 13% and the refinement was consequently carried out. First all non-hydrogen atoms have been found and assigned from the Fourier maps and their thermal parameters refined anisotropically. Next, the hydrogen atoms bonded to C-atoms have been added to the refinement as riding models and their thermal parameters refined isotropically. The main crystallographic details are summarized in Table 6.

**Table 6**. Crystal data and structure refinement for **LCoN$^t$Bu**.

| | |
|---|---|
| Empirical formula | $[C_{32}H_{48}BCoN_7]$ 1/2 $(C_6H_4O_2)$ |
| Formula weight | 654.09 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Monoclinic, P21/n (#14) |
| Unit cell dimensions | a = 9.6389(3) A alpha = 90 deg.<br>b = 20.8449(7) A beta = 100.028(2) deg.<br>c = 17.1780(6) A gamma = 90 deg. |
| Volume, Z | 3398.7(2) A^3 , 4 |
| Calculated density | 1.201 g/cm^3 |
| Absorption coefficient | 0.538 mm^-1 |
| F(000) | 1312 |
| Crystal size | 0.15 x 0.14 x 0.10 mm |
| Theta range for data collection | 1.55 to 22.00 deg. |
| Limiting indices | -10<=h<=9, -20<=k<=21, -18<=l<=18 |
| Reflections collected / unique | 42722 / 4150 [R(int) = 0.0304] |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4150 / 0 / 399 |
| Goodness-of-fit on F^2 | 1.150 |
| Final R indices [I>2sigma(I)] | R1 = 0.0519, wR2 = 0.1651 |
| R indices (all data) | R1 = 0.0593, wR2 = 0.1783 |
| Extinction coefficient | 0.0130(17) |
| Largest diff. peak and hole | 0.970 and -0.357 e.A^-3 |

**Table 2.** Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **LCoN$^t$Bu**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Co(1) | 3452(1) | 2392(1) | 9652(1) | 21(1) |
| B(1) | 3968(5) | 3543(2) | 8562(3) | 26(1) |
| N(11) | 578(3) | 3064(2) | 9043(2) | 32(1) |
| N(12) | 2377(3) | 3454(2) | 8607(2) | 27(1) |
| C(11) | 2004(4) | 2978(2) | 9069(2) | 26(1) |
| C(12) | 120(4) | 3589(2) | 8580(2) | 39(1) |
| C(13) | 1232(4) | 3835(2) | 8314(2) | 35(1) |
| C(14) | -347(5) | 2677(2) | 9473(3) | 39(1) |
| C(15) | -1868(5) | 2915(3) | 9275(3) | 59(2) |
| C(16) | -280(5) | 1987(2) | 9215(3) | 53(1) |
| C(17) | 168(5) | 2771(3) | 359(3) | 49(1) |
| N(21) | 4475(3) | 2885(2) | 8306(2) | 23(1) |
| N(22) | 5045(3) | 1878(2) | 8366(2) | 27(1) |
| C(21) | 4398(4) | 2346(2) | 8738(2) | 23(1) |
| C(22) | 5098(4) | 2755(2) | 7659(2) | 29(1) |
| C(23) | 5452(4) | 2135(2) | 7693(2) | 33(1) |
| C(24) | 5343(4) | 1202(2) | 8628(2) | 30(1) |
| C(25) | 3965(5) | 834(2) | 8521(3) | 42(1) |
| C(26) | 6334(6) | 892(2) | 8144(3) | 50(1) |
| C(27) | 6061(5) | 1206(2) | 9489(3) | 40(1) |
| N(31) | 5230(3) | 3398(2) | 693(2) | 29(1) |
| N(32) | 4657(3) | 3636(2) | 9447(2) | 26(1) |
| C(31) | 4567(4) | 3158(2) | 9977(2) | 24(1) |
| C(32) | 5645(5) | 4025(2) | 600(3) | 40(1) |
| C(33) | 5283(5) | 4167(2) | 9831(3) | 36(1) |
| C(34) | 5494(4) | 3052(2) | 1467(2) | 35(1) |
| C(35) | 4089(5) | 2938(3) | 1728(3) | 55(1) |
| C(36) | 6268(6) | 2432(2) | 1356(3) | 51(1) |
| C(37) | 6436(5) | 3455(3) | 2088(3) | 51(1) |
| N(41) | 3145(3) | 1778(2) | 213(2) | 27(1) |
| C(41) | 2882(5) | 1235(2) | 707(2) | 35(1) |
| C(42) | 1924(9) | 1443(3) | 1274(4) | 95(3) |
| C(43) | 2183(9) | 696(3) | 209(4) | 94(3) |
| C(44) | 4248(7) | 988(4) | 1178(5) | 110(3) |
| C(51) | 4318(4) | 4092(2) | 7960(2) | 31(1) |
| C(52) | 3448(5) | 4197(2) | 7235(3) | 40(1) |

