Supporting information belonging to the publication

'Benzylic Metalation of Phenethylamine Derivatives: Potassium as the Key to both Generation and Stabilization of a "Labile Anion"'

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Experimental Details

General remarks
All manipulations were conducted under an atmosphere of dry argon using standard Schlenk techniques. THF, diethyl ether, toluene and *n*-pentane were purified by distillation from sodium/benzophenone and stored under an atmosphere of argon. NMR spectra were recorded on a Bruker Avance-400 DR X or Bruker Avance-300 DP X, chemical shifts are referred to TMS with the deuterium signal of the solvent serving as internal lock and the residual solvent signals as additional reference. GC/MS analyses were performed on an Agilent 6890 5972 GC MS system (temperature program: 50 °C (2 min) – 300 °C (5 min) with 40 °C/min and a HP Mass Selective Detector 5973 (EI(+)-MS, 70 eV). Elemental analyses were performed with a Leco CHNS-932/O VTF-900 analyzer. Powder diffraction spectra were recorded on a Siemens D500 diffractometer.

Synthesis of *N*,*N*-dimethyl-2-phenylethylamine 1
The compound was synthesized according to a literature procedure[i] in 83 % yield.

Preparation of 5-K
n-BuLi (670 µL of a 1.6 M solution in hexanes, 1.07 mmol) and *t*-BuOK (123 mg, 1.07 mmol) were dissolved in THF (2 mL) at –78 °C. **1** (150 mg, 1.02 mmol) was added to the reaction mixture. The volume of the solution was halved by slow evaporation of THF *in vacuo* at –78 °C upon which the mixture was stored at this temperature. After 48 h, red hexagonal crystals of **5**-K were obtained which were suitable for X-ray crystal structure determination. ^{1}H-NMR (500.1 MHz, C_4D_8O): δ = 2.04 [s, 6H; N(CH_3)$_2$], 2.59 [d, 2H, ^3J(H,H) = 6.6 Hz; NCH_2], 2.98 [t, 1H, ^3J(H,H) = 6.6 Hz, ^1J(H,C) = 154 Hz; PhC*H*CH$_2$], 4.85 (m, 1H, *para*-H), 5.34 [d, 1H; *ortho*-H], 5.64 [m, 1H; *ortho*-H], 6.09 (m, 1H; *meta*-H), 6.28 (m, 1H; *meta*-H) (ar. H).

Synthesis of *N*-methyl-1,2,3,4-tetrahydroisoquinoline (MTHIQ) 7
The compound was synthesized following a literature procedure[i] in 95 % yield.

Crystallization of 8
MTHIQ (150 mg, 1.02 mmol) and TMEDA (120 mg, 1.03 mmol) in Et_2O (1 mL) were cooled to –60 °C and pentane (3 mL) was added slowly to the solution. Consecutively, *n*-BuLi (670 µL of a 1.6 M solution in hexanes, 1.07 mmol) was added to the reaction mixture and the solution was stored at –78 °C. After 36 h, red block-shaped crystals of **8** were obtained which were suitable for X-ray crystal structure determination.

Crystallization of 9

n-BuLi (670 µL of a 1.6 M solution in hexanes, 1.07 mmol) and *t*-BuOK (123 mg, 1.07 mmol) were dissolved in THF (2 mL) at –78 °C. MTHIQ (150 mg, 1.02 mmol) was added to the reaction mixture. The volume of the solution was halved by slow evaporation of THF *in vacuo* at –78 °C upon which the mixture was stored at this temperature. After 72 h, deep red, block-shaped crystals of **9** were obtained which were suitable for X-ray crystal structure determination.

Synthesis of 1-methyl-4-tributylstannyl-1,2,3,4-tetrahydroisoquinoline (7·$SnBu_3$)

7 (3.00 g, 20.4 mmol) and TMEDA (2.38 g, 20.5 mmol) were dissolved in pentane (30 mL) and cooled to –78 °C. *n*-BuLi (9.00 mL of a 2.5 M solution in hexanes, 22.5 mmol) was added. Within 1 h, the mixture was allowed to warm to –60 °C upon which the solution turned intensively red. Tributyltin chloride (7.36 g, 22.6 mmol) was added and the reaction mixture was allowed to warm to rt. The volatile components were removed by distillation and the residue was taken up in Et_2O (100 mL) and washed with brine (3 x 20 mL). The organic phase was dried over Na_2SO_4 and the solvent removed. The crude product was purified by Kugelrohr distillation (210 °C, 2.10^{-2} mbar) which afforded **7**·$SnBu_3$ as a colourless oil (yield: 7.27 g, 16.7 mmol, 82 %): ^{1}H-NMR (300.1 MHz, C_6D_6): δ = 0.71-1.02 {m, 15H; Sn[CH_2(CH$_2$)$_2$CH_3]$_3$}, 1.29-1.62 {m, 12 H; Sn[CH$_2$(CH_2)$_2$CH$_3$]$_3$}, 2.20 (s, 3H; NCH_3), 2.64-2.69 (m, 1H; NCH$_2$C*H*Sn), 2.79-2.86 (m, 2H; NCH_2CHSn), 3.23, 3.72 [„AB-System“, 2H, ^2J(H,H) = 14.6 Hz; C$_{ar}$CH_2N], 6.84-7.06 (m, 4H; ar. H). – {^{1}H}^{13}C-NMR (75.5 MHz, C_6D_6): δ = 10.5 {Sn[*C*H$_2$(CH$_2$)$_2$CH$_3$]$_3$}, 14.4 {Sn[(CH$_2$)$_3$*C*H$_3$]$_3$}, 28.3 {Sn[(CH$_2$)$_2$*C*H$_2$CH$_3$]$_3$}, 29.9 [Sn(CH$_2$*C*H$_2$CH$_2$CH$_3$)$_3$], 32.7 [C$_{ar}$*C*(H)Sn], 46.6 (N*C*H$_3$), 57.1 (N*C*H$_2$CHSn), 59.3 (C$_{ar}$*C*H$_2$N), 124.1 [C$_{ar}$(3)], 126.6 [C$_{ar}$(4)], 126.8 [C$_{ar}$(5)], 127.0 [C$_{ar}$(1)], 132.8 [C$_{ar}$(6)], 141.5 [C$_{ar}$(2)]. – {^{1}H}^{119}Sn-NMR (111.9 MHz, C_6D_6): δ = –8.0. – $C_{22}H_{39}NSn$ (436.26); calc. C 60.57 H 9.01 N 3.21; found C 59.3 H 8.9 N 2.7. – GC/MS retention time: 7.20. – EI-MS m/z (%): 437 (1) (M^+), 380 (17) [(M – Bu)$^+$], 144 (100) [(M – HSnBu_3)$^+$].

General procedure for the metalation of *N*,*N*-dimethyl-2-phenylethylamine

N,*N*-dimethyl-2-phenylethylamine (2.00 g, 13.4 mmol) and Kot*B*u (1.50 g, 13.4 mmol) were dissolved in THF (20 mL) and cooled to –78 °C. *t*-BuLi (7.10 mL of a 1.9 M solution in pentanes, 22.5 mmol) was added upon which the solution turned intensively red. Within 1 h, the mixture was allowed to warm to –60 °C upon which the respective electrophile (13.4 mmol) was added and the reaction mixture was allowed to warm to rt.

Synthesis of *N*,*N*-dimethyl-2-deutero-2-phenylethylamine D-1

The solvent was removed from the reaction mixture and the residue taken up in Et_2O and extracted with aq. HCl (1M, 3 x 20 mL). The aqueous phases were combined, made basic (pH 13) by the addition of aq. NaOH (1M) and extracted with Et_2O (3 x 20 mL). The organic phases were combined and dried over Na_2SO_4. After removal of the solvent, the crude product was analyzed by NMR and GCMS: ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 2.28 [s, 6 H; N(CH_3)$_2$], 2.49-2.53 (m, 2H; Me$_2$NCH_2), 2.73-2.79 (m, 1H; PhC(D)*H*), 7.16-7.29 (m, 5H; ar. *H*). – {^{1}H}^{13}C-NMR (100 MHz, $CDCl_3$): δ = 34.0 [t, 1H, ^1J(C,D) = 19.4 Hz; Ph*C*DH], 45.5 [2C; N(*C*H$_3$)$_2$], 61.6 (N*C*H$_2$), 126.0 (Ph-C$_p$), 128.3 (2C, Ph-C$_o$), 128.6 (2C; Ph-C$_m$), 140.4 (Ph-C$_i$). – GC/MS retention time: 4.20. – EI-MS m/z (%): 150 (2) (M^+), 106 (5) [(M – NMe$_2$)$^+$], 92 (7) (Bn$^+$), 77 (5) (Ph$^+$), 58 (100) (Me$_2$NCH$_2^+$).

***N*,*N*-dimethyl-2-phenyl-1-hexylamine 6a**

The solvent was removed from the reaction mixture and the residue taken up in Et_2O and extracted with aq. HCl (1M, 3 x 20 mL). The aqueous phases were combined, made basic (pH 13) by the addition of aq. NaOH (1M) and extracted with Et_2O (3 x 20 mL). The organic phases were combined and dried over Na_2SO_4. After removal of the solvent, the crude product was purified by Kugelrohr distillation (150 °C, 32 mbar) which afforded **6a** as a colourless oil (yield: 2.53 g, 12.3 mmol, 92 %): ^{1}H-NMR (400.1 MHz, $CDCl_3$): δ = 0.81-0.84 [m, 3H; *C*H$_3$CH$_2$], 1.07-1.34 [m, 4H; CH$_3$*C*H$_2$*C*H$_2$CH$_2$], 1.45-1.56 [m, 1H; CH$_2$*C*H$_2$CH], 1.74-1.82 [m, 1H; CH$_2$*C*H$_2$CH], 2.22 (s, 1H; N(CH$_3$)$_2$), 2.45-2.51 [m, 2H; CH*C*H$_2$N], 2.71-2.77 [m, 1H; Ph*C*HCH$_2$], 7.16-7.33 [m, 5H; *Ph*CH]. – {^{1}H}^{13}C-NMR (125.7 MHz, $CDCl_3$): δ = 14.0 (*C*H$_3$CH$_2$), 22.8 (CH$_3$*C*H$_2$CH$_2$), 29.7 (CH$_2$*C*H$_2$CH$_2$), 34.3 (CH$_2$*C*H$_2$CH), 44.3 (CH$_2$Ph*C*HCH$_2$), 45.9 [2C; N(*C*H$_3$)$_2$], 66.7 (N*C*H$_2$CH), 126.1 (C-*p*-Ph), 127.7 [2C; C-*o*-Ph], 128.3 [2C; C-*m*-Ph], 144.8 (C-*i*-Ph). – $C_{14}H_{23}N$ (205.34); calc. C 81.89 H 11.29 N 6.82; found C 81.8 H 11.5 N

7.0. – GC/MS retention time: 5.13. – EI-MS m/z (%): 205 (2) (M^+), 104 (23) [$(C_9H_8)^+$], 91 (35) [$(C_7H_7)^+$], 58 (100) [$(C_3H_8N)^+$].

***N,N*-dimethyl-2-phenyl-2-(trimethylsilyl)ethylamine 6b**

The solvent was removed from the reaction mixture and the residue taken up in Et_2O and extracted with aq. HCl (1M, 3 x 20 mL). The aqueous phases were combined, made basic (pH 13) by the addition of aq. NaOH (1M) and extracted with Et_2O (3 x 20 mL). The organic phases were combined and dried over Na_2SO_4. After removal of the solvent, the crude product was purified by Kugelrohr distillation (100 °C, 1 mbar) which afforded **6b** as a colorless oil (yield: 2.28 g, 8.03 mmol, 60 %): ^{1}H-NMR (300.1 MHz, $CDCl_3$): δ = –0.04 [s, 9H; Si*(CH$_3$)$_3$*], 2.17 [s, 6H; N(CH$_3$)$_2$], 2.31-2.38 [m, 2H; CH*CH$_2$*N], 2.89-2.98 [m, 1H; Ph*CH*CH$_2$], 7.03-7.25 (m, 5H; *Ph*CH). – {^{1}H}^{13}C-NMR (100.6 MHz, $CDCl_3$): δ = –2.8 [3C; CHSi(*Me*)$_3$)], 35.8 (SiPh*C*HCH$_2$), 45.4 [2C; N*(CH$_3$)$_2$*], 59.8 (CH*CH$_2$*N), 124.5 [2C; C-*o*-Ph], 127.4 (C-*p*-Ph), 128.1 [2C; C-*m*-Ph], 142.7 (C-*i*-Ph). – $C_{13}H_{23}NSi$ (221.41); calc. C 70.52 H 10.47 N 6.33; found C 70.6 H 10.6 N 6.4. – GC/MS retention time: 4.95. – EI-MS m/z (%): 221 (3) [M^+], 102 (43) [$(C_8H_7\text{-}H)^+$], 73 (37) [$(C_3H_9Si)^+$], 58 (100) [$(C_3H_8N)^+$].

***N,N*-Dimethyl-2-(dimethyl(phenyl)silyl)-2-phenylethanamine 6c**

The solvent was removed from the reaction mixture and the residue taken up in Et_2O and extracted with aq. HCl (1M, 3 x 20 mL). The aqueous phases were combined, made basic (pH 13) by the addition of aq. NaOH (1M) and extracted with Et_2O (3 x 20 mL). The organic phases were combined and dried over Na_2SO_4. After removal of the solvent, the crude product was purified by Kugelrohr distillation (150 °C, 1 mbar) which afforded **6c** as a pale yellow oil (yield: 2.28 g, 8.03 mmol, 60 %): ^{1}H-NMR (500.1 MHz, $CDCl_3$): δ = –0.02 [s, 3H; *CH$_3$*SiCH$_3$Ph], .0.04 [s, 3H; CH$_3$Si*CH$_3$*Ph], 1.93 [s, 3H; N*(CH$_3$)$_2$*], 2.33-2.44 [m, 2H; CH*CH$_2$*N], 2.68-2.74 [m, 1H; Ph*CH*CH$_2$], 6.74-7.03 [m, 5H; *Ph*Si(CH$_3$)$_2$], 7.12-7.22 [m, 5H; *Ph*CH]. – {^{1}H}^{13}C-NMR (75.5 MHz, $CDCl_3$): δ = 0.0 [2C; PhSi*(CH$_3$)$_2$*] 34.2 (PhSi*C*HCH$_2$), 45.3 [2C; N*(CH$_3$)$_2$*], 61.5 (N*CH$_2$*CH), 126.0 [2C; *o*-PhCHCH$_2$)], 127.5 (*p*-PhCHCH$_2$), 127.8 [2C, C-*m*-PhCHCH$_2$], 128.1 (C-*p*-PhSi(CH$_3$)$_2$), 128.4 [2C, C-*o*-PhSi(CH$_3$)$_2$], 128.6 [2C, C-*m*-PhSi(CH$_3$)$_2$], 133.0 (C-*p*-PhSi(CH$_3$)$_2$), 133.1 (C-*p*-PhCHCH$_2$). – $C_{19}H_{27}NSi$ (283.48); calc. C 76.26 H 8.89 N 4.94; found C 76.4 H 9.2 N 5.1. – GC/MS retention time: 6.55. – EI-MS m/z (%): 283 (4) [M^+], 105 (38) [$(C_8H_9)^+$], 58 (100) [$(C_3H_8N)^+$].

3-(Dimethylamino)-1,1,2-triphenyl-1-propanol 6d

The solvent was removed from the reaction mixture and the residue taken up in Et_2O and extracted with aq. HCl (1M, 3 x 20 mL). The aqueous phases were combined, made basic (pH 13) by the addition of aq. NaOH (1M) and extracted with Et_2O (3 x 20 mL). The organic phases were combined and dried over Na_2SO_4. After removal of the solvent, the crude product was purified by Kugelrohr distillation (280 °C, 1 mbar) which afforded **6d** as a pale yellow oil which could be recrystallized from Et_2O to afford colorless needles (yield: 3.29 g, 9.93 mmol, 74 %): ^{1}H-NMR (400.1 MHz, $CDCl_3$): δ = 2.08 [s, 6H; N*(CH$_3$)$_2$*], 2.79-2.82 [m, 2H; CH*CH$_2$*N], 3.95-4.01 [m, 1H; Ph*CH*CH$_2$], 7.06-7.22 [m, 5H; *Ph*CH], 7.29-7.84 (m, 10H; *Ph$_2$*COHCH). – {^{1}H}^{13}C-NMR (126.7 MHz, $CDCl_3$): δ = 46.4 [2C; N*(CH$_3$)$_2$*], 50.8 (Ph*CH*CH$_2$), 63.2 (CH*CH$_2$*N), 81.9 (CH*C*(Ph)$_2$OH), 125.9 (C-*p*-PhCHCH$_2$), 126.1 [2C; C-*o*-PhCHCH$_2$)], 126.5 (C-*p*-PhCPhOH), 127.4 [4C, C-*o*-PhCPhOH], 127.6 [2C, C-*m*-PhCHCH$_2$], 128.0 [4C, C-*m*-PhCPhOH], 145.8 (C-*i*-PhCPhOH), 148.5 (C-*i*-PhCHCH$_2$). – $C_{23}H_{25}NO$ (331.45); calc. C 83.34 H 7.60 N 4.23; found C 83.4 H 7.7 N 3.8. – GC/MS retention time: 8.03. – EI-MS m/z (%): 105 (23) [$(C_9H_9)^+$], 77 (21) [$(C_6H_5)^+$], 58 (100) [$(C_3H_8N)^+$].

1-(2-Dimethylamino)-1-phenylethylcyclohexanol 6e

The solvent was removed from the reaction mixture and the residue taken up in Et_2O and extracted with aq. HCl (1M, 3 x 20 mL). The aqueous phases were combined, made basic (pH 13) by the addition of aq. NaOH (1M) and extracted with Et_2O (3 x 20 mL). The organic phases were combined and dried over Na_2SO_4. After removal of the solvent, the crude product was recrystallized from Et_2O to afford colorless blocks of **6e** (yield: 2.78 g, 11.3 mmol, 84 %): ^{1}H-NMR (400.1 MHz, $CDCl_3$): δ = 1.31-1.90 [m, H; CH*Cy*OH], 2.33 [s, 6H; N*(CH$_3$)$_2$*], 2.51-2.57 [m, 2H; CH*CH$_2$*N], 2.77-2.82 [m, 1H; Ph*CH*CH$_2$], 7.25-7.32 (m, 5H; *Ph*CH). – GC/MS retention time: 6.51. – EI-MS m/z (%): 247 (2) [M^+], 104 (28) [$(C_9H_9 - H)^+$], 81 (15) [$(C_6H_{10} - H)^+$], 58 (100) [$(C_3H_8N)^+$].