| | | | | |
|---|---|---|---|---|
| C(53) | 3766(6) | 4641(3) | 6699(3) | 53(1) |
| C(54) | 4978(6) | 5001(2) | 6866(3) | 57(2) |
| C(55) | 5894(6) | 4891(2) | 7552(3) | 54(1) |
| C(56) | 5572(5) | 4437(2) | 8089(3) | 41(1) |
| C(61) | 4616(10) | 256(4) | 5700(5) | 37(2) |
| C(62) | 5986(10) | 361(4) | 5502(5) | 41(2) |
| C(63) | 3643(9) | -130(4) | 5150(5) | 40(2) |
| O(61) | 4279(8) | 490(3) | 6292(4) | 59(2) |

**Table 3.** Bond lengths [A] and angles [deg] for **LCoN$^t$Bu**.

| | |
|---|---|
| Co(1)-N(41)#1 | 1.660(3) |
| Co(1)-C(21) | 1.949(4) |
| Co(1)-C(31) | 1.952(4) |
| Co(1)-C(11) | 1.988(4) |
| B(1)-N(21) | 1.544(6) |
| B(1)-N(12) | 1.560(5) |
| B(1)-N(32) | 1.561(5) |
| B(1)-C(51) | 1.617(6) |
| N(11)-C(11) | 1.379(5) |
| N(11)-C(12) | 1.379(6) |
| N(11)-C(14) | 1.491(6) |
| N(12)-C(11) | 1.359(5) |
| N(12)-C(13) | 1.381(5) |
| C(12)-C(13) | 1.339(6) |
| C(14)-C(16) | 1.510(7) |
| C(14)-C(17)#1 | 1.528(7) |
| C(14)-C(15) | 1.528(7) |
| C(17)-C(14)#2 | 1.528(7) |
| N(21)-C(21) | 1.356(5) |
| N(21)-C(22) | 1.379(5) |
| N(22)-C(21) | 1.375(5) |
| N(22)-C(23) | 1.390(5) |
| N(22)-C(24) | 1.492(5) |
| C(22)-C(23) | 1.335(6) |
| C(24)-C(25) | 1.517(6) |
| C(24)-C(26) | 1.517(6) |
| C(24)-C(27) | 1.519(6) |
| N(31)-C(31)#2 | 1.378(5) |
| N(31)-C(32) | 1.383(5) |
| N(31)-C(34) | 1.496(5) |
| N(32)-C(31) | 1.361(5) |
| N(32)-C(33) | 1.373(5) |
| C(31)-N(31)#1 | 1.378(5) |
| C(32)-C(33)#2 | 1.341(6) |
| C(33)-C(32)#1 | 1.341(6) |
| C(34)-C(35) | 1.518(6) |
| C(34)-C(36) | 1.520(7) |
| C(34)-C(37) | 1.527(6) |
| N(41)-C(41) | 1.463(5) |
| N(41)-Co(1)#2 | 1.660(3) |
| C(41)-C(43) | 1.500(7) |
| C(41)-C(44) | 1.511(8) |

| | |
|---|---|
| C(41)-C(42) | 1.517(7) |
| C(51)-C(56) | 1.390(6) |
| C(51)-C(52) | 1.393(6) |
| C(52)-C(53) | 1.377(6) |
| C(53)-C(54) | 1.375(8) |
| C(54)-C(55) | 1.364(8) |
| C(55)-C(56) | 1.395(7) |
| C(61)-O(61) | 1.223(10) |
| C(61)-C(62) | 1.437(14) |
| C(61)-C(63) | 1.452(13) |
| C(62)-C(63)#3 | 1.323(13) |
| C(63)-C(62)#3 | 1.323(13) |