Crystal-Structure Determination

The crystals of **5**-K, **6d**, **6e**, **8** and **9** were mounted in an inert oil (perfluoropolyalkylether) at –80 °C (N_2 stream) using the X-TEMP 2 device.[ii] Crystal structure determination of **5**-K, **6d**, **6e**, **8** and **9** was accomplished on a Oxford Diffraction Xcalibur S diffractometer; data collection: CrysAlis CCD (Oxford Diffraction, 2006); cell refinement: CrysAlis RED (Oxford Diffraction, 2006); data reduction: CrysAlis RED; absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006). The structure was solved by applying direct and Fourier methods, using SHELXS97[iii] and SHELXL-97.[iv] The non-hydrogen atoms were refined anisotropically. All of the H-atoms – except H(9), H(10a) and H(10b) – were placed in geometrically calculated positions and each was assigned a fixed isotropic displacement parameter based on a riding-model. The hydrogen-atoms H(1O) in **6e**, H(9), H(10a) and H(10b) in compound **8**, H(2a), H(2b), H(9), H(10a), H(10b), H(20a), H20b), H(27), H(28a) and H(28b) in compound **9** were found and could be freely refined via Difference-Fourier-Synthesis. CCDC 856271 (**6d**), CCDC 856272 (**6e**), CCDC 856273(**8**) and CCDC 856274 (**9**) contain the detailed crystallographic data for this publication. This data may be obtained free of charge from the Cambridge Crystallographic Data Center through www.ccdc.cam.ac.uk/data_request/cif.

Table 1 Crystal Data and Structural Refinement Details for compounds **5-K**.

compound	**5-K**
empirical formula	$C_{32}H_{44}NO_3K_2$
molecular mass [g·mol^{-1}]	582.89
temperature [K]	173(2)
wave length [Å]	0.71073
crystal system	hexagonal
space group (Nr.)	$P3_221$ (154)
a [Å]	9.3923(3)
b [Å]	9.3923(3)
c [Å]	67.355(3)
α	90°
β	90°
γ	120°
cell volume V [Å^3]	5145.7(3)
Z	6
calculated density *ρ* [g·cm^{-3}]	1.129
absorption coefficient *μ* [mm^{-1}]	0.447
F(000)	2848
crystal size [mm^3]	0.60 x 0.60 x 0.60
range for data collection 2*θ* [°]	2.50 – 27.00.
index ranges	–7 < h < 5 –8 < k < 11 –69 < l < 85
reflections collected	12753
independent reflections	7361 [R_{int}= 0.0523]
refinement method	Full-matrix least-squares on F^2
data / restraints / parameter	7361/0/362
goodness-of-fit on F^2	0.990
final *R*-values [$I > 2\sigma(I)$]	*R*1 = 0.1101 w*R*2 = 0.3135
R-values (all data)	*R*1 = 0.1848 w*R*2 = 0.3419

Absolute structure parameter	0.94(14)
largest diff. peak and hole [e· Å^{-3}]	0.507 and –0.678

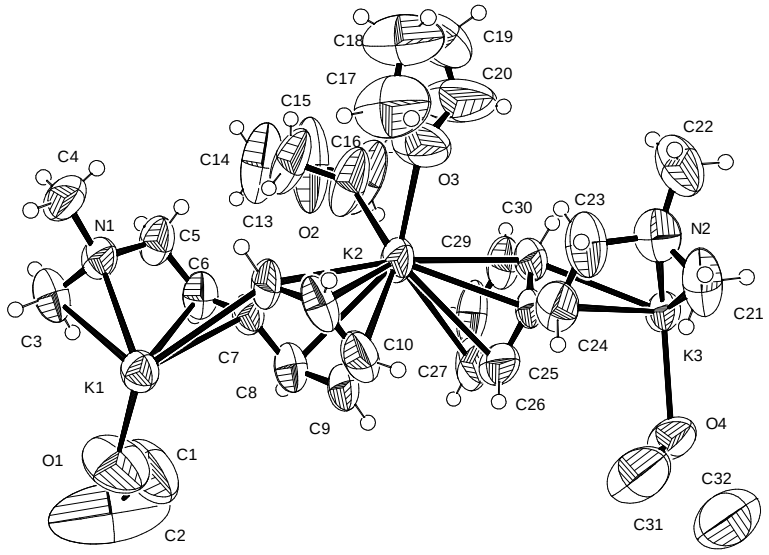


Fig. 1 ORTEP plot of **5-K** at 50% probability level.

Table 2 Atomic coordinates (·10^4) and equivalent isotropic displacement parameters (Å^2 ·10^3) for **5-K**.

Atom	x	y	z	U(eq)
C(1)	610(30)	5600(30)	3187(2)	185(8)
C(2)	577(17)	6904(18)	3284(6)	313(19)
C(3)	3540(13)	4039(11)	3506(1)	93(3)
C(4)	3957(13)	1759(15)	3513(1)	107(3)
C(5)	4003(10)	3001(12)	3194(1)	83(2)
C(6)	3101(11)	3474(11)	3052(1)	81(2)
C(7)	1792(10)	2345(12)	2950(1)	71(2)
C(8)	862(12)	2750(12)	2811(1)	83(2)
C(9)	–466(12)	1591(15)	2702(1)	90(3)
C(10)	–977(12)	–31(14)	2716(1)	92(3)
C(11)	–155(13)	–492(12)	2846(1)	94(3)
C(12)	1189(12)	674(14)	2954(1)	85(2)
C(13)	5945(15)	2990(20)	2727(1)	145(5)
C(14)	7230(20)	4600(20)	2754(2)	184(8)
C(15)	7690(30)	5177(19)	2556(2)	220(11)
C(16)	6617(15)	4230(20)	2421(2)	170(7)
C(17)	2820(20)	–2300(20)	2634(2)	190(8)
C(18)	3984(19)	–2730(20)	2595(3)	171(7)
C(19)	4825(19)	–1840(20)	2423(2)	157(6)
C(20)	4060(20)	–1090(30)	2348(3)	204(9)
C(21)	–2227(13)	–3769(15)	1790(2)	124(4)
C(22)	256(19)	–3946(15)	1815(2)	128(4)
C(23)	–399(18)	–2506(16)	2072(1)	122(4)
C(24)	–802(11)	–1228(15)	2116(1)	97(3)
C(25)	434(11)	444(13)	2107(1)	78(2)
C(26)	107(17)	1730(20)	2161(1)	105(3)
C(27)	1310(20)	3320(20)	2162(1)	119(4)
C(28)	2910(20)	3838(18)	2110(1)	129(5)
C(29)	3198(14)	2590(17)	2046(1)	101(3)
C(30)	2028(12)	1008(15)	2044(1)	88(3)
C(31)	–3710(20)	50(40)	1841(2)	236(13)
C(32)	–4960(40)	–220(60)	1575(4)	321(19)
K(1)	0	1626(3)	3333	68(1)
K(2)	2186(2)	1239(3)	2491(1)	84(1)

K(3)	5(3)	0	1667	81(1)
N(1)	3267(7)	2588(8)	3394(1)	68(2)
N(2)	–572(10)	–3000(10)	1860(1)	96(2)
O(1)	0	4453(11)	3333	159(6)
O(2)	5401(8)	2905(13)	2537(1)	145(4)
O(3)	2928(12)	–1179(13)	2494(1)	141(3)
O(4)	–2453(15)	703(19)	1658(3)	110(6)

Table 3 Anisotropic Displacement parameters ($Å^2 \cdot 10^3$) for **5-K**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	300(20)	209(19)	112(10)	32(11)	67(13)	173(18)
C(2)	107(15)	68(9)	710(60)	93(19)	10(30)	1(9)
C(3)	116(7)	86(6)	60(5)	–4(4)	17(5)	39(6)
C(4)	114(7)	174(10)	63(5)	24(6)	–2(5)	95(7)
C(5)	70(5)	108(6)	47(4)	11(4)	5(4)	28(5)
C(6)	84(6)	86(6)	57(4)	–3(4)	–2(4)	31(5)
C(7)	71(5)	110(7)	36(3)	2(4)	10(3)	47(5)
C(8)	105(7)	86(6)	48(4)	–4(4)	4(4)	41(5)
C(9)	107(7)	136(10)	37(4)	–12(5)	–1(4)	69(7)
C(10)	88(6)	107(8)	67(5)	–21(5)	15(5)	38(6)
C(11)	114(8)	97(6)	58(5)	–15(4)	22(5)	43(6)
C(12)	119(7)	116(8)	27(3)	4(4)	–2(4)	64(6)
C(13)	119(8)	214(14)	55(5)	36(7)	–13(5)	50(10)
C(14)	167(13)	187(14)	86(8)	3(9)	–20(9)	3(13)
C(15)	260(20)	141(12)	69(7)	2(7)	6(10)	–38(13)
C(16)	105(8)	200(14)	96(8)	59(9)	–5(7)	–5(10)
C(17)	211(17)	250(20)	146(13)	113(14)	74(13)	147(16)
C(18)	149(12)	195(15)	205(17)	103(13)	79(12)	114(12)
C(19)	131(10)	167(13)	181(15)	–20(12)	53(11)	82(10)
C(20)	229(18)	350(30)	166(14)	87(16)	91(14)	240(20)
C(21)	101(8)	126(9)	82(6)	–34(6)	8(6)	9(7)
C(22)	220(14)	119(8)	64(5)	10(6)	21(7)	99(10)
C(23)	157(10)	126(9)	56(5)	1(6)	8(6)	52(8)
C(24)	65(5)	142(9)	62(5)	2(6)	22(4)	36(7)
C(25)	91(6)	135(8)	29(3)	–18(4)	–8(3)	72(7)
C(26)	120(9)	192(13)	43(4)	13(7)	3(5)	107(10)
C(27)	196(15)	150(12)	39(5)	–1(6)	–21(7)	107(12)
C(28)	169(13)	118(9)	43(5)	2(6)	–23(7)	30(9)
C(29)	111(8)	125(9)	48(5)	–3(5)	–5(5)	44(8)
C(30)	97(7)	136(9)	43(4)	–13(5)	4(4)	68(7)
C(31)	164(14)	530(40)	79(8)	7(15)	22(9)	220(20)
C(32)	240(30)	660(60)	180(30)	–110(30)	–60(20)	310(30)
K(1)	68(1)	78(1)	56(1)	3(1)	6(1)	34(1)
K(2)	82(1)	129(2)	39(1)	1(1)	5(1)	53(1)
K(3)	87(1)	128(2)	42(1)	–5(1)	–2(1)	64(1)
N(1)	68(4)	90(4)	42(3)	20(3)	14(3)	38(4)
N(2)	93(6)	93(5)	82(5)	10(4)	18(4)	31(5)
O(1)	225(16)	107(6)	185(15)	20(6)	39(12)	113(8)
O(2)	85(4)	217(9)	53(3)	29(5)	2(3)	16(5)
O(3)	189(8)	212(8)	95(5)	42(6)	49(6)	156(7)
O(4)	83(8)	184(18)	73(7)	19(13)	9(8)	75(9)

Table 4 Crystal Data and Structural Refinement Details for compounds **6d** and **6e**.

compound	**6d**	**6e**
empirical formula	$C_{23}H_{25}NO$	$C_{16}H_{24}NO$
molecular mass [$g \cdot mol^{-1}$]	331.44	247.37

temperature [K]	173(2)	173(2)
wave length [Å]	0.71073	0.71073
crystal system	orthorhombic	orthorhombic
space group (Nr.)	*Fdd*2 (43)	$Pma2_1$ (33)
a [Å]	39.761(4)	8.3576(10)
b [Å]	30.556(3)	19.611(2)
c [Å]	5.9332(5)	8.8256(9)
cell volume V [$Å^3$]	7208.5(11)	1446.5(3
Z	16	4
calculated density ρ [$g \cdot cm^{-3}$]	1.222	1.136
absorption coefficient μ [mm^{-1}]	0.074	0.070
F(000)	2848	544
crystal size [mm^3]	0.60 x 0.20 x 0.20	0.40 x 0.40 x 0.20
range for data collection 2θ [°]	2.44 – 25.99	2.53 – 26.99
index ranges	–48 < h < 48 –34 < k < 37 –7 < l < 7	–10 < h < 7 –23 < k < 24 –11 < l < 5
reflections collected	9834	5187
independent reflections	3448 [R_{int}=0.0563]	2204 [R_{int} = 0.0389]
refinement method	Full-matrix least-squares on F^2	
data / restraints / parameter	3448/1/232	2204/1/169
goodness-of-fit on F^2	0.843	1.010
final *R*-values [$I > 2\sigma(I)$]	*R*1 = 0.0375 w*R*2 = 0.0344	*R*1 = 0.0369 w*R*2 = 0.0531
R-values (all data)	*R*1 = 0.0881 w*R*2 = 0.0368	*R*1 = 0.0674 w*R*2 = 0.0555
Absolute structure parameter	0.9(13)	–1.1(15)
largest diff. peak and hole [$e \cdot Å^{-3}$]	0.187 and –0.151	0.166 and –0.216

2.) Crystallographic data for compound **8**.

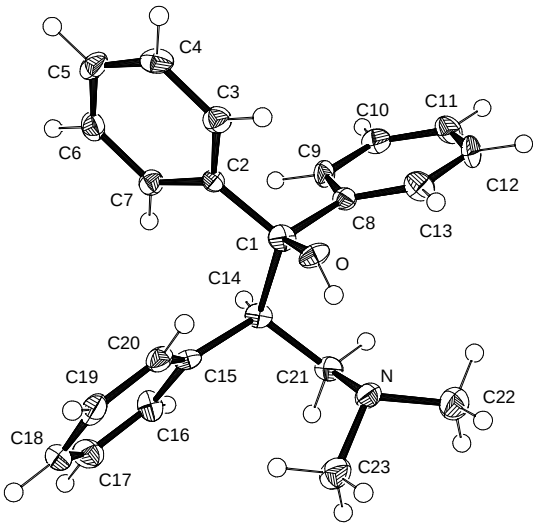


Fig. 2 ORTEP plot of **6d** at 50% probability level.

Table 5 Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters ($Å^2 \cdot 10^3$) for **6d**.

Atom	x	y	z	U(eq)
C(1)	3274(1)	778(1)	5497(4)	20(1)
C(2)	3122(1)	328(1)	5107(4)	17(1)
C(3)	2939(1)	135(1)	6858(4)	22(1)
C(4)	2775(1)	–258(1)	6535(4)	23(1)
C(5)	2793(1)	–470(1)	4471(4)	24(1)
C(6)	2972(1)	–281(1)	2723(4)	24(1)
C(7)	3136(1)	117(1)	3032(4)	20(1)
C(8)	3000(1)	1129(1)	5102(4)	17(1)
C(9)	2833(1)	1148(1)	3028(4)	21(1)
C(10)	2585(1)	1459(1)	2677(4)	25(1)
C(11)	2496(1)	1749(1)	4379(4)	27(1)
C(12)	2658(1)	1722(1)	6407(4)	28(1)
C(13)	2907(1)	1411(1)	6785(5)	26(1)
C(14)	3577(1)	880(1)	3886(4)	16(1)
C(15)	3854(1)	535(1)	3776(4)	22(1)
C(16)	4049(1)	524(1)	1842(4)	23(1)
C(17)	4323(1)	246(1)	1626(4)	30(1)
C(18)	4403(1)	–33(1)	3388(4)	27(1)
C(19)	4207(1)	–34(1)	5313(4)	25(1)
C(20)	3933(1)	244(1)	5508(4)	20(1)
C(21)	3720(1)	1342(1)	4335(4)	21(1)
C(22)	3788(1)	1850(1)	7457(4)	35(1)
C(23)	4208(1)	1293(1)	6849(4)	30(1)
N	3847(1)	1400(1)	6679(3)	22(1)
O	3388(1)	796(1)	7794(2)	19(1)

Table 6 Anisotropic Displacement parameters ($Å^2 \cdot 10^3$) for **6d**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(2)	28(2)	10(2)	–3(2)	4(1)	–4(2)
C(2)	13(2)	15(2)	23(2)	–1(2)	–1(1)	2(1)
C(3)	19(2)	23(2)	25(2)	2(2)	–2(1)	1(2)
C(4)	19(2)	23(2)	28(2)	14(2)	2(2)	0(2)
C(5)	22(2)	14(2)	38(2)	5(2)	–8(2)	–2(2)
C(6)	21(2)	23(2)	28(2)	–7(2)	–4(1)	6(2)
C(7)	22(2)	17(2)	21(2)	2(2)	1(1)	0(1)
C(8)	16(2)	16(2)	19(2)	3(2)	2(1)	0(1)
C(9)	23(2)	22(2)	18(2)	–8(2)	–2(1)	2(1)
C(10)	22(2)	26(2)	26(2)	6(2)	–4(2)	–1(2)
C(11)	20(2)	26(2)	34(2)	1(2)	0(2)	8(2)
C(12)	33(2)	28(2)	25(2)	–12(2)	6(2)	2(2)
C(13)	23(2)	29(2)	24(2)	4(2)	–3(1)	5(2)
C(14)	19(2)	21(2)	7(2)	5(1)	–2(1)	0(1)
C(15)	15(2)	22(2)	29(2)	–5(2)	–3(1)	–6(1)
C(16)	29(2)	22(2)	17(2)	2(2)	3(1)	4(2)
C(17)	26(2)	37(2)	28(2)	–5(2)	6(2)	–3(2)
C(18)	18(2)	24(2)	38(2)	–6(2)	–1(2)	3(2)
C(19)	29(2)	17(2)	30(2)	–3(2)	–6(2)	–2(2)
C(20)	23(2)	20(2)	19(2)	–2(2)	4(1)	–6(2)
C(21)	18(2)	19(2)	25(2)	7(2)	–1(1)	1(1)
C(22)	31(2)	32(2)	41(2)	–11(2)	–6(2)	3(2)
C(23)	28(2)	19(2)	44(2)	3(2)	–8(2)	0(2)
N	19(1)	19(1)	27(1)	–1(1)	–4(1)	–2(1)
O	20(1)	23(1)	14(1)	0(1)	–6(1)	–5(1)

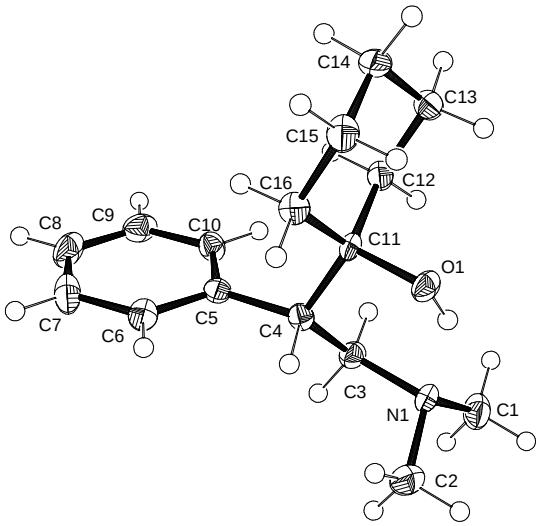


Fig. 3 ORTEP plot of **6e** at 50% probability level.

Table 7 Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters ($Å^2 \cdot 10^3$) for **6e**.

Atom	x	y	z	U(eq)
O(1)	4325(2)	652(1)	7583(2)	22(1)
N(1)	2434(2)	–350(1)	6426(2)	20(1)
C(4)	2762(3)	814(1)	5300(2)	18(1)
C(11)	4363(3)	973(1)	6111(2)	18(1)
C(14)	7500(3)	1672(1)	6406(3)	29(1)
C(3)	2518(3)	46(1)	5021(2)	21(1)
C(13)	7383(3)	912(1)	6105(3)	25(1)
C(10)	3169(3)	1020(1)	2453(3)	23(1)
C(9)	2841(3)	1376(1)	1150(3)	30(1)
C(16)	4501(2)	1736(1)	6408(3)	23(1)
C(12)	5850(3)	728(1)	5261(2)	22(1)
C(5)	2472(3)	1204(1)	3831(3)	21(1)
C(6)	1449(3)	1761(1)	3845(3)	24(1)
C(1)	2608(3)	–1078(1)	6055(3)	32(1)
C(7)	1123(3)	2122(1)	2529(3)	33(1)
C(15)	6035(3)	1923(1)	7239(3)	27(1)
C(2)	901(3)	–251(1)	7186(2)	33(1)
C(8)	1828(3)	1930(1)	1182(3)	35(1)

Table 8 Anisotropic Displacement parameters ($Å^2 \cdot 10^3$) for **6e**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	28(1)	25(1)	14(1)	4(1)	–3(1)	–5(1)
N(1)	24(1)	18(1)	19(1)	6(1)	0(1)	0(1)
C(4)	19(2)	20(1)	16(1)	–1(1)	1(1)	3(1)
C(11)	21(2)	17(1)	16(1)	6(1)	0(1)	1(1)
C(14)	22(2)	31(1)	34(1)	6(1)	–7(2)	–9(1)
C(3)	22(2)	23(1)	19(1)	3(1)	–2(1)	–3(1)
C(13)	21(2)	30(1)	24(1)	4(1)	0(2)	2(1)
C(10)	23(2)	27(1)	20(1)	1(1)	–2(1)	3(1)
C(9)	29(2)	41(1)	20(1)	5(1)	1(2)	–7(1)
C(16)	25(2)	21(1)	22(1)	–3(1)	0(1)	1(1)
C(12)	21(2)	22(1)	21(1)	3(1)	–1(1)	2(1)
C(5)	17(1)	21(1)	24(1)	1(1)	–4(1)	–4(1)
C(6)	28(2)	22(1)	23(1)	–1(1)	–4(1)	–2(1)
C(1)	37(2)	23(1)	36(2)	6(1)	–8(2)	0(1)
C(7)	38(2)	24(1)	38(2)	4(2)	–13(2)	5(1)

C(15)	33(2)	21(1)	29(2)	–2(1)	–9(1)	–3(1)
C(2)	30(2)	34(2)	33(2)	6(1)	8(2)	0(1)
C(8)	41(2)	37(2)	26(2)	14(2)	–10(2)	–8(1)

Table 9 Crystal Data and Structural Refinement Details for compounds **8** and **9**.

compound	**8**	**9**
empirical formula	$C_{16}H_{28}LiN_3$	$C_{18}H_{28}KNO_2$
molecular mass [g·mol^{-1}]	269.35	329.51
temperature [K]	173(2)	173(2)
wave length [Å]	0.71073	0.71073
crystal system	monoclinic	triklin
space group (Nr.)	$P2_1/c$	$P1$ (1)
a [Å]	11.9709(7)	9.5449(6)
b [Å]	8.4897(5)	9.8534(5)
c [Å]	16.7872(11)	11.6027(6)
α [°]		81.047(5)
β [°]	104.660(6)	74.192(5)
γ [°]		61.176(6)
cell volume V [Å^3]	1650.54(17)	919.49(9)
Z	4	2
calculated density ρ [g·cm^{-3}]	1.084	1.161
absorption coefficient μ [mm^{-1}]	0.064	0.295
F(000)	592	340
crystal size [mm^3]	0.30 x 0.30 x 0.20	0.50 x 0.40 x 0.30
range for data collection 2θ [°]	2.51 – 26.99	2.36 – 27.00
index ranges	$-15 \le h \le 15$	$-12 \le h \le 12$
	$-10 \le k \le 10$	$-12 \le k \le 12$
	$-21 \le l \le 21$	$-14 \le l \le 14$
reflections collected	21704	14339
independent reflections	3599 (R_{int} = 0.0535)	7893 (R_{int} = 0.0320)
refinement method	Full-matrix least-squares on F^2	
data / restraints / parameter	3599 / 0 / 198	7893 / 3 / 431
goodness-of-fit on F^2	1.000	1.004
final R-values [$I > 2\sigma(I)$]	$R1$ = 0.0435 $wR2$ = 0.0764	$R1$ = 0.0432 w$R2$ = 0.0613
R-values (all data)	$R1$ = 0.0933 $wR2$ = 0.0813	$R1$ = 0.0853 w$R2$ = 0.0645
Absolute structure parameter		–0.03(3)
largest diff. peak and hole [e·Å^{-3}]	0.161 and –0.199	0.336 and –0.231

2.) Crystallographic data for compound **8**.

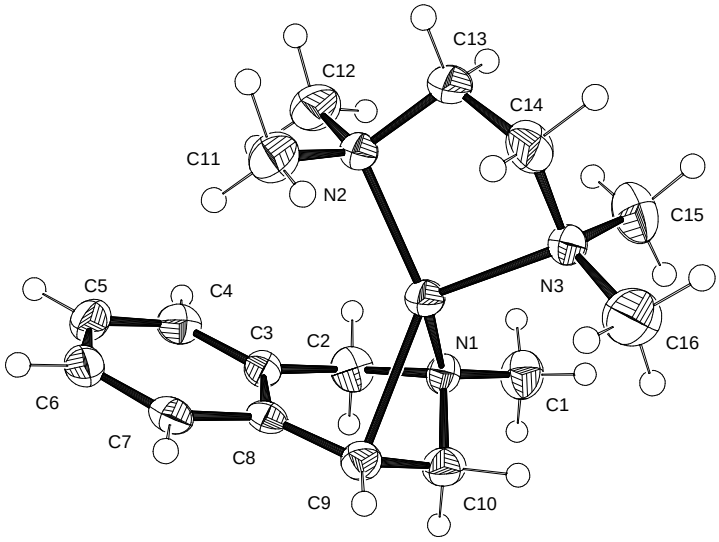


Fig. 4 ORTEP plot of **8** at 50% probability level

Table 10 Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters ($Å^2 \cdot 10^3$) for **8**.

Atom	x	y	z	U(eq)
Li	2193(2)	1969(3)	1406(1)	28(1)
C(1)	3899(1)	831(2)	3134(1)	43(1)
N(1)	3229(1)	516(1)	2294(1)	27(1)
C(2)	3891(1)	–527(2)	1885(1)	35(1)
N(2)	2588(1)	3283(1)	479(1)	28(1)
C(3)	3230(1)	–902(2)	1018(1)	26(1)
N(3)	1603(1)	4032(1)	1851(1)	28(1)
C(4)	3798(1)	–1234(2)	418(1)	34(1)
C(5)	3220(1)	–1568(2)	–384(1)	37(1)
C(6)	2021(1)	–1552(2)	–583(1)	35(1)
C(7)	1428(1)	–1222(2)	0(1)	30(1)
C(8)	1997(1)	–861(2)	828(1)	25(1)
C(9)	1434(1)	–421(2)	1431(1)	29(1)
C(10)	2125(1)	–264(2)	2295(1)	33(1)
C(11)	1761(1)	2906(2)	–297(1)	44(1)
C(12)	3761(1)	3073(2)	386(1)	46(1)
C(13)	2440(1)	4916(2)	728(1)	46(1)
C(14)	1456(1)	5055(2)	1129(1)	43(1)
C(15)	2521(1)	4640(2)	2524(1)	53(1)
C(16)	535(1)	4003(2)	2116(1)	60(1)

Table 11 Anisotropic Displacement parameters ($Å^2 \cdot 10^3$) for **8**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Li	33(1)	24(1)	29(1)	2(1)	10(1)	0(1)
C(1)	47(1)	46(1)	32(1)	1(1)	4(1)	4(1)
N(1)	28(1)	30(1)	21(1)	–1(1)	5(1)	2(1)
C(2)	29(1)	34(1)	41(1)	1(1)	6(1)	10(1)
N(2)	35(1)	24(1)	30(1)	–1(1)	13(1)	–1(1)
C(3)	31(1)	21(1)	28(1)	3(1)	8(1)	5(1)
N(3)	30(1)	26(1)	31(1)	–2(1)	12(1)	–1(1)
C(4)	31(1)	29(1)	43(1)	3(1)	12(1)	5(1)
C(5)	49(1)	33(1)	36(1)	0(1)	22(1)	3(1)
C(6)	51(1)	27(1)	26(1)	1(1)	7(1)	–4(1)
C(7)	31(1)	22(1)	34(1)	1(1)	5(1)	–4(1)
C(8)	30(1)	14(1)	31(1)	4(1)	7(1)	1(1)

C(9)	27(1)	29(1)	31(1)	–1(1)	8(1)	–1(1)
C(10)	36(1)	29(1)	38(1)	4(1)	14(1)	1(1)
C(11)	56(1)	42(1)	33(1)	6(1)	10(1)	2(1)
C(12)	44(1)	50(1)	52(1)	0(1)	25(1)	–5(1)
C(13)	77(1)	23(1)	47(1)	3(1)	34(1)	–1(1)
C(14)	58(1)	26(1)	45(1)	2(1)	16(1)	14(1)
C(15)	60(1)	48(1)	47(1)	–14(1)	6(1)	2(1)
C(16)	53(1)	52(1)	90(1)	–7(1)	45(1)	1(1)

3.) Crystallographic data for compound **9**.

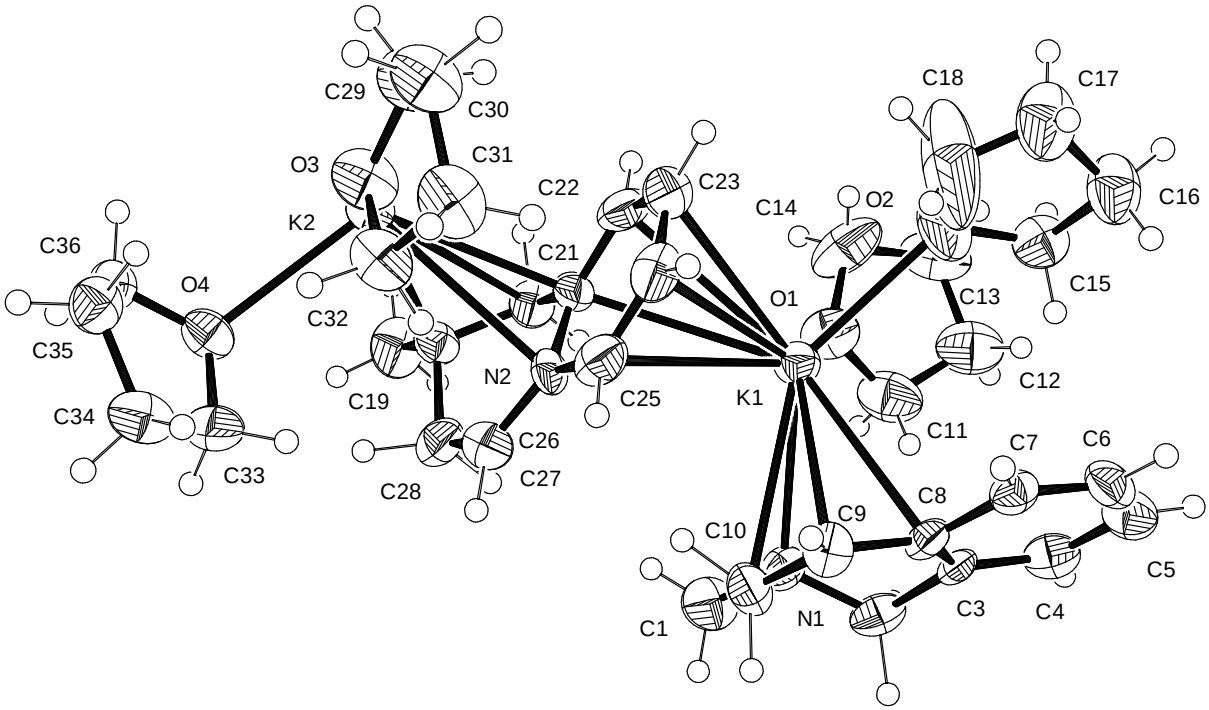


Fig. 5 ORTEP plot of **9** at 50% probability level.

Table 12 Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters ($Å^2 \cdot 10^3$) for **9**.

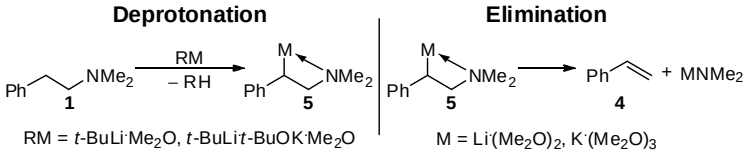
Atom	x	y	z	U(eq)
C(1)	–3486(4)	5404(4)	5559(3)	60(1)
K(1)	–337(1)	6876(1)	3960(1)	41(1)
N(1)	–2116(3)	5558(3)	5734(2)	39(1)
O(1)	–3141(3)	9555(2)	4109(2)	59(1)
C(2)	–2423(4)	6050(4)	6950(3)	46(1)
K(2)	752(1)	4352(1)	–826(1)	37(1)
N(2)	–2315(3)	5388(3)	822(2)	39(1)
O(2)	941(3)	8801(3)	3905(2)	75(1)
C(3)	–1037(3)	6331(3)	7056(2)	29(1)
O(3)	3986(2)	2457(2)	–932(2)	53(1)
C(4)	–1278(4)	7454(4)	7759(3)	45(1)
O(4)	443(2)	1815(2)	–992(2)	47(1)
C(5)	–39(5)	7660(4)	7909(3)	51(1)
C(6)	1544(4)	6711(4)	7302(3)	47(1)
C(7)	1899(4)	5561(3)	6575(3)	39(1)
C(8)	574(4)	5304(3)	6426(3)	36(1)
C(9)	806(4)	4190(4)	5704(3)	44(1)
C(10)	–614(5)	4080(4)	5526(3)	45(1)
C(11)	–4096(4)	9966(4)	5263(3)	70(1)
C(12)	–4226(5)	11435(4)	5525(3)	71(1)

Table 13 Anisotropic Displacement parameters ($Å^2 \cdot 10^3$) for **9**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	56(2)	82(3)	62(2)	3(2)	–21(2)	–44(2)
K(1)	51(1)	39(1)	36(1)	–3(1)	–7(1)	–23(1)
N(1)	39(2)	45(2)	36(2)	–1(1)	–12(1)	–20(1)
O(1)	66(2)	44(1)	49(2)	–4(1)	–3(1)	–16(1)
C(2)	49(2)	50(2)	34(2)	–1(2)	1(2)	–24(2)
K(2)	33(1)	35(1)	37(1)	–6(1)	–4(1)	–13(1)
N(2)	36(2)	41(2)	40(2)	–7(1)	–4(1)	–17(1)
O(2)	65(2)	104(2)	79(2)	–45(2)	9(2)	–59(2)
C(3)	37(2)	32(2)	16(2)	0(1)	–5(1)	–16(2)
O(3)	38(1)	59(2)	61(2)	–5(1)	–13(1)	–20(1)
C(4)	49(2)	39(2)	39(2)	3(2)	–12(2)	–14(2)
O(4)	53(2)	38(1)	52(2)	–7(1)	–10(1)	–21(1)
C(5)	63(3)	46(2)	52(2)	–4(2)	–19(2)	–28(2)
C(6)	44(2)	51(2)	53(3)	4(2)	–13(2)	–29(2)
C(7)	45(2)	36(2)	33(2)	3(2)	–11(2)	–16(2)
C(8)	51(3)	29(2)	26(2)	–1(2)	–9(2)	–17(2)
C(9)	40(2)	39(2)	42(2)	1(2)	–9(2)	–11(2)
C(10)	54(3)	47(2)	46(2)	–5(2)	–18(2)	–27(2)
C(11)	73(3)	53(2)	79(3)	–2(2)	–2(2)	–32(2)
C(12)	61(3)	71(3)	73(3)	3(2)	–10(2)	–28(2)

Computational Details

If not otherwise mentioned, all calculations were performed without symmetry restrictions. Starting coordinates were obtained with Chem3D Ultra 10.0, optimisation and frequency analyses were conducted with Gaussian *03* Revision B.04 at the M052X/6-31+G(d) level or, in selected cases at the B3LYP/6-31+G(d) level for comparative purposes (indicated by a * in the Table below).[v] Harmonic vibrational frequency analyses (to establish the nature of stationary points on the potential energy surface) were performed on the same level. Table 6 lists the total (SCF) and zero-point energies (ZPE) of all compounds in Hartree and, in addition, the relative energies of the respective reaction species (starting material, transition state and product; ZPE differences) for ease of comparison. The vibrational frequency of all compounds analyses showed no imaginary frequencies for ground state structures and exactly one imaginary frequence for transition states.