| | |
|---|---|
| N(41)#1-Co(1)-C(21) | 125.82(15) |
| N(41)#1-Co(1)-C(31) | 127.58(16) |
| C(21)-Co(1)-C(31) | 87.67(15) |
| N(41)#1-Co(1)-C(11) | 125.81(16) |
| C(21)-Co(1)-C(11) | 90.64(15) |
| C(31)-Co(1)-C(11) | 86.84(15) |
| N(21)-B(1)-N(12) | 105.8(3) |
| N(21)-B(1)-N(32) | 106.6(3) |
| N(12)-B(1)-N(32) | 102.8(3) |
| N(21)-B(1)-C(51) | 109.5(3) |
| N(12)-B(1)-C(51) | 115.6(3) |
| N(32)-B(1)-C(51) | 115.7(3) |
| C(11)-N(11)-C(12) | 109.9(3) |
| C(11)-N(11)-C(14) | 126.3(3) |
| C(12)-N(11)-C(14) | 123.8(3) |
| C(11)-N(12)-C(13) | 110.9(3) |
| C(11)-N(12)-B(1) | 118.5(3) |
| C(13)-N(12)-B(1) | 130.1(3) |
| N(12)-C(11)-N(11) | 104.4(3) |
| N(12)-C(11)-Co(1) | 120.6(3) |
| N(11)-C(11)-Co(1) | 134.8(3) |
| C(13)-C(12)-N(11) | 107.8(4) |
| C(12)-C(13)-N(12) | 106.9(4) |
| N(11)-C(14)-C(16) | 108.0(4) |
| N(11)-C(14)-C(17)#1 | 107.8(4) |
| C(16)-C(14)-C(17)#1 | 113.0(4) |
| N(11)-C(14)-C(15) | 110.3(4) |
| C(16)-C(14)-C(15) | 109.4(4) |
| C(17)#1-C(14)-C(15) | 108.2(4) |
| C(21)-N(21)-C(22) | 110.5(3) |
| C(21)-N(21)-B(1) | 122.0(3) |
| C(22)-N(21)-B(1) | 127.5(3) |
| C(21)-N(22)-C(23) | 109.2(3) |

| | |
|---|---|
| C(21)-N(22)-C(24) | 127.5(3) |
| C(23)-N(22)-C(24) | 123.3(3) |
| N(21)-C(21)-N(22) | 105.1(3) |
| N(21)-C(21)-Co(1) | 118.5(3) |
| N(22)-C(21)-Co(1) | 136.3(3) |
| C(23)-C(22)-N(21) | 107.4(3) |
| C(22)-C(23)-N(22) | 107.6(3) |
| N(22)-C(24)-C(25) | 108.9(3) |
| N(22)-C(24)-C(26) | 110.1(3) |
| C(25)-C(24)-C(26) | 109.8(4) |
| N(22)-C(24)-C(27) | 108.7(3) |
| C(25)-C(24)-C(27) | 111.2(4) |
| C(26)-C(24)-C(27) | 108.2(4) |
| C(31)#2-N(31)-C(32) | 109.8(3) |
| C(31)#2-N(31)-C(34) | 126.8(3) |
| C(32)-N(31)-C(34) | 123.4(3) |
| C(31)-N(32)-C(33) | 110.0(3) |
| C(31)-N(32)-B(1) | 119.6(3) |
| C(33)-N(32)-B(1) | 130.1(3) |
| N(32)-C(31)-N(31)#1 | 105.0(3) |
| N(32)-C(31)-Co(1) | 120.2(3) |
| N(31)#1-C(31)-Co(1) | 134.4(3) |
| C(33)#2-C(32)-N(31) | 107.0(4) |
| C(32)#1-C(33)-N(32) | 108.2(4) |
| N(31)-C(34)-C(35) | 108.4(3) |
| N(31)-C(34)-C(36) | 108.0(3) |
| C(35)-C(34)-C(36) | 112.8(4) |
| N(31)-C(34)-C(37) | 110.1(4) |
| C(35)-C(34)-C(37) | 109.5(4) |
| C(36)-C(34)-C(37) | 108.1(4) |
| C(41)-N(41)-Co(1)#2 | 179.7(3) |
| N(41)-C(41)-C(43) | 110.7(4) |
| N(41)-C(41)-C(44) | 110.6(4) |
| C(43)-C(41)-C(44) | 108.2(6) |
| N(41)-C(41)-C(42) | 109.8(4) |
| C(43)-C(41)-C(42) | 108.5(5) |
| C(44)-C(41)-C(42) | 108.9(5) |
| C(56)-C(51)-C(52) | 115.6(4) |
| C(56)-C(51)-B(1) | 122.5(4) |
| C(52)-C(51)-B(1) | 121.6(4) |
| C(53)-C(52)-C(51) | 122.4(5) |
| C(54)-C(53)-C(52) | 120.4(5) |
| C(55)-C(54)-C(53) | 119.2(4) |
| C(54)-C(55)-C(56) | 120.0(5) |
| C(51)-C(56)-C(55) | 122.2(5) |

| | |
|---|---|
| O(61)-C(61)-C(62) | 121.6(8) |
| O(61)-C(61)-C(63) | 121.9(9) |
| C(62)-C(61)-C(63) | 116.5(7) |
| C(63)#3-C(62)-C(61) | 122.7(8) |
| C(62)#3-C(63)-C(61) | 120.8(9) |