Scheme 1 Computed reaction pathways

Table 14 SCF and Zero-Point-Energies for the computed compounds. [* designates the respective B3LYP energies].

Structure	Properties	E_{rel} (kJ·mol^{-1})	SCF Energy	Zero-Point Energy
	Deprotonation			
[**1**·*t*-BuLi]	starting material	0	–610.118760132	–609.771404
[**1**·*t*-BuLi]	transition state	+83	–610.093353578	–609.739670
[**1**·*t*-BuLi]	product	–59	–610.153144546	–609.793857
[**1**·*t*-BuLi]*	starting material	0	–610.224996102	–609.873100
[**1**·*t*-BuLi]*	transition state	+91	–610.190347108	–609.843494
[**1**·*t*-BuLi]*	product	–67	–610.250463641	–609.898000
[**1**·*t*-BuK]	starting material	0	–1202.45091362	–1202.095217
[**1**·*t*-BuK]	transition state	+34	–1202.43369158	–1202.082182
[**1**·*t*-BuK]	product	–96	–1202.48805081	–1202.131653
[**1**·*t*-BuK]*	starting material	0	–1202.57357058	–1202.224554
[**1**·*t*-BuK]*	transition state	+48	–1202.55521376	–1202.210109
[**1**·*t*-BuK]*	product	–96	–1202.61024361	–1202.261102
[**1**·*t*-BuLi·Me_2O]	starting material	0	–765.147427767	–764.705185
[**1**·*t*-BuLi·Me_2O]	transition state	+73	–765.114557611	–764.677246
[**1**·*t*-BuLi·Me_2O]	product	–77	–765.176311806	–764.734606
[**1**·*t*-BuK·Me_2O]	starting material	0	–1357.46497339	–1357.027354
[**1**·*t*-BuK·Me_2O]	transition state	+36	–1357.44880654	–1357.013778
[**1**·*t*-BuK·Me_2O]	product	–97	–1357.50360018	–1357.064245
[**1**·*t*-BuK·$(Me_2O)_2$]	starting material	0	–1512.47004582	–1511.949579
[**1**·*t*-BuK·$(Me_2O)_2$]	transition state	+20	–1512.45934995	–1511.941824
[**1**·*t*-BuK·$(Me_2O)_2$]	product	–116	–1512.51556154	–1511.993631
[**1**·*t*-BuLi·*t*-BuOK]	starting material	0	–1443.12766261	–1442.641920
[**1**·*t*-BuLi·*t*-BuOK]	transition state	+40	–1443.10886345	–1442.626847
[**1**·*t*-BuLi·*t*-BuOK]	product	–105	–1443.16886642	–1442.682440
[**1**·*t*-BuLi·*t*-BuOK·Me_2O]	starting material	0	–1598.14009170	–1597.571256
[**1**·*t*-BuLi·*t*-BuOK·Me_2O]	transition state	+42	–1598.10778023	–1597.543084

[**1**·*t*-BuLi·*t*-BuOK·Me_2O]	product	–87	–1598.18133949	–1597.612333
	Elimination			
[**5**-Li]	starting material	0	–451.704827240	–451.481009
[**5**-Li]	transition state	+27	–451.690441069	–451.470547
[**5**-Li]	product	+10	–451.696139284	–451.477024
[**5**-Li]*	starting material	0	–451.781794936	–451.561987
[**5**-Li]*	transition state	+44	–451.764874499	–451.548383
[**5**-Li]*	product	+26	–451.771927139	–451.556767
[**5**-K]	starting material	0	–1044.05920318	–1043.837952
[**5**-K]	transition state	+81	–1044.02414243	–1043.807026
[**5**-K]	product	+71	–1044.02771886	–1043.810762
[**5**-K]*	starting material	0	–1044.13488318	–1043.921562
[**5**-K]*	transition state	+53	–1044.12567778	–1043.912064
[**5**-K]*	product	+51	–1044.12666579	–1043.914256
[**5**-Li·$(Me_2O)_2$]	starting material	0	–761.762787974	–761.372262
[**5**-Li·$(Me_2O)_2$]	transition state	+67	–761.734617073	–761.346776
[**5**-Li·$(Me_2O)_2$]	product	+52	–761.738435272	–761.352338
[**5**-K·$(Me_2O)_2$]	starting material	0	–1354.08805198	–1353.701016
[**5**-K·$(Me_2O)_2$]	transition state	+85	–1354.05162367	–1353.668544
[**5**-K·$(Me_2O)_2$]	product	+74	–1354.05649822	–1353.672963
[**5**-K·$(Me_2O)_3$]	starting material	0	–1509.09738968	–1508.627148
[**5**-K·$(Me_2O)_3$]	transition state	+87	–1509.06027423	–1508.594142
[**5**-K·$(Me_2O)_3$]	product	+73	–1509.06576641	–1508.599445
1 (*β*-anion)	starting material	0	–444.170539101	–443.951915
1 (*β*-anion)	transition state	+119	–444.119448481	–443.906768
1 (*β*-anion)	product	+92	–444.130745925	–443.917011
1 (*β*-anion)*	starting material	0	–444.240239182	–444.025974
1 (*β*-anion)*	transition state		(*no transition state found using B3LYP*)	
1 (*β*-anion)*	product	+56	–444.213881207	–444.004598

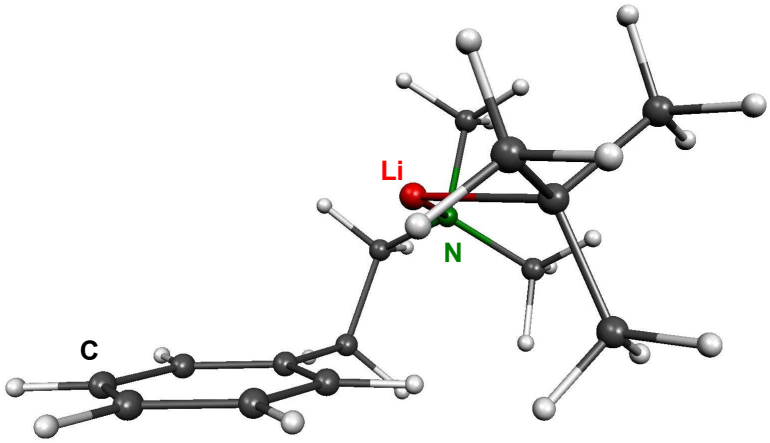


Fig. 6 Molekel plot of [**1**·*t*-BuLi] (starting material)

Table 15 Cartesian coordinates of [**1**·*t*-BuLi] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–2.35948900	1.45496300	–0.28438000
C	–3.49762800	0.71377800	0.01544400
C	–3.34716800	–0.65784200	0.24602500
C	–2.09875100	–1.25562100	0.18780500
C	–0.92070800	–0.52432000	–0.10296500

C	–1.10165500	0.85540200	–0.34324000
C	0.36421900	–1.21403700	–0.13567500
C	1.57849900	–0.56894500	–0.75917700
Li	1.61586100	–1.26078900	1.47415700
N	2.57737700	–0.05476900	0.26738800
C	3.90477100	0.08431700	–0.32305900
C	2.13687200	1.24195700	0.79096800
H	–2.44433100	2.51806400	–0.48329500
H	–4.47241900	1.18265100	0.06245600
H	–4.21635600	–1.26647700	0.47136500
H	–2.00795900	–2.32180900	0.37250200
H	–0.25313700	1.47691700	–0.60240700
H	0.25370500	–2.25445000	–0.43884100
H	2.13316300	–1.31330500	–1.33671300
H	1.35261700	0.27061900	–1.43895300
H	4.60520900	0.46428000	0.42262500
H	3.89036300	0.77931700	–1.17503900
H	4.25775300	–0.88639300	–0.67234900
H	2.83004300	1.58646300	1.56130300
H	2.09346800	1.99790800	–0.00684000
H	1.13488700	1.15404300	1.21952500

Table 16 Cartesian coordinates of [**1**·*t*-BuLi] (starting material) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	4.65827500	–0.13930700	0.27157900
C	4.65074300	–1.39188000	–0.34870400
C	3.43265400	–2.02539500	–0.61007400
C	2.22987900	–1.40789100	–0.25677500
C	2.22473300	–0.14972100	0.36319900
C	3.45355800	0.47404900	0.62480300
C	0.91799400	0.53309900	0.71730200
C	0.45100500	1.46873500	–0.41349100
Li	–2.21730700	0.50760300	0.06881900
C	–3.37769400	–1.17117500	0.10329900
C	–2.52203800	–2.43454900	–0.08286800
C	–4.14141900	–1.31121100	1.42930300
C	–4.41124600	–1.13272400	–1.03402200
N	–0.89959200	2.05123600	–0.20386000
C	–0.92175900	2.97990600	0.94297300
C	–1.31994600	2.76880000	–1.42483200
H	5.60098300	0.35754900	0.48698000
H	5.58676200	–1.87331000	–0.61977000
H	3.41673800	–3.00403100	–1.08299100
H	1.28657800	–1.91357100	–0.45408300
H	3.46936200	1.44475500	1.11761600
H	1.04432900	1.09821000	1.64799600
H	0.14614200	–0.22615500	0.90387100
H	0.41487800	0.89868700	–1.34877900
H	1.18984400	2.27659600	–0.55778500
H	–3.13959500	–3.36389800	–0.08385500
H	–1.97104800	–2.43285700	–1.03738100
H	–1.77962400	–2.56240400	0.72138100
H	–4.78132500	–2.22505700	1.44951000
H	–4.81477400	–0.46022000	1.61818700
H	–3.46728300	–1.38857600	2.29698500
H	–5.05477900	–2.04425100	–1.04638100
H	–5.09656000	–0.27430600	–0.95058500
H	–3.94142900	–1.07557700	–2.02902400
H	–0.19364200	3.79885200	0.81463200
H	–0.69277800	2.45086400	1.87115300

H	–1.92055500	3.41729600	1.03792600
H	–0.63622100	3.59998200	–1.66544800
H	–1.33936200	2.07815400	–2.27361500
H	–2.32601300	3.17738500	–1.28612200

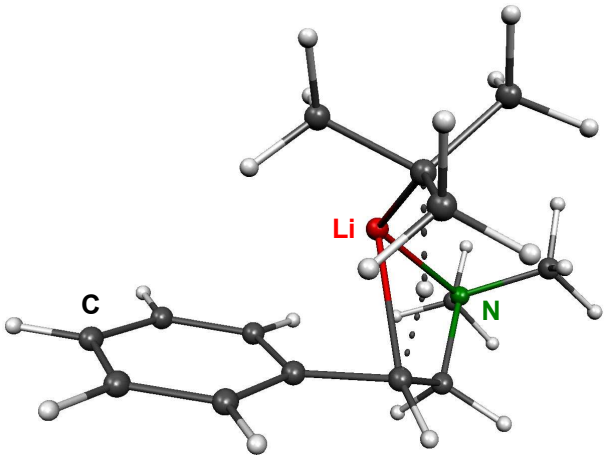


Fig. 7 Molekel plot of [**1**·*t*-BuLi] (transition state)

Table 17 Cartesian coordinates of [**1**·*t*-BuLi] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	2.24192700	1.52773500	0.14614600
C	3.39628100	0.89826400	–0.30859100
C	3.39425000	–0.48936500	–0.47236800
C	2.25701200	–1.23147200	–0.18792200
C	1.08137500	–0.61596600	0.28487700
C	1.09684600	0.78637400	0.43598900
C	–0.12491000	–1.41531100	0.52537100
C	–1.27956000	–0.90997000	1.05440300
Li	–0.86229600	–0.05669100	–1.01700200
N	–2.56710100	0.33626800	–0.53522200
C	–3.66205400	–0.57995200	–0.73212000
C	–3.02961100	1.49147600	0.18626700
H	2.22572400	2.60284900	0.27885900
H	4.28382600	1.47541800	–0.53412800
H	4.28622300	–0.99314900	–0.82505900
H	2.26707800	–2.30816300	–0.31691700
H	0.21694800	1.30423500	0.80540300
H	–0.10167700	–2.44401500	0.18039900
H	–2.13541100	–1.55538100	1.20037500
H	–1.30060700	0.02404800	1.60262100
H	–4.43801800	–0.16800600	–1.39868200
H	–4.17418600	–0.84266900	0.21495700
H	–3.31099600	–1.51484900	–1.18467900
H	–3.84533400	2.01697100	–0.33780700
H	–3.42568400	1.23198100	1.18951600
H	–2.22062200	2.21605300	0.33040000

Table 18 Cartesian coordinates of [**1**·*t*-BuLi] (transition state) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	3.75687900	–0.25672400	–1.00767300
C	4.20033800	–0.41179700	0.31046000
C	3.25428200	–0.65100900	1.31245100
C	1.89528400	–0.73034400	1.00368200
C	1.42214400	–0.58422400	–0.32111700
C	2.39912100	–0.34673400	–1.31429500

C	–0.02462200	–0.58605500	–0.66236600
C	–0.81210800	–1.76756200	–0.08375300
Li	–1.85781500	0.38260600	0.63787300
N	–2.27956700	–1.48012300	0.09511000
C	–2.95545600	–1.42152400	–1.21472300
C	–2.91521900	–2.50548100	0.93575000
H	4.47448000	–0.07332200	–1.80491200
H	5.25829100	–0.34810500	0.55136600
H	3.57532000	–0.76927100	2.34557400
H	1.18869500	–0.89611300	1.81591200
H	2.07684100	–0.23144200	–2.34791300
H	–0.13638300	–0.56464500	–1.75440600
H	–0.43189700	–2.02573200	0.91065900
H	–0.71714700	–2.68397600	–0.69967500
H	–0.50393100	0.72486900	–0.29630300
H	–2.87721700	–2.38387700	–1.74876500
H	–2.50165600	–0.64598700	–1.83758700
H	–4.01546400	–1.18376000	–1.07594800
H	–2.82871400	–3.51107100	0.49058500
H	–2.44113400	–2.52476000	1.92251600
H	–3.97797500	–2.27406500	1.06423500
C	–1.00365800	2.12818000	0.10057800
C	–0.95323000	2.35541100	1.61786600
C	0.06049400	2.96406600	–0.59904600
C	–2.39744900	2.48452500	–0.43447100
H	–1.22371400	3.38961200	1.90822700
H	–1.66434000	1.72146400	2.19793700
H	0.04564300	2.14910200	2.02195700
H	–0.08728600	4.05061400	–0.44388300
H	0.05315600	2.79103900	–1.68423600
H	1.06678800	2.71576000	–0.23929700
H	–2.67762800	3.53688700	–0.23008800
H	–2.46366900	2.33699600	–1.52110100
H	–3.22145100	1.88845000	0.01568600

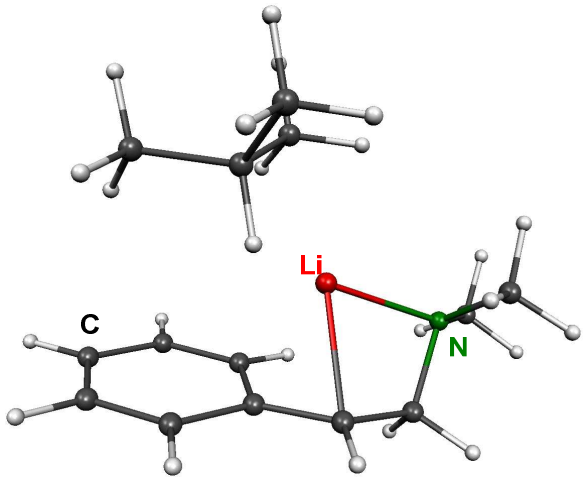


Fig. 8 Molekel plot of [**5**-Li] (product)

Table 19 Cartesian coordinates of [**1**·*t*-BuLi] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	1.42685800	–1.24286500	–1.08094700
C	2.20145200	–1.59730800	0.02829700
C	2.44559900	–0.65214100	1.02738400
C	1.91088700	0.63430100	0.92160400
C	1.10564800	0.99103500	–0.17003500
C	0.88531100	0.03895200	–1.17812100

C	0.42561700	2.30294100	–0.20673800
C	–0.86698400	2.41717500	–0.52176100
Li	–0.16268700	–0.88145000	0.73197700
N	–1.92218300	–0.79684400	0.40551100
C	–2.95969300	–0.25986500	1.24398400
C	–2.51136000	–1.23924500	–0.82874500
H	1.22640900	–1.96974500	–1.85784000
H	2.60893400	–2.59659600	0.11135100
H	3.04306100	–0.91727900	1.89062300
H	2.08361600	1.35766000	1.70996700
H	0.25928900	0.30301600	–2.02048100
H	1.00943000	3.17055500	0.08538600
H	–1.35387500	3.38450800	–0.52440000
H	–1.46878200	1.53360600	–0.71810500
H	–3.75088900	–0.99774600	1.48294000
H	–3.48585300	0.60055800	0.77680700
H	–2.55327000	0.09593900	2.19761700
H	–3.27836600	–2.02664500	–0.69139200
H	–3.02460300	–0.42049700	–1.38110500
H	–1.75176500	–1.65294900	–1.50540800

Table 20 Cartesian coordinates of [**1**·*t*-BuLi] (product) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	–1.63875000	2.66444500	–0.58478400
C	–1.79616300	2.58100200	0.81890900
C	–0.76841100	2.00658800	1.55736600
C	0.38365300	1.49355400	0.93507900
C	0.57225500	1.56549000	–0.49298300
C	–0.51142100	2.17840000	–1.21680100
C	1.67350400	0.95950800	–1.15882400
C	2.89194300	0.51428500	–0.40710900
Li	0.74384200	–0.52698200	0.01966200
N	2.72924400	–0.88778600	0.18464000
C	3.04721300	–1.90118000	–0.83143700
C	3.56273300	–1.08750300	1.37497800
H	–2.41918900	3.13142300	–1.18360400
H	–2.68505800	2.97411200	1.30388000
H	–0.84200000	1.95628300	2.64278700
H	1.19905600	1.14870300	1.57300900
H	–0.41612500	2.27056100	–2.29739400
H	1.75947500	1.10484400	–2.23213200
H	3.11646500	1.16522300	0.45180400
H	3.78579700	0.51418300	–1.05028300
H	4.11500400	–1.87217200	–1.11467000
H	2.45050800	–1.71393200	–1.73070400
H	2.81624100	–2.90407400	–0.45393500
H	4.63897200	–0.98683200	1.14992900
H	3.30158500	–0.34916900	2.14012700
H	3.39072600	–2.08845100	1.78648600
C	–2.59401700	–1.46874700	0.01032200
C	–3.30346600	–2.10160200	1.21633500
C	–3.45767200	–1.55604600	–1.25651700
C	–1.22438700	–2.12796100	–0.22276300
H	–3.49627200	–3.16987100	1.04526500
H	–2.70207000	–2.01048800	2.12973900
H	–4.26788200	–1.61478200	1.40443800
H	–3.65866900	–2.60225200	–1.52621900
H	–2.96451000	–1.07543200	–2.11013000
H	–4.42341500	–1.05870500	–1.10714700

H	–1.32502500	–3.19294100	–0.46915000
H	–0.70192200	–1.66338400	–1.07454000
H	–0.60428300	–2.08290400	0.68783500
H	–2.42572200	–0.40590200	0.23251600

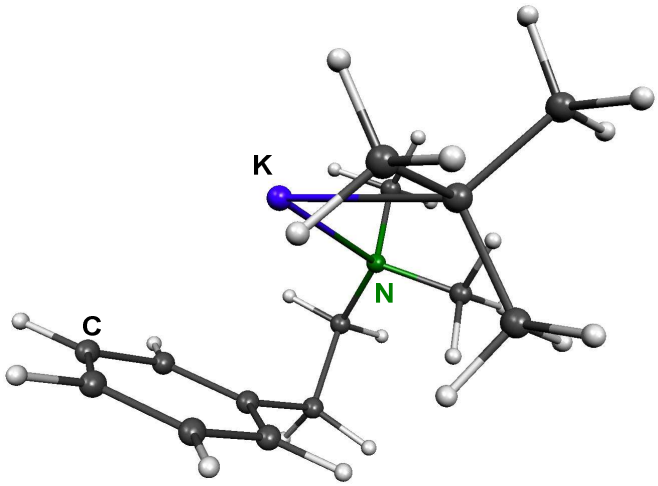


Fig. 9 Molekel plot of [**1**·*t*-BuK] (starting material)

Table 21 Cartesian coordinates of [**1**·*t*-BuK] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	2.16970900	–2.38477600	–0.92619100
C	1.09340900	–3.02714400	–0.30865800
C	0.50580500	–2.45206800	0.81634000
C	0.98938500	–1.24187800	1.31701400
C	2.06151800	–0.58658900	0.70587800
C	2.64732800	–1.17663300	–0.42131200
C	2.56476300	0.73877900	1.22850100
C	2.33860300	1.89559900	0.24643700
K	–0.46652000	–0.23818400	–1.31389700
C	–2.88600300	–0.02350900	0.09175800
C	–3.44244400	–1.34937000	–0.41994000
C	–2.76756000	–0.14395800	1.60347000
C	–3.92475400	1.04932100	–0.19818900
N	0.96064600	2.00849400	–0.22228200
C	0.03730500	2.31854400	0.86964500
C	0.87247500	3.05214100	–1.23815800
H	2.64366000	–2.83166400	–1.79193200
H	0.72294800	–3.96791300	–0.69660100
H	–0.33668000	–2.93139800	1.29917300
H	0.51420500	–0.80085300	2.18557900
H	3.49105500	–0.69219800	–0.90177600
H	3.64028700	0.67615700	1.41873400
H	2.09322900	0.95576000	2.18849000
H	2.97136900	1.74301000	–0.63307500
H	2.66749600	2.83543100	0.72348500
H	–4.41855100	–1.60594200	0.05829400
H	–3.63116400	–1.33771500	–1.50263200
H	–2.77405900	–2.19986600	–0.21185600
H	–3.75191300	–0.37343700	2.07867600
H	–2.41114700	0.78281100	2.07205900
H	–2.08630600	–0.94991200	1.91259000
H	–4.12398400	1.16161900	–1.27113600
H	–3.62193800	2.03434000	0.18010600
H	–4.90574200	0.81708700	0.28312800

H	0.30276400	3.26878100	1.36168200
H	0.04021600	1.52078000	1.60999400
H	–0.97974200	2.37685200	0.47876000
H	1.15771000	4.03970700	–0.84095600
H	1.53240800	2.81460300	–2.07558500
H	–0.15399600	3.11924200	–1.60475400

Table 22 Cartesian coordinates of [**1**·*t*-BuK] (starting material) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	4.60464700	–1.36177800	–1.23154300
C	5.49174800	–1.29208200	–0.15373000
C	5.04073900	–0.81496900	1.08006700
C	3.71228300	–0.40923100	1.23200000
C	2.81226300	–0.47017300	0.15778900
C	3.27767300	–0.95373200	–1.07394700
C	1.38206000	0.00568400	0.31646900
C	1.24268900	1.50228200	–0.01873700
K	–2.24240400	0.38078700	–1.41067900
C	–4.01805100	–1.13443200	0.20413400
C	–3.52124800	–1.05871700	1.64657300
C	–5.44585200	–0.59449900	0.14387200
C	–4.02075800	–2.59636900	–0.24093800
N	–0.14141000	2.00867800	0.02527200
C	–0.68417900	2.01004100	1.39120500
C	–0.18893300	3.36685900	–0.52828700
H	4.94295600	–1.73991700	–2.19308900
H	6.52334800	–1.61310400	–0.27246000
H	5.72060800	–0.76444100	1.92692300
H	3.36796600	–0.04827900	2.19943500
H	2.59210000	–1.02109800	–1.91713700
H	1.04776100	–0.18588400	1.34176000
H	0.72263200	–0.57216900	–0.34505900
H	1.62059900	1.66782500	–1.03495400
H	1.89184400	2.08888300	0.65972000
H	–4.16263400	–1.65754900	2.34207700
H	–2.49902100	–1.45232600	1.76518500
H	–3.52479200	–0.03083700	2.04226800
H	–6.13990700	–1.17552600	0.80297300
H	–5.87297400	–0.64464600	–0.86913400
H	–5.51636800	0.45313000	0.47499400
H	–4.67956100	–3.22831100	0.40740800
H	–4.39167300	–2.72412200	–1.26922700
H	–3.02058100	–3.05476400	–0.19637700
H	–0.06953600	2.61895200	2.08035800
H	–0.74924500	0.99338900	1.78555800
H	–1.69774000	2.42431800	1.38204400
H	0.42644400	4.08081900	0.05030800
H	0.17447100	3.36280100	–1.56188800
H	–1.22163600	3.73384900	–0.52526000

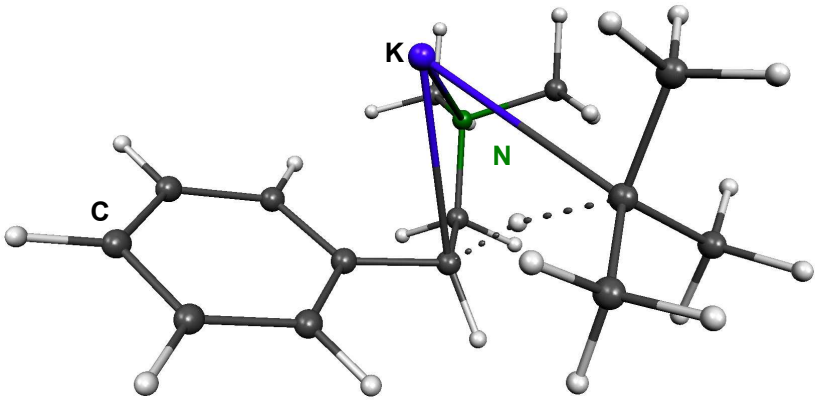


Fig. 10 Molekel plot of [**1**·*t*-BuK] (transition state)

Table 23 Cartesian coordinates of [**1**·*t*-BuK] (transition state) [M052X/6-31+G(d)]

a

atom	X	Y	Z
C	–3.41425900	0.42751500	0.44636400
C	–3.85191200	–0.89182000	0.35990100
C	–3.05279000	–1.81497700	–0.32133600
C	–1.84454200	–1.42916900	–0.88769600
C	–1.37440100	–0.09752700	–0.81376600
C	–2.20158800	0.81848800	–0.12438400
C	–0.02459800	0.23535300	–1.30869400
C	0.29880400	1.71920100	–1.35283200
K	0.09584500	–0.03948800	1.62140200
C	1.98033500	–1.52653600	–0.06910200
C	2.61134400	–1.67078100	1.31643500
C	1.37634200	–2.86952500	–0.46271500
C	3.08720000	–1.20800100	–1.06728900
N	0.67314400	2.27281600	–0.02583500
C	2.09200200	2.03671500	0.22506900
C	0.41233000	3.70620600	0.02511300
H	–4.02410200	1.16794700	0.95250400
H	–4.79365400	–1.19366600	0.80071700
H	–3.37630900	–2.84571500	–0.41230500
H	–1.23992700	–2.16233900	–1.40784200
H	–1.89744600	1.85471500	–0.03873500
H	0.15653500	–0.23492200	–2.27874400
H	0.89068800	–0.47916700	–0.59776200
H	–0.56050100	2.30158200	–1.70813500
H	1.11847800	1.90785100	–2.06284600
H	3.43155900	–2.41399700	1.32039300
H	3.05397600	–0.73365200	1.68555900
H	1.89931800	–2.03327200	2.07540300
H	2.13931600	–3.67118300	–0.48545000
H	0.93812400	–2.82682500	–1.46674600
H	0.58737700	–3.19685800	0.22592200
H	3.68089200	–0.33285900	–0.77846800
H	2.67912300	–1.00938700	–2.06663100
H	3.79740700	–2.04865200	–1.17084600
H	2.72842900	2.57602100	–0.49545400
H	2.30765200	0.97286400	0.13107500
H	2.35657200	2.37775900	1.23103300
H	0.96018800	4.25134400	–0.76047500
H	–0.65421500	3.89970100	–0.10289500
H	0.72184900	4.10242500	0.99452900

Table 24 Cartesian coordinates of [**1**·*t*-BuK] (transition state) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	–3.41490700	0.62417100	0.59443200
C	–4.03016400	–0.60550600	0.35356600
C	–3.35809100	–1.54272900	–0.44808500
C	–2.10497600	–1.25847400	–0.98048000
C	–1.44794900	–0.01951900	–0.75141900
C	–2.15189500	0.91221600	0.05975800
C	–0.07601900	0.20488300	–1.25918100
C	0.36409300	1.66739200	–1.35649300
K	0.24637400	0.04297600	1.69145600
C	1.86367800	–1.71083800	–0.06134500
C	2.75675700	–1.66584900	1.18762300
C	1.03873500	–3.00034600	–0.02179900
C	2.76482400	–1.74079400	–1.29530300
N	0.97483600	2.22355500	–0.10499900
C	2.41831400	1.96157400	–0.08225800
C	0.73977500	3.66532300	0.00704700
H	–3.92393900	1.37926300	1.19131800
H	–5.01092100	–0.82789600	0.76521200
H	–3.82274200	–2.50290800	–0.66312100
H	–1.61013300	–2.00090800	–1.60229600
H	–1.72489300	1.89586500	0.24402500
H	0.04692900	–0.28648700	–2.23140900
H	0.82858900	–0.56708200	–0.58017000
H	–0.49167900	2.31327700	–1.60039800
H	1.08367700	1.78902800	–2.18417500
H	3.47314200	–2.51566000	1.22104600
H	3.37106600	–0.75370200	1.24902100
H	2.19187700	–1.75050900	2.13632700
H	1.67843000	–3.90876500	0.01500300
H	0.40014800	–3.10314000	–0.90912100
H	0.37402700	–3.05889400	0.85669900
H	3.42434200	–2.63346000	–1.31424700
H	2.17831200	–1.76272300	–2.22560300
H	3.42731100	–0.86377800	–1.35329400
H	2.94894300	2.49421300	–0.89439800
H	2.60263800	0.89283800	–0.20427500
H	2.84770600	2.29227000	0.87252800
H	1.16583700	4.23097800	–0.84319600
H	–0.33495700	3.87200800	0.04785300
H	1.19827600	4.04571500	0.92762600

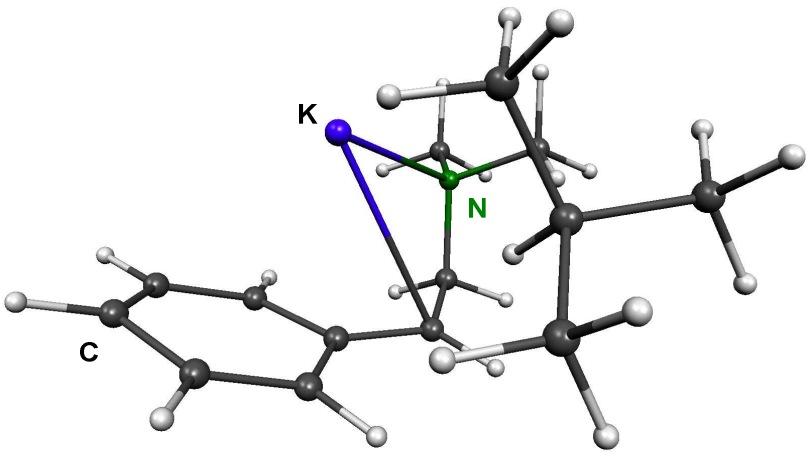


Fig. 11 Molekel plot of [**1**·*t*-BuK] (product)

Table 25 Cartesian coordinates of [**1**·*t*-BuK] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	1.64323200	2.85597700	0.43932800
C	0.39484800	3.49023800	0.47916900
C	–0.60850800	2.97890700	–0.36958400
C	–0.41078000	1.84680000	–1.13507400
C	0.80567900	1.07144700	–1.06432700
C	1.86059600	1.70241100	–0.30321500
C	0.88243500	–0.23128300	–1.55434900
C	2.05953100	–1.10396800	–1.28486300
K	0.27502700	0.15573600	1.45600200
C	–2.79179500	–0.82363600	–0.07563900
C	–2.88783300	–0.60916200	1.43715500
C	–3.75063800	0.12004200	–0.80079400
C	–3.09429700	–2.28065500	–0.42665200
N	2.04374000	–1.71552300	0.08874900
C	1.05563900	–2.78559600	0.12320700
C	3.35531700	–2.26211000	0.41112400
H	2.47187600	3.27315100	1.00444100
H	0.23642500	4.39035100	1.05776600
H	–1.56322300	3.49246000	–0.43521900
H	–1.20978900	1.48547300	–1.77492000
H	2.84201500	1.24300300	–0.27607700
H	0.08166500	–0.60541300	–2.18305700
H	–1.77450000	–0.59429900	–0.41809000
H	3.00468600	–0.55431800	–1.35115700
H	2.12490700	–1.92273500	–2.02007300
H	–3.90398600	–0.81759000	1.78466100
H	–2.22373500	–1.28759000	1.98719300
H	–2.66293200	0.42772400	1.71092800
H	–4.78502500	–0.09468800	–0.51332600
H	–3.66927800	0.00199200	–1.88387000
H	–3.53638100	1.16334900	–0.55730400
H	–2.41870800	–2.96749300	0.09089200
H	–2.99190800	–2.45218600	–1.50055600
H	–4.11883200	–2.53698000	–0.13892200
H	1.32572400	–3.61637100	–0.55091300
H	0.08937400	–2.39465200	–0.20579300
H	0.96262400	–3.18979600	1.13634800
H	3.67525200	–3.02359500	–0.31963000
H	4.09564500	–1.46011400	0.41829700
H	3.33585300	–2.72647200	1.40016500

Table 26 Cartesian coordinates of [**1**·*t*-BuK] (product) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	1.61108800	2.65827500	–0.63150400
C	1.72477800	2.65643900	0.77875500
C	0.68024800	2.11207000	1.51644400
C	–0.44566100	1.54980100	0.88886000
C	–0.58793400	1.53515700	–0.54631200
C	0.51041900	2.12166300	–1.26970100
C	–1.65782500	0.87364500	–1.21035600
C	–2.89344600	0.45115100	–0.47387900
K	–0.74376800	–0.52427900	0.08527700
C	2.64586500	–1.43841000	0.00852700
C	3.40436800	–1.74111500	–1.29200200
C	3.45180000	–1.87298500	1.24128300
C	1.26331500	–2.11168900	–0.00291700

N	–2.72723500	–0.91131400	0.20319200
C	–3.59391600	–1.05610400	1.37781200
C	–2.99786400	–1.98750000	–0.76060300
H	2.40449600	3.10123000	–1.23156700
H	2.59353400	3.08738800	1.26799900
H	0.71936100	2.12549300	2.60472200
H	–1.27828200	1.23280200	1.51910500
H	0.44896900	2.15086700	–2.35624500
H	–1.71110600	0.95620300	–2.29243100
H	2.49249200	–0.35194400	0.06732700
H	–3.15830800	1.14685300	0.33725700
H	–3.76481300	0.39642900	–1.14493500
H	3.58386900	–2.81965300	–1.40212800
H	2.84343800	–1.40083400	–2.17112000
H	4.37836200	–1.23755300	–1.30445200
H	3.63020700	–2.95731600	1.23473000
H	2.92748500	–1.62348000	2.17224400
H	4.42826700	–1.37475500	1.26686700
H	1.34643400	–3.20446700	–0.06534000
H	0.67996700	–1.79581600	–0.88284500
H	0.71406200	–1.89738500	0.92842200
H	–4.66420100	–0.98882100	1.11505900
H	–3.36895800	–0.26931900	2.10520600
H	–3.41814000	–2.02767200	1.85327900
H	–4.05718900	–1.99453800	–1.07517600
H	–2.37808800	–1.84165000	–1.65181900
H	–2.76132400	–2.96240800	–0.31877600

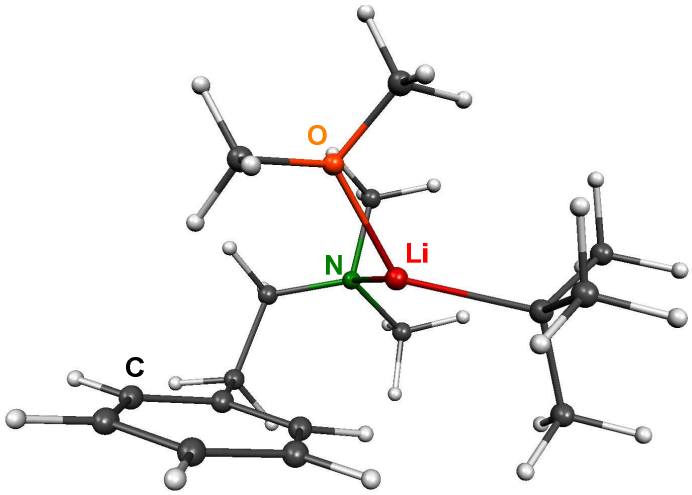


Fig. 12 Molekel plot of [**1**·*t*-BuLi·Me_2O] (starting material)