---

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z+1  #2 x,y,z-1  #3 -x+1,-y,-z+1

**Table 4**. Anisotropic displacement parameters (A^2 x 10^3) for **LCoN$^t$Bu**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Co(1) | 22(1) | 20(1) | 22(1) | 1(1) | 7(1) | -2(1) |
| B(1) | 25(2) | 25(2) | 29(2) | 1(2) | 6(2) | 0(2) |
| N(11) | 21(2) | 41(2) | 33(2) | 3(2) | 5(1) | 0(2) |
| N(12) | 27(2) | 25(2) | 30(2) | 3(1) | 6(1) | 3(1) |
| C(11) | 26(2) | 28(2) | 25(2) | -2(2) | 7(2) | -2(2) |
| C(12) | 27(2) | 52(3) | 39(2) | 8(2) | 5(2) | 12(2) |
| C(13) | 34(2) | 37(2) | 34(2) | 9(2) | 6(2) | 11(2) |
| C(14) | 24(2) | 50(3) | 43(3) | 5(2) | 9(2) | -5(2) |
| C(15) | 22(2) | 85(4) | 72(4) | 11(3) | 13(2) | -3(3) |
| C(16) | 39(3) | 53(3) | 68(3) | 0(3) | 11(2) | -18(2) |
| C(17) | 38(3) | 70(3) | 44(3) | 9(2) | 18(2) | 1(2) |
| N(21) | 23(2) | 23(2) | 24(2) | 3(1) | 6(1) | -1(1) |
| N(22) | 29(2) | 23(2) | 31(2) | 0(1) | 12(1) | 1(1) |
| C(21) | 20(2) | 25(2) | 25(2) | 0(2) | 3(2) | -2(2) |
| C(22) | 34(2) | 30(2) | 26(2) | 5(2) | 13(2) | -1(2) |
| C(23) | 38(2) | 35(3) | 30(2) | -1(2) | 18(2) | 3(2) |
| C(24) | 32(2) | 20(2) | 38(2) | 2(2) | 12(2) | 2(2) |
| C(25) | 39(2) | 29(2) | 57(3) | 5(2) | 4(2) | -3(2) |
| C(26) | 64(3) | 31(3) | 60(3) | 3(2) | 29(3) | 10(2) |
| C(27) | 37(2) | 35(2) | 48(3) | 5(2) | 2(2) | 7(2) |
| N(31) | 33(2) | 25(2) | 27(2) | -3(1) | 4(1) | -5(2) |
| N(32) | 28(2) | 21(2) | 29(2) | 0(2) | 8(1) | -2(1) |
| C(31) | 21(2) | 25(2) | 28(2) | 1(2) | 8(2) | 3(2) |
| C(32) | 52(3) | 31(3) | 36(3) | -6(2) | 6(2) | -15(2) |
| C(33) | 46(3) | 22(2) | 42(3) | -2(2) | 12(2) | -9(2) |
| C(34) | 39(2) | 40(3) | 25(2) | -2(2) | 1(2) | -7(2) |
| C(35) | 58(3) | 75(4) | 32(3) | -2(2) | 11(2) | -17(3) |
| C(36) | 63(3) | 44(3) | 40(3) | 5(2) | -10(3) | 7(2) |
| C(37) | 57(3) | 57(3) | 34(3) | -5(2) | -4(2) | -14(3) |
| N(41) | 29(2) | 26(2) | 26(2) | -1(1) | 10(1) | -1(1) |
| C(41) | 48(3) | 27(2) | 31(2) | 5(2) | 15(2) | -6(2) |
| C(42) | 174(7) | 47(3) | 93(5) | 20(3) | 102(5) | 4(4) |
| C(43) | 168(7) | 53(4) | 58(4) | 8(3) | 11(4) | -61(4) |
| C(44) | 71(4) | 96(5) | 159(7) | 99(5) | 6(4) | 3(4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(51) | 35(2) | 24(2) | 36(2) | 4(2) | 13(2) | 4(2) |
| C(52) | 38(2) | 47(3) | 38(3) | 13(2) | 14(2) | 8(2) |
| C(53) | 56(3) | 59(3) | 49(3) | 26(3) | 23(2) | 26(3) |
| C(54) | 88(4) | 35(3) | 58(3) | 20(2) | 46(3) | 18(3) |
| C(55) | 75(4) | 36(3) | 62(3) | -7(2) | 43(3) | -20(3) |
| C(56) | 49(3) | 38(3) | 39(2) | -1(2) | 19(2) | -7(2) |
| C(61) | 51(6) | 21(4) | 34(5) | 6(4) | -8(4) | 23(4) |
| C(62) | 60(6) | 25(5) | 25(5) | -1(4) | -30(4) | 16(4) |
| C(63) | 33(5) | 36(5) | 48(6) | 16(4) | -3(4) | 25(4) |
| O(61) | 97(5) | 52(4) | 28(3) | -15(3) | 13(3) | 21(4) |