Table 27 Cartesian coordinates of [**1**·*t*-BuLi·Me_2O] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–3.52722900	–1.44158000	–0.20937100
C	–2.55310600	–2.25854100	–0.77978900
C	–1.41848300	–1.68137500	–1.34823000
C	–1.26412900	–0.29556700	–1.34768800
C	–2.22121200	0.53380100	–0.75123700
C	–3.35603700	–0.05802700	–0.18861400
C	–2.03115900	2.03028000	–0.69555900
C	–1.06975300	2.47615900	0.41426500
C	2.42121900	–0.75334600	–0.82869200
C	3.74264600	–0.09422000	–0.43229700
C	2.57646400	–2.24964300	–0.54840700

C	2.29714000	–0.60833600	–2.34574800
N	0.31102000	2.02244500	0.23122200
C	0.92636600	2.63951300	–0.94694000
C	1.10102500	2.38541600	1.41203700
H	–4.41938200	–1.87962900	0.22192600
H	–2.68076200	–3.33392000	–0.79095800
H	–0.65266900	–2.29976000	–1.80028500
H	–0.39160600	0.13451100	–1.83028800
H	–4.11661900	0.57173300	0.26136000
H	–2.99436600	2.50816100	–0.50041200
H	–1.68976000	2.40524200	–1.66259000
H	–1.42444500	2.07227900	1.36699300
H	–1.09476300	3.57651300	0.48817200
H	4.60717400	–0.54780800	–0.96552300
H	3.76887500	0.97820100	–0.66856600
H	3.95983500	–0.19229800	0.64045400
H	3.42770000	–2.68863200	–1.11454000
H	1.68519500	–2.82570800	–0.83176700
H	2.77377500	–2.46016600	0.51010500
H	3.18034200	–1.03121400	–2.87315200
H	1.42281800	–1.13830600	–2.74871900
H	2.21974000	0.43867900	–2.66833200
H	0.87310500	3.73813400	–0.89039300
H	0.43639400	2.30904000	–1.86131700
H	1.96882000	2.33031500	–1.00280000
H	1.14374800	3.47715100	1.54505900
H	0.65934700	1.93350500	2.30015000
H	2.11793000	2.00573000	1.29246800
C	1.42906800	–1.12858500	2.72590100
H	1.32949900	–0.86815700	3.78439200
H	1.51605700	–2.21259200	2.61695500
H	2.31043100	–0.65529500	2.29934800
C	–0.89977200	–1.29941800	2.40056500
H	–0.83566800	–2.37194500	2.19491300
H	–1.07565300	–1.14007400	3.46920300
H	–1.71217500	–0.86766700	1.82116100
O	0.29948800	–0.65128000	2.00324900
Li	0.73191600	–0.03069100	0.19042100

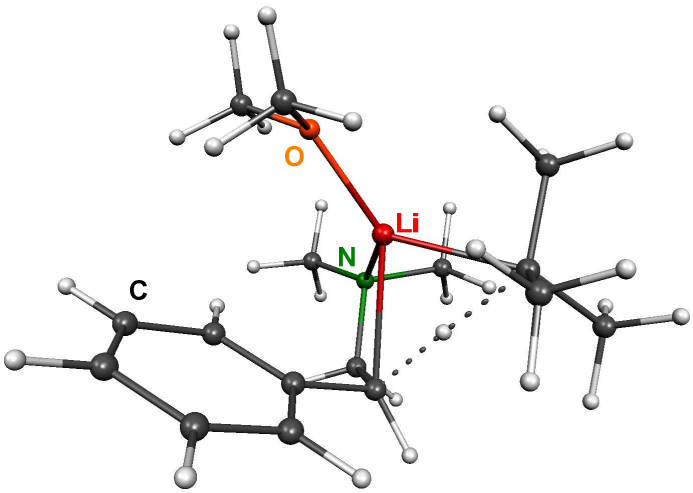


Fig. 13 Molekel plot of [**1**·*t*-BuLi·Me_2O] (transition state)

Table 28 Cartesian coordinates of [**1**·*t*-BuLi·Me_2O] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–3.15659000	0.72562900	–0.33555300
C	–3.82248800	–0.48988200	–0.45251800
C	–3.13205700	–1.58024500	–0.99139700
C	–1.81436000	–1.44994600	–1.40450300
C	–1.11788200	–0.22572100	–1.30679000
C	–1.82770300	0.85343200	–0.74316600
C	0.30233600	–0.14476400	–1.71445900
C	0.84574600	1.26172700	–1.89684100
C	1.80911100	–1.72869400	0.25253300
C	2.37641800	–1.43425600	1.64601600
C	0.88833200	–2.94503400	0.33927500
C	2.96939000	–2.11244100	–0.66222500
N	1.37795200	1.82233400	–0.61308700
C	2.82033700	1.57044900	–0.52783700
C	1.15206500	3.26275900	–0.53108000
H	–3.67435700	1.58993600	0.06739200
H	–4.85486400	–0.58842200	–0.14091800
H	–3.63080600	–2.53673100	–1.09780200
H	–1.30058600	–2.30493900	–1.82898400
H	–1.34747600	1.81912900	–0.63855500
H	0.49672400	–0.77780600	–2.58111800
H	1.04786400	–0.82011600	–0.76690400
H	0.07206900	1.95056100	–2.25493600
H	1.64903100	1.27373400	–2.64389600
H	2.95044400	–2.29776200	2.03178300
H	3.06720600	–0.58123400	1.64512200
H	1.60071600	–1.22608500	2.39314000
H	1.42022600	–3.82140600	0.75219000
H	0.52386300	–3.23343400	–0.65239300
H	0.00729200	–2.77593600	0.96707400
H	3.42727000	–3.06553700	–0.34630600
H	2.63893700	–2.24301200	–1.70059900
H	3.77459200	–1.36954800	–0.66311200
H	3.36673300	2.13376800	–1.29911600
H	3.00942600	0.50906900	–0.67001800
H	3.19365800	1.86851300	0.45443800
H	1.61929500	3.79167600	–1.37467500
H	0.08334300	3.48192200	–0.53767400
H	1.58254600	3.64989000	0.39479500
C	–1.26054800	–0.38624000	2.61490500
H	–1.40752000	–0.26343500	3.69149200
H	–2.21155300	–0.29324400	2.08550400
H	–0.82271100	–1.36022100	2.41436900
C	–0.78906800	1.91536600	2.43098400
H	–1.77133600	2.08798300	1.98269400
H	–0.84744100	2.05872700	3.51362800
H	–0.06377800	2.60619600	2.00715300
O	–0.34112700	0.59890400	2.14224900
Li	0.67543800	0.21244700	0.54859500

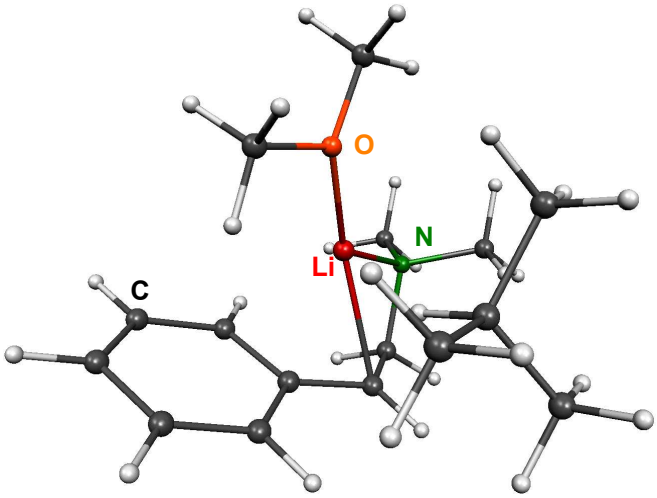


Fig. 14 Molekel plot of [**1**·*t*-BuLi·Me_2O] (product)

Table 29 Cartesian coordinates of [**1**·*t*-BuLi·Me_2O] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	0.77321600	3.17219600	0.58596100
C	–0.50384000	3.65505300	0.33685400
C	–1.27774700	2.98864200	–0.63628100
C	–0.79919400	1.88869500	–1.31221200
C	0.51566200	1.35362500	–1.07913900
C	1.27888100	2.05065600	–0.07990300
C	0.96047100	0.17101800	–1.70288800
C	2.37324000	–0.29044700	–1.55379700
C	–2.42755000	–1.33717000	–0.59565700
C	–2.36934500	–2.47535800	0.42322200
C	–3.72462700	–0.54257800	–0.44292600
C	–2.29653200	–1.88378600	–2.01691800
N	2.59421500	–1.06499100	–0.27571100
C	2.13481100	–2.44014300	–0.46146400
C	4.00004500	–1.05944400	0.11141100
H	1.40712500	3.67367500	1.31033600
H	–0.88706500	4.52443200	0.85469600
H	–2.27367000	3.35247400	–0.86770900
H	–1.41419500	1.41128400	–2.06833400
H	2.30728700	1.75701300	0.11625700
H	0.33942000	–0.27443600	–2.46906000
H	–1.58390500	–0.66208100	–0.41603500
H	3.07501100	0.55218400	–1.51400300
H	2.68122800	–0.92536000	–2.39645600
H	–3.17468500	–3.19416500	0.23966700
H	–1.41811500	–3.01249200	0.36358800
H	–2.48365300	–2.09953200	1.44361900
H	–4.59127600	–1.18948300	–0.61643000
H	–3.76778700	0.28168600	–1.15893700
H	–3.81568000	–0.11907500	0.56106200
H	–3.12846800	–2.55887900	–2.24413400
H	–2.30655100	–1.07485600	–2.75189200
H	–1.36302100	–2.43882300	–2.14199700
H	2.74349400	–2.96621500	–1.21348000
H	1.09771900	–2.42788200	–0.80514500
H	2.19490600	–2.98980100	0.48085400
H	4.63564400	–1.50811200	–0.66691000
H	4.33067000	–0.03345400	0.28073000
H	4.13240600	–1.62557200	1.03557000
C	0.13935800	–1.32857200	3.07406400

H	0.54512200	–0.78699100	3.93353500
H	–0.78725900	–1.83268000	3.36190100
H	0.86222300	–2.06526500	2.72881800
C	–1.05109700	0.58342200	2.33763000
H	–1.99990600	0.12016700	2.62225500
H	–0.66603700	1.18776700	3.16300000
H	–1.18750800	1.21171100	1.45942200
O	–0.10557200	–0.43401300	2.00095900
Li	0.94236200	–0.13168600	0.45659000

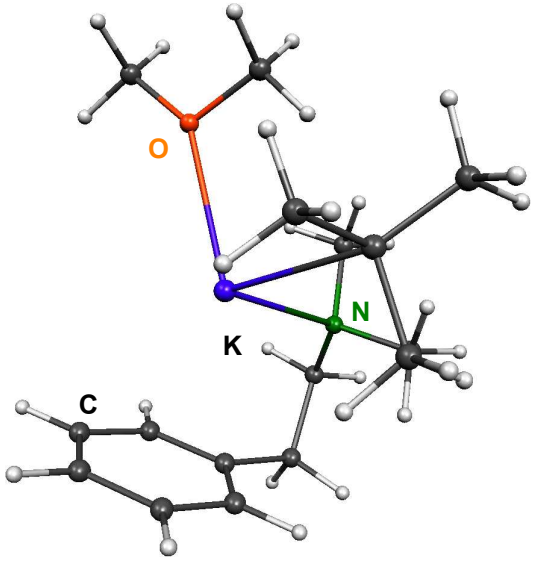


Fig. 15 Molekel plot of [**1**·*t*-BuK·Me_2O] (starting material)

Table 30 Cartesian coordinates of [**1**·*t*-BuK·Me_2O] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	2.72480300	1.01040800	–2.08273900
C	2.35539500	–0.17397600	–2.72445300
C	2.26301800	–1.35246200	–1.98653100
C	2.53045100	–1.34390400	–0.61577200
C	2.89075500	–0.16366700	0.03956900
C	2.99032100	1.01167800	–0.71506600
C	3.14517200	–0.13857200	1.52877800
C	2.10718000	0.70449100	2.28357300
C	–2.25731600	–1.78572100	–0.09085400
C	–3.42450000	–2.10469700	0.82731800
C	–2.81118300	–1.65820300	–1.50658500
C	–1.33086000	–2.99534000	–0.09108400
N	0.73510000	0.34310800	1.95938200
C	0.39294800	–1.00254500	2.41643400
C	–0.19771700	1.30095800	2.54210200
H	2.81523500	1.92905200	–2.65005900
H	2.15374900	–0.17891700	–3.78843800
H	1.97908200	–2.27882600	–2.47096500
H	2.44801500	–2.26640000	–0.05187300
H	3.28349000	1.93561500	–0.22738500
H	4.13192500	0.28912600	1.72902300
H	3.16335800	–1.15895000	1.91551100
H	2.24265600	1.75572200	2.01200200
H	2.29502100	0.62121300	3.36845800
H	–3.96778400	–3.02929500	0.51627300
H	–3.10329700	–2.26759300	1.86427900
H	–4.17532400	–1.30245800	0.84548900

H	–3.35549800	–2.57633700	–1.83325100
H	–2.02450700	–1.50710200	–2.26635800
H	–3.52367100	–0.82845700	–1.61225100
H	–1.84312200	–3.92050300	–0.44943700
H	–0.45573000	–2.86686500	–0.75113000
H	–0.94517900	–3.22825500	0.90962600
H	0.50805900	–1.09944000	3.50882300
H	1.02697400	–1.74314900	1.92920700
H	–0.63814900	–1.21888500	2.12667300
H	–0.12779100	1.32805100	3.64210600
H	0.00475600	2.30202800	2.15452700
H	–1.21668400	1.01868400	2.26990000
C	–3.24482200	1.69859700	0.04596100
H	–3.49031500	2.25199800	0.95888300
H	–4.09186800	1.74438700	–0.64595200
H	–3.01332100	0.65649700	0.28100000
C	–2.28782700	3.60834200	–0.93511100
H	–3.10661500	3.69033500	–1.65781700
H	–2.52489600	4.21790000	–0.05638400
H	–1.36664600	3.97103700	–1.38875000
O	–2.08322800	2.25976100	–0.56556600
K	–0.34930100	0.18882200	–0.68348000

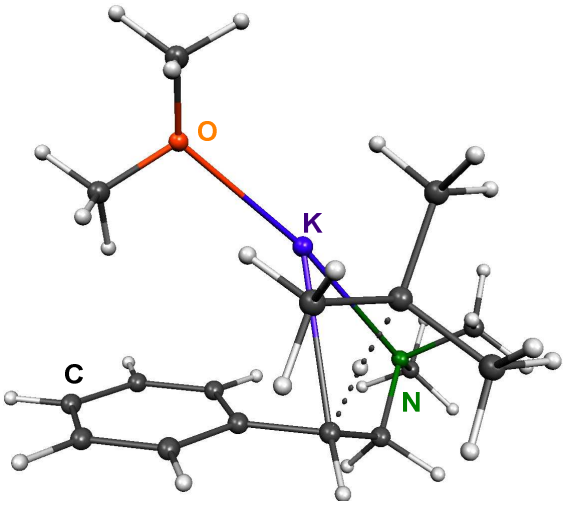


Fig. 16 Molekel plot of [**1**·*t*-BuK·Me_2O] (transition state)

Table 31 Cartesian coordinates of [**1**·*t*-BuK·Me_2O] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–1.35440200	–3.10510400	–0.45451300
C	–2.39508800	–3.07441300	0.46901500
C	–2.23996200	–2.29842300	1.62345500
C	–1.07689200	–1.57442400	1.84155400
C	0.00365900	–1.59960300	0.93047000
C	–0.18040300	–2.38104900	–0.23353400
C	1.22011100	–0.80273000	1.18376800
C	2.46460000	–1.29939800	0.45874400
C	0.70658300	2.08998900	1.07985300
C	0.67684900	3.19044600	0.01998500
C	–0.63164700	2.08823900	1.80749100
C	1.80155400	2.42374600	2.08155000
N	2.61251600	–0.76606600	–0.91776000
C	3.23402200	0.55551500	–0.86443800
C	3.44458200	–1.65385800	–1.72051400

H	–1.44356800	–3.70895400	–1.35116400
H	–3.30017600	–3.64535900	0.30308800
H	–3.03278600	–2.26563200	2.36257300
H	–0.97370300	–0.98938200	2.74855400
H	0.62346000	–2.45177700	–0.95944200
H	1.40430600	–0.74594600	2.25937300
H	1.00650100	0.50793900	0.95913400
H	2.44822600	–2.39282200	0.37382700
H	3.36594700	–1.04207700	1.03639300
H	0.54227000	4.19199100	0.47439400
H	1.60424500	3.24430900	–0.56599700
H	–0.16140700	3.08516900	–0.68670200
H	–0.85797300	3.07064200	2.26766900
H	–0.64414900	1.34960500	2.61626200
H	–1.46932800	1.85029100	1.13749800
H	1.61158100	3.38232900	2.60020900
H	1.88464700	1.65238600	2.85706600
H	2.78616400	2.51316000	1.60577600
H	4.26318900	0.50162700	–0.47312700
H	2.65270300	1.20453000	–0.20926900
H	3.27478400	0.99142700	–1.86752700
H	4.44059900	–1.79981500	–1.27168000
H	2.96575200	–2.62983400	–1.81904500
H	3.57875800	–1.23062000	–2.71818300
C	–3.10483700	2.55804500	–1.47860400
H	–4.08808300	2.52616500	–1.95910100
H	–3.20555300	2.95575600	–0.46402200
H	–2.44085800	3.20034000	–2.05357300
C	–3.35373200	0.34268800	–0.73990500
H	–3.51061700	0.68268800	0.28814700
H	–4.31960400	0.23680300	–1.24393300
H	–2.84643900	–0.62068900	–0.72060000
O	–2.52959500	1.26178600	–1.44839500
K	0.02633100	0.46768000	–1.23902100