**Table 5.** Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **LCoN$^t$Bu**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(12) | -798 | 3744 | 8472 | 47 |
| H(13) | 1234 | 4195 | 7993 | 42 |
| H(15A) | -1911 | 3354 | 9438 | 88 |
| H(15B) | -2455 | 2657 | 9548 | 88 |
| H(15C) | -2192 | 2884 | 8716 | 88 |
| H(16A) | -609 | 1956 | 8656 | 80 |
| H(16B) | -863 | 1728 | 9489 | 80 |
| H(16C) | 676 | 1838 | 9336 | 80 |
| H(17A) | 1147 | 2658 | 487 | 74 |
| H(17B) | -368 | 2503 | 650 | 74 |
| H(17C) | 50 | 3212 | 495 | 74 |
| H(22) | 5245 | 3045 | 7271 | 35 |
| H(23) | 5891 | 1915 | 7333 | 39 |
| H(25A) | 3532 | 841 | 7974 | 63 |
| H(25B) | 3346 | 1029 | 8834 | 63 |
| H(25C) | 4147 | 398 | 8689 | 63 |
| H(26A) | 5899 | 885 | 7597 | 74 |
| H(26B) | 6536 | 460 | 8325 | 74 |
| H(26C) | 7194 | 1133 | 8203 | 74 |
| H(27A) | 6928 | 1442 | 9539 | 60 |
| H(27B) | 6256 | 773 | 9665 | 60 |
| H(27C) | 5454 | 1406 | 9805 | 60 |
| H(32) | 6091 | 4296 | 996 | 48 |
| H(33) | 5430 | 4558 | 9597 | 44 |
| H(35A) | 3644 | 3342 | 1789 | 82 |
| H(35B) | 4239 | 2713 | 2223 | 82 |
| H(35C) | 3495 | 2686 | 1337 | 82 |
| H(36A) | 7146 | 2531 | 1191 | 77 |
| H(36B) | 5701 | 2175 | 959 | 77 |
| H(36C) | 6445 | 2200 | 1846 | 77 |
| H(37A) | 7323 | 3530 | 1922 | 76 |
| H(37B) | 6592 | 3231 | 2584 | 76 |
| H(37C) | 5986 | 3858 | 2149 | 76 |
| H(42A) | 2356 | 1790 | 1595 | 143 |
| H(42B) | 1775 | 1088 | 1606 | 143 |
| H(42C) | 1037 | 1582 | 979 | 143 |

| | | | | |
|---|---|---|---|---|
| H(43A) | 1326 | 847 | -108 | 141 |
| H(43B) | 1973 | 354 | 545 | 141 |
| H(43C) | 2804 | 540 | -130 | 141 |
| H(44A) | 4713 | 1327 | 1501 | 166 |
| H(44B) | 4846 | 839 | 824 | 166 |
| H(44C) | 4054 | 640 | 1510 | 166 |
| H(52) | 2623 | 3960 | 7109 | 48 |
| H(53) | 3157 | 4698 | 6221 | 63 |
| H(54) | 5170 | 5315 | 6515 | 68 |
| H(55) | 6734 | 5119 | 7662 | 65 |
| H(56) | 6218 | 4362 | 8549 | 49 |
| H(62) | 6640 | 600 | 5846 | 50 |
| H(63) | 2749 | -217 | 5258 | 48 |

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