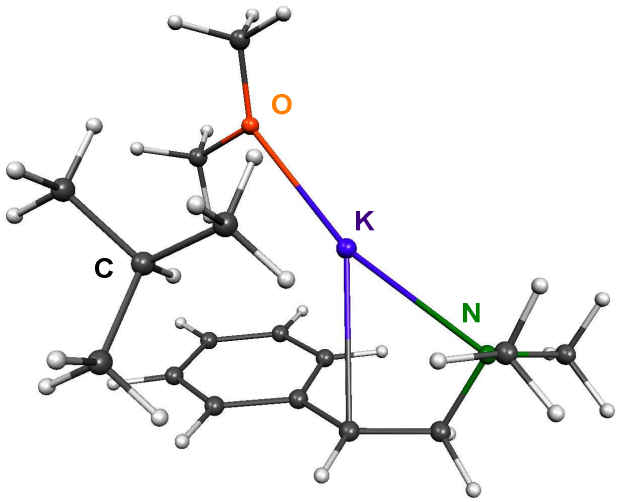


Fig. 17 Molekel plot of [**1**·*t*-BuK·Me_2O] (product)

Table 32 Cartesian coordinates of [**1**·*t*-BuK·Me_2O] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	0.91789100	2.99311800	0.96342000
C	–0.28768600	3.44058700	0.41903200
C	–0.69224200	2.86621600	–0.80084000

C	0.05369200	1.88786000	–1.42760800
C	1.29287400	1.38630300	–0.89017300
C	1.68412700	2.00402100	0.35282800
C	1.97840700	0.31904400	–1.48476500
C	3.27705200	–0.18345100	–0.95295800
C	–2.66448000	–0.77570500	–1.50770800
C	–3.96817000	–1.33037000	–0.93512300
C	–2.85556300	–0.35145200	–2.96404600
C	–1.54313300	–1.81103800	–1.40122400
N	3.15320500	–1.20596000	0.14333100
C	2.73274500	–2.47670000	–0.42889700
C	4.43384700	–1.37709200	0.81494200
H	1.28225000	3.43116900	1.88820900
H	–0.86854500	4.21897700	0.89659800
H	–1.61218900	3.20060400	–1.27211100
H	–0.28938600	1.48079300	–2.37370800
H	2.61904800	1.70917000	0.81958100
H	1.66537900	0.00571400	–2.47486800
H	–2.37089300	0.10926600	–0.93292600
H	3.88121600	0.62667900	–0.52568500
H	3.88287600	–0.63205600	–1.75841700
H	–4.28971200	–2.20779100	–1.50562400
H	–3.84666800	–1.63802300	0.10651200
H	–4.76990400	–0.58870800	–0.98153200
H	–3.19183800	–1.20282900	–3.56459900
H	–1.92198000	0.01611600	–3.39485000
H	–3.60376400	0.44000100	–3.05102400
H	–1.74821500	–2.66607900	–2.05350500
H	–0.58107900	–1.38211400	–1.70255200
H	–1.46705000	–2.19842100	–0.37838200
H	3.49365900	–2.89269600	–1.11105300
H	1.81858000	–2.32626300	–1.01004600
H	2.54919300	–3.21063500	0.36203900
H	5.22704400	–1.68959400	0.11466900
H	4.73569900	–0.43522400	1.27675600
H	4.35018200	–2.13668200	1.59594500
C	–2.64714600	–1.41243500	3.00969600
H	–2.71872700	–0.99150100	4.01761600
H	–3.65479200	–1.55609500	2.60752600
H	–2.13532000	–2.37224400	3.05331300
C	–2.51525600	0.71646800	2.02405600
H	–3.48860100	0.60317800	1.53657100
H	–2.64752500	1.18369900	3.00450700
H	–1.86863000	1.34433500	1.41085700
O	–1.89301400	–0.55757800	2.16793300
K	0.49787400	–0.56382300	0.96366300

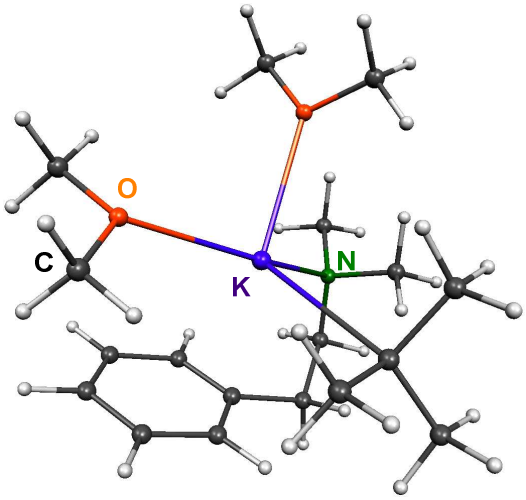


Fig. 18 Molekel plot of [**1**·*t*-BuK·$(Me_2O)_2$] (starting material)

Table 33 Cartesian coordinates of [**1**·*t*-BuK·$(Me_2O)_2$] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–2.39906200	–0.85633800	–2.37126200
C	–3.28793600	–0.77600400	–1.30161300
C	–2.96028200	–1.38630200	–0.09171600
C	–1.75188800	–2.06725700	0.04474500
C	–0.85522500	–2.16748700	–1.02635400
C	–1.19557100	–1.55033600	–2.23361500
C	0.43895900	–2.92927200	–0.82565300
C	1.61812400	–2.42555200	–1.65516500
K	0.00293500	0.55663100	0.16686500
C	0.38408000	–0.82018800	2.67772900
C	1.44912500	0.07227400	3.30112300
C	–0.94135500	–0.42812500	3.31550300
C	0.69026300	–2.24635100	3.10026800
N	2.01753200	–1.05744800	–1.32251900
C	2.75533800	–1.03159700	–0.05782100
C	2.85080800	–0.50959300	–2.38350100
H	–2.64260000	–0.38742200	–3.31752200
H	–4.22654500	–0.24540300	–1.41135700
H	–3.63594200	–1.32424000	0.75330000
H	–1.48104700	–2.50110300	0.99944800
H	–0.51929400	–1.59650600	–3.07831800
H	0.27597500	–3.98247600	–1.07991100
H	0.68676600	–2.89997800	0.23887900
H	1.36101800	–2.45440800	–2.71657600
H	2.46995100	–3.11403800	–1.52222300
H	1.51086500	–0.05149100	4.41036100
H	2.45823400	–0.13686400	2.91668900
H	1.24704000	1.14222500	3.13539000
H	–0.93281900	–0.55105600	4.42661700
H	–1.78526800	–1.03025700	2.94914900
H	–1.19198900	0.62934500	3.13791900
H	0.72902100	–2.35560900	4.21150500
H	–0.06616100	–2.96421000	2.75308900
H	1.66267400	–2.59813500	2.72708300
H	3.63609800	–1.69402800	–0.09448700
H	2.10475200	–1.31811800	0.77271000
H	3.09943400	–0.01233100	0.13074500
H	3.76782100	–1.10255600	–2.54082500
H	2.29060200	–0.48272700	–3.32071800
H	3.14119100	0.50988900	–2.12341800

C	2.80211600	2.82140300	0.67821700
H	2.61430500	2.13983200	1.50523400
H	3.84056900	2.71669800	0.34554400
H	2.62864700	3.85166200	1.00538700
C	2.08366800	3.30949900	–1.50167000
H	1.85689800	4.35186900	–1.25324200
H	3.11171100	3.24649600	–1.87541400
H	1.39982700	2.96139800	–2.27453400
C	–2.43697300	3.15216200	–0.95086100
H	–3.21988500	2.70399600	–1.57289700
H	–2.77648300	4.12957100	–0.59152000
H	–1.53305300	3.28216300	–1.54485800
C	–3.22718300	2.10258100	0.99103800
H	–3.52639300	3.04836600	1.45467300
H	–4.07273700	1.68888900	0.43117000
H	–2.92211200	1.39715400	1.76062700
O	1.91062500	2.47669500	–0.37248400
O	–2.11582300	2.30436100	0.13287800

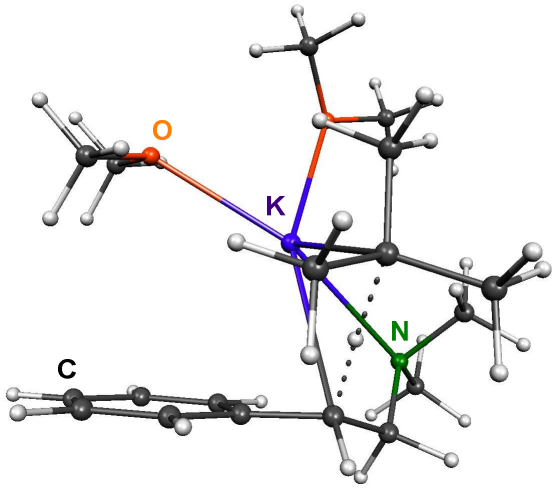


Fig. 19 Molekel plot of [**1**·*t*-BuK·$(Me_2O)_2$] (transition state)

Table 34 Cartesian coordinates of [**1**·*t*-BuK·$(Me_2O)_2$] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–2.97745700	–0.08397800	–1.90903200
C	–3.91142700	0.38576200	–0.98829800
C	–3.81583700	–0.04985400	0.33728100
C	–2.80853000	–0.92145600	0.72881000
C	–1.85325800	–1.42083600	–0.18618800
C	–1.96909800	–0.96671900	–1.51978100
C	–0.75108400	–2.27767100	0.28942600
C	0.01948500	–3.00465000	–0.80118600
K	0.42041500	0.42851100	–0.26997600
C	0.81240000	–0.92231700	2.37600700
C	1.75323500	0.27862600	2.44850600
C	–0.35378700	–0.68244100	3.32595000
C	1.55963100	–2.15481400	2.86823500
N	1.04375500	–2.16371100	–1.46611800
C	2.25975000	–2.13232000	–0.66097200
C	1.35459400	–2.68728600	–2.78888500
H	–3.03865000	0.22527400	–2.94722700
H	–4.70231600	1.05954100	–1.29511300
H	–4.53784800	0.29087100	1.07171600
H	–2.75216500	–1.24490700	1.76167300

H	–1.26347000	–1.31594800	–2.26496100
H	–1.11942200	–2.98727200	1.03544700
H	0.04452300	–1.56286900	1.10508100
H	–0.65810900	–3.35748900	–1.58904100
H	0.50810400	–3.89969400	–0.38411400
H	2.18806700	0.40462400	3.46016700
H	2.60741800	0.19154100	1.75915900
H	1.24343800	1.22920600	2.22861600
H	–0.01533300	–0.55037500	4.37274200
H	–1.04521400	–1.53399100	3.32687100
H	–0.93546000	0.20841000	3.05957000
H	1.81130200	–2.08054500	3.94336500
H	0.95695200	–3.06457600	2.74428900
H	2.50610000	–2.31688000	2.33897800
H	2.72145000	–3.13052100	–0.57941700
H	2.02378000	–1.78908400	0.34610300
H	2.99015000	–1.45502400	–1.11446900
H	1.71780200	–3.72767100	–2.74577200
H	0.46556000	–2.65993700	–3.42181800
H	2.12947000	–2.07437500	–3.25506300
C	2.68086900	3.13038200	–0.02191100
H	1.71556700	3.38747300	0.40912200
H	3.35774500	2.78688800	0.76688000
H	3.11254800	4.00673000	–0.51673100
C	3.65974600	1.68387200	–1.59151700
H	4.13271400	2.52694600	–2.10556200
H	4.35636700	1.27476000	–0.85204400
H	3.40689900	0.91450700	–2.31933600
C	–1.71800600	2.99750400	1.22386600
H	–1.85028500	4.06026500	1.45232500
H	–2.67327700	2.56002300	0.92095800
H	–1.34446400	2.47855300	2.10423900
C	–1.15191000	3.46738000	–1.00861700
H	–2.07945400	3.02354200	–1.38387800
H	–1.29901200	4.54066700	–0.84730700
H	–0.35210800	3.32009200	–1.73407300
O	2.45551400	2.09406900	–0.96882200
O	–0.75044600	2.83473300	0.19517700

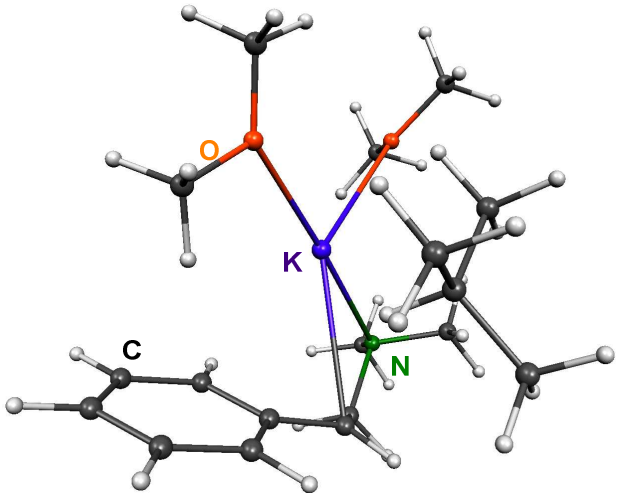


Fig. 20 Molekel plot of [**1**·*t*-BuK·$(Me_2O)_2$] (product)

Table 35 Cartesian coordinates of [**1**·*t*-BuK·$(Me_2O)_2$] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–2.38592300	–2.02688000	–2.06743300
C	–3.62596100	–1.57750800	–1.61450700
C	–3.74592700	–1.29029400	–0.24208900
C	–2.68772500	–1.45423600	0.62953700
C	–1.40712800	–1.96254700	0.21061800
C	–1.30274500	–2.19189000	–1.20705000
C	–0.35855500	–2.16566900	1.12311200
C	0.85529400	–2.95884200	0.77200100
K	0.57224200	0.07644200	–0.58940200
C	–1.04411500	1.57633500	2.16922100
C	0.28837900	2.27268000	1.88252700
C	–2.19566500	2.57456700	2.05487800
C	–1.02203000	0.92487100	3.55102000
N	2.06082100	–2.16972600	0.34268100
C	2.59075800	–1.45331400	1.49460100
C	3.07916100	–3.07571100	–0.16781700
H	–2.25191900	–2.25909000	–3.11990900
H	–4.46378900	–1.45927800	–2.28931100
H	–4.69514400	–0.93748600	0.14969700
H	–2.83123000	–1.25193000	1.68711200
H	–0.37189800	–2.57744000	–1.61579900
H	–0.59459000	–2.05105000	2.17583400
H	–1.21154900	0.78173900	1.43333800
H	0.64828200	–3.64660600	–0.05664700
H	1.16980600	–3.58256200	1.62814100
H	0.46005900	3.07318400	2.60946100
H	1.13207400	1.57821700	1.95896100
H	0.28826100	2.72328400	0.88471900
H	–2.10631900	3.35017500	2.82277400
H	–3.15921200	2.07610400	2.18411000
H	–2.19472300	3.06461000	1.07751000
H	–0.86680200	1.68124500	4.32762100
H	–1.96627100	0.41546800	3.75756800
H	–0.22033800	0.18606100	3.62344900
H	2.96426300	–2.14695900	2.26781400
H	1.79239700	–0.85755500	1.94397800
H	3.41033600	–0.79444600	1.19410300
H	3.36536200	–3.83329500	0.58149500
H	2.70310400	–3.59469900	–1.05187900
H	3.97777400	–2.51842400	–0.44496400
C	3.47399000	2.59395800	–0.41452600
H	2.65224300	3.15237900	0.02889100
H	4.24613500	2.42212100	0.34248600
H	3.90229100	3.16577700	–1.24455300
C	3.95359400	0.55709700	–1.47637800
H	4.36188700	1.05012100	–2.36457300
H	4.76427300	0.36108600	–0.76674900
H	3.49096600	–0.38716600	–1.75913300
C	–2.22946100	1.68068000	–1.73538100
H	–2.92167900	2.35588200	–1.22228700
H	–2.46506300	1.65644800	–2.80368800
H	–2.33021700	0.67908800	–1.32203200
C	–0.67938400	3.43424900	–1.99106600
H	–0.92319300	3.52137700	–3.05536700
H	–1.29944800	4.13660300	–1.42292100
H	0.37261800	3.67456900	–1.84074900
O	2.95087800	1.36125400	–0.87746900
O	–0.88418400	2.11160200	–1.53831000

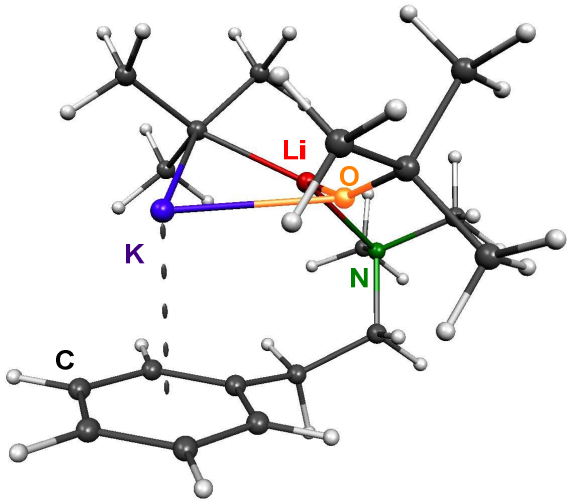


Fig. 21 Molekel plot of [**1**·*t*-BuLi·*t*-BuOK] (starting material)

Table 36 Cartesian coordinates of [**1**·*t*-BuLi·*t*-BuOK] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	3.67500600	0.15622900	0.02492300
C	3.59857000	1.53242400	–0.19256100
C	2.62877100	2.03379500	–1.06363700
C	1.76014700	1.16613600	–1.72398300
C	1.83573800	–0.21709700	–1.52664600
C	2.79483400	–0.70495800	–0.63212500
C	1.00581600	–1.18772000	–2.34241000
C	–0.49384500	–0.88151500	–2.50078200
N	–1.36568300	–1.59466100	–1.55495800
C	–1.35213100	–3.03726800	–1.79410900
C	–2.73651400	–1.11022800	–1.74812200
Li	–0.99889900	–0.72202700	0.32365300
O	–1.15118600	1.05467500	0.17516400
C	–1.90709200	2.21161400	0.26736200
C	–2.01208300	2.89282300	–1.10759700
C	–1.24393500	3.20821500	1.24061200
C	–3.31800500	1.89999900	0.79170600
H	4.42097800	–0.25016400	0.69797200
H	4.29108000	2.20475900	0.30023200
H	2.55581400	3.10051000	–1.24043300
H	1.01845700	1.57462700	–2.39928900
H	2.85427400	–1.77175100	–0.45041800
H	1.14536300	–2.18400700	–1.92283600
H	1.44880400	–1.21744600	–3.34323700
H	–0.80613400	–1.13443500	–3.52749700
H	–0.67861100	0.18278700	–2.34534400
H	–2.06295600	–3.51872100	–1.12232900
H	–0.37155100	–3.46269000	–1.59448800
H	–1.63869800	–3.26746600	–2.83271200
H	–3.40315600	–1.61192900	–1.04346100
H	–3.09029700	–1.31322100	–2.77151400
H	–2.76275000	–0.03951100	–1.55558500
H	–2.58135700	3.82707600	–1.06807900
H	–2.50027100	2.22297700	–1.82109400
H	–1.00602700	3.11055900	–1.47965400
H	–1.80944700	4.13941700	1.33887000
H	–0.23971300	3.46509000	0.88008900

H	–1.16912300	2.75682900	2.23723600
H	–3.93342000	2.80031500	0.89086500
H	–3.24275200	1.41522000	1.76928200
H	–3.82405700	1.20999300	0.11122000
C	–0.10271200	–1.82356700	1.93027600
C	0.74322900	–3.04700700	1.59605500
C	0.30329000	–1.36893500	3.33195600
C	–1.55923400	–2.28831900	2.04150200
K	1.00718900	0.90764600	1.54252500
H	0.48717400	–3.47213700	0.61762800
H	0.61529100	–3.86496800	2.33915600
H	1.81535000	–2.81235400	1.57555400
H	–0.29916200	–0.52113300	3.69292200
H	1.36634600	–1.08199300	3.39598000
H	0.17890500	–2.17288300	4.08776400
H	–2.23885100	–1.47423000	2.33296700
H	–1.68848800	–3.08916700	2.80014300
H	–1.94072000	–2.71165200	1.10002900

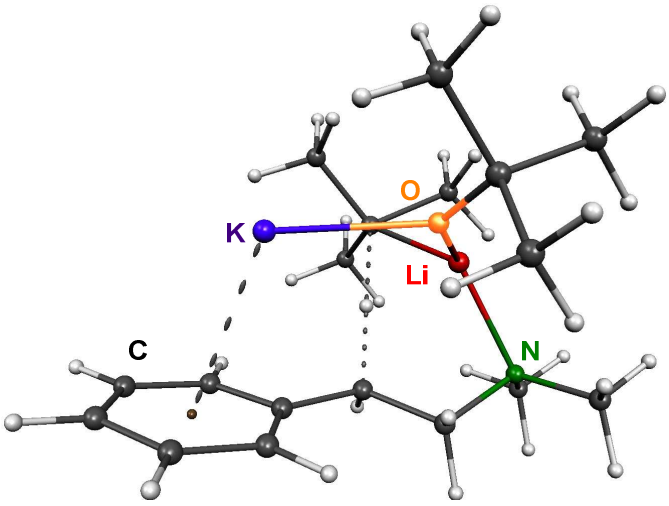


Fig. 22 Molekel plot of [**1**·*t*-BuLi·*t*-BuOK] (transition state)

Table 37 Cartesian coordinates of [**1**·*t*-BuLi·*t*-BuOK] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–4.12880800	–0.37871900	0.08664400
C	–4.08379400	–1.59527900	–0.60406300
C	–3.04468300	–1.80247500	–1.51192200
C	–2.05019100	–0.84229700	–1.70120800
C	–2.04704500	0.37361700	–0.97856400
C	–3.14033800	0.57953000	–0.09991900
C	–0.94066700	1.33565400	–0.95942500
C	0.15839400	1.14596800	–1.98947700
N	1.43545000	1.75556700	–1.55520100
C	1.33253800	3.21244000	–1.53379600
C	2.50455300	1.36019300	–2.46899100
Li	1.31685900	0.67294500	0.20878800
O	1.35043700	–1.09912800	0.27523000
C	2.35485300	–2.05781800	0.20226500
C	2.31377900	–2.76006800	–1.16337100
C	2.14960200	–3.11007500	1.30536700
C	3.73270400	–1.40624900	0.39489100

H	–4.94238400	–0.17715800	0.77448400
H	–4.85521600	–2.34173600	–0.46361800
H	–3.00736500	–2.71962300	–2.08924500
H	–1.26629800	–1.05083200	–2.41742800
H	–3.18800500	1.51214900	0.45180400
H	–0.42510900	1.34057900	0.34463600
H	–1.33400800	2.35557700	–0.95224600
H	–0.10994200	1.54224500	–2.98702100
H	0.37388700	0.08181700	–2.10491300
H	2.28627900	3.64174200	–1.22200200
H	0.56628800	3.52538900	–0.82748100
H	1.07782800	3.60576700	–2.53049300
H	3.44948800	1.79444500	–2.13798400
H	2.30225100	1.69972600	–3.49664100
H	2.59984300	0.27409900	–2.46873400
H	3.06722900	–3.54950700	–1.24867500
H	2.48287400	–2.03096300	–1.96040800
H	1.32430500	–3.20173200	–1.31657200
H	2.93434100	–3.87253300	1.30943300
H	1.19064300	–3.62188100	1.15721300
H	2.13777500	–2.61639100	2.28192400
H	4.55053900	–2.13037600	0.32646400
H	3.77769100	–0.92343700	1.37577900
H	3.88648500	–0.64087900	–0.37276700
C	0.06213100	1.71325900	1.81308200
C	–0.77721700	2.98223100	1.90379900
C	–0.29837600	0.82306400	3.00250800
C	1.53422300	2.11080000	1.97654200
K	–1.00473000	–1.39773300	1.08747700
H	–0.55163900	3.68400800	1.09370800
H	–0.59995300	3.51837800	2.85187000
H	–1.84943700	2.76432500	1.85310700
H	0.31785100	–0.08508400	3.04112900
H	–1.36126400	0.54330200	3.00524600
H	–0.12582700	1.34578500	3.96092800
H	2.20732900	1.24163500	2.03306400
H	1.69464800	2.66670500	2.91664200
H	1.88657900	2.76393800	1.16875100

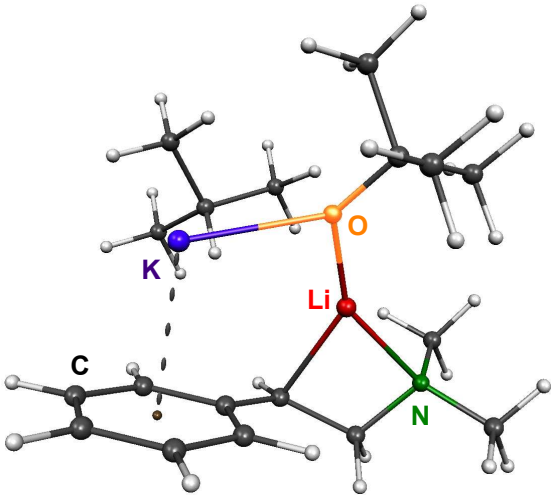


Fig. 23 Molekel plot of [**1**·*t*-BuLi·*t*-BuOK] (product)

Table 38 Cartesian coordinates of [**1**·*t*-BuLi·*t*-BuOK] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–3.61807700	0.78803200	–0.65001900
C	–3.32989800	1.24394600	–1.95068500
C	–2.10341300	1.89227400	–2.14538100
C	–1.18812300	2.06216400	–1.11304700
C	–1.46077700	1.62876200	0.23331000
C	–2.72258800	0.94923000	0.39219200
C	–0.58248200	1.81692200	1.31526000
C	0.53074600	2.81949000	1.25733300
N	1.86817200	2.22149100	0.93742300
C	2.43445300	1.62075800	2.14399900
C	2.78487400	3.22147200	0.40545500
Li	0.92800400	0.59706400	0.14365200
O	1.06295900	–0.87535900	–0.83846400
C	2.24347700	–1.40424600	–1.35906200
C	2.42094200	–0.95251500	–2.81684900
C	2.19378600	–2.93829700	–1.31194300
C	3.45207900	–0.92212700	–0.54142600
H	–4.57205200	0.31036400	–0.44867500
H	–4.05071300	1.15001000	–2.75230900
H	–1.84987900	2.27393200	–3.12941300
H	–0.25143800	2.56340100	–1.33452800
H	–2.99702600	0.61374600	1.38683500
H	–1.02697100	–1.00320900	1.39732100
H	–0.93665600	1.51188500	2.29397600
H	0.62009400	3.36619200	2.20908400
H	0.33792400	3.56707900	0.48103900
H	3.36976700	1.11141100	1.90636100
H	1.73022800	0.89232600	2.55263900
H	2.62817000	2.38325700	2.91481300
H	3.74657200	2.75676000	0.18059900
H	2.95073600	4.04103600	1.12158900
H	2.37769100	3.64104200	–0.51575700
H	3.34434000	–1.33633300	–3.26169900
H	2.43586200	0.14013200	–2.86189100
H	1.57865600	–1.30656000	–3.42127100
H	3.09851700	–3.39543600	–1.72413200
H	1.33547200	–3.29798000	–1.89046000
H	2.07234600	–3.27296200	–0.27823100
H	4.39646300	–1.32851100	–0.91621300
H	3.33321300	–1.22762100	0.50285400
H	3.50906200	0.17121300	–0.57869900
C	–1.00523500	–1.94098200	1.96381400
C	–2.09817800	–1.87735600	3.02961900
C	–1.24888500	–3.11147200	1.00966200
C	0.37892200	–2.05713000	2.59999300
K	–1.32386500	–1.03091500	–1.54859700
H	–1.95844700	–1.01205300	3.68288100
H	–2.07685500	–2.77755800	3.65252300
H	–3.09157200	–1.80430900	2.57798200
H	–0.46003400	–3.16590000	0.25354700
H	–2.22764000	–3.03049600	0.52063500
H	–1.24544700	–4.05839500	1.55854800
H	1.15455800	–2.02284700	1.83065700
H	0.47190900	–2.99975100	3.14999000
H	0.55196200	–1.23877800	3.30419000

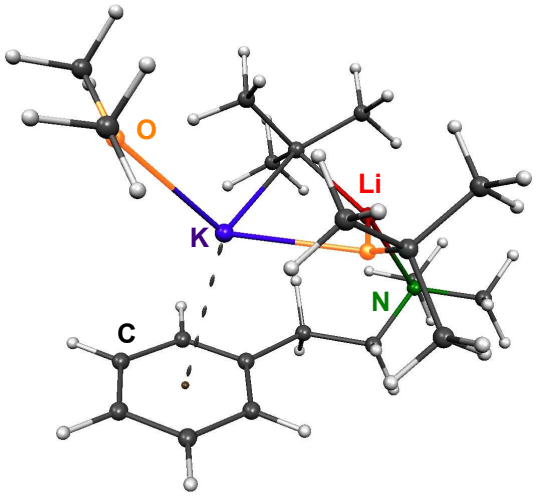


Fig. 24 Molekel plot of [**1**·*t*-BuLi·*t*-BuOK·Me_2O] (starting material)

Table 39 Cartesian coordinates of [**1**·*t*-BuLi·*t*-BuOK·Me_2O] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–1.30403100	3.76995300	0.01015800
C	–1.62117400	3.66756700	–1.34579100
C	–0.73745300	3.01898000	–2.20444800
C	0.44809700	2.46565200	–1.71569100
C	0.77081100	2.54647500	–0.35881500
C	–0.12226900	3.21375100	0.49287000
C	1.99682500	1.90693400	0.25993600
C	2.76767500	0.92953600	–0.63394500
N	3.29895600	–0.19627300	0.14835700
C	4.24970800	0.25052400	1.16186000
C	3.95272300	–1.14207500	–0.75342000
Li	1.37449300	–1.04680900	0.58715500
O	0.50387000	–1.23077100	–0.96888900
C	0.15798300	–2.14703000	–1.94959500
C	0.71614000	–1.70644900	–3.31319100
C	–1.37563100	–2.24150300	–2.06759500
C	0.70240300	–3.54157300	–1.60195700
H	–1.97718100	4.27886000	0.68982700
H	–2.54077300	4.09447500	–1.72647600
H	–0.96707900	2.93808600	–3.26014100
H	1.10958800	1.95632000	–2.40388700
H	0.11413800	3.28088500	1.55020700
H	1.64868000	1.34863300	1.13855200
H	2.65685700	2.69882500	0.62778200
H	3.58328500	1.44210500	–1.17110000
H	2.09435800	0.47692300	–1.36299100
H	4.63023000	–0.61491600	1.70614000
H	3.76267200	0.91113800	1.87731400
H	5.10028900	0.78239900	0.70542600
H	4.30831800	–2.00280800	–0.18380200
H	4.81134600	–0.68299200	–1.26885600
H	3.22874500	–1.48252400	–1.49270500
H	0.42684800	–2.38588300	–4.12150000
H	1.80802200	–1.66304800	–3.27461100
H	0.34507400	–0.70357600	–3.54727200
H	–1.69614800	–2.97732000	–2.81183100
H	–1.78185600	–1.26690200	–2.36572600
H	–1.80011200	–2.52549900	–1.09807800
H	0.45006400	–4.29042800	–2.35994000
H	0.29162200	–3.86363000	–0.64046600

H	1.79142800	–3.49836500	–1.50839300
C	0.46154300	–0.72535400	2.50472100
C	0.94771700	0.28984700	3.53248500
C	–0.98243400	–1.06957600	2.86178400
C	1.27438400	–2.00770400	2.71301300
K	–1.29859800	0.23587600	0.15328000
H	2.01126300	0.52981200	3.40945000
H	0.83065100	–0.07640700	4.57643900
H	0.39583100	1.23820500	3.47236600
H	–1.42721500	–1.80699200	2.17565700
H	–1.62972800	–0.17887900	2.86717400
H	–1.07064400	–1.50162700	3.88220000
H	0.95105600	–2.82490200	2.04918400
H	1.18446600	–2.40326100	3.74696700
H	2.35176700	–1.85408200	2.54553300
C	–4.66496900	–1.21667900	–0.56857000
H	–4.18414400	–1.00600200	–1.52110900
H	–4.63484700	–2.29468200	–0.38019000
H	–5.70732100	–0.88317800	–0.60293300
C	–4.53357000	–0.73398500	1.71814500
H	–4.48250300	–1.79406900	1.98534400
H	–3.96531200	–0.15598200	2.44248300
H	–5.57803300	–0.40563000	1.72353900
O	–3.95554100	–0.51474600	0.43969100

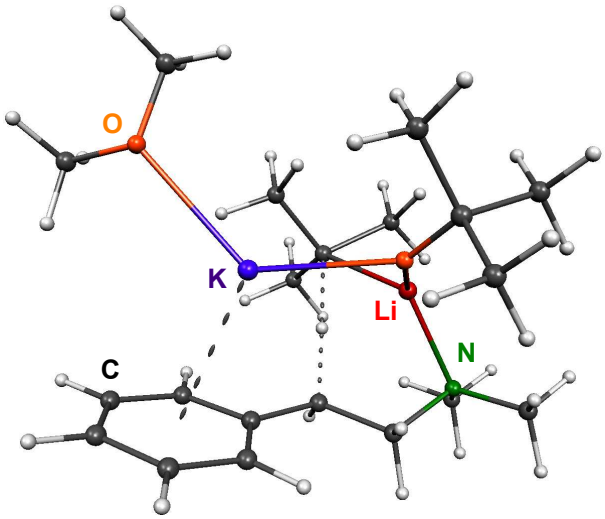


Fig. 25 Molekel plot of [**1**·*t*-BuLi·*t*-BuOK·Me_2O] (transition state)

Table 40 Cartesian coordinates of [**1**·*t*-BuLi·*t*-BuOK·Me_2O] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	2.74804500	–2.72673000	–0.65509000
C	2.86225000	–2.41847400	–2.01580400
C	1.69945100	–2.11412800	–2.72357100
C	0.45715800	–2.07928900	–2.08905400
C	0.32334400	–2.33719700	–0.70492400
C	1.51353600	–2.68976800	–0.02018300
C	–0.90502300	–2.13469100	0.07087600
C	–2.16290800	–1.80059800	–0.71051000
N	–3.15361000	–1.07715700	0.11727400
C	–3.70656100	–1.95028300	1.14835700
C	–4.23091900	–0.57711600	–0.73265000
Li	–1.72414000	0.32888700	0.61032900

O	–1.03731400	1.42926000	–0.59565600
C	–1.40054500	2.66589500	–1.11419900
C	–1.67461500	2.54540900	–2.62122200
C	–0.26132300	3.67793200	–0.89486600
C	–2.66292400	3.19533000	–0.41583500
H	3.63002200	–3.00047700	–0.08611200
H	3.82295100	–2.44996500	–2.51412700
H	1.75327400	–1.91147100	–3.78754900
H	–0.41652100	–1.84924600	–2.68492300
H	1.44880100	–2.92065400	1.03730000
H	–0.65381300	–1.15225100	1.02817700
H	–1.05067700	–2.96509600	0.76732100
H	–2.64735400	–2.68852200	–1.15971100
H	–1.91597100	–1.11415700	–1.52369100
H	–4.44454300	–1.40037500	1.73508400
H	–2.91636800	–2.28736400	1.81664900
H	–4.19591500	–2.83069600	0.70263100
H	–4.95258400	–0.02810400	–0.12514200
H	–4.75506500	–1.39847300	–1.24548700
H	–3.81491900	0.09997800	–1.47955000
H	–1.94722200	3.50447000	–3.07321800
H	–2.48828700	1.83496500	–2.79107000
H	–0.78306700	2.16241700	–3.12762600
H	–0.50900400	4.67699400	–1.26658300
H	0.64331200	3.34266900	–1.41707000
H	–0.04150300	3.74678100	0.17522600
H	–2.98523600	4.16324200	–0.81257000
H	–2.47111900	3.30830700	0.65564700
H	–3.48126900	2.48028300	–0.54602800
C	–0.43422500	–0.30455700	2.35437500
C	–0.27499400	–1.52023100	3.25873500
C	0.83445700	0.53846900	2.44974600
C	–1.59359300	0.53450400	2.90194100
K	1.30676100	0.45787200	–0.62561000
H	–1.16563700	–2.15848600	3.25008100
H	–0.10137600	–1.22524000	4.30835300
H	0.57221200	–2.14554300	2.95735300
H	0.75237400	1.46748600	1.87108000
H	1.72280100	–0.01155400	2.11117000
H	1.03965000	0.84233700	3.49447600
H	–1.72443300	1.48710100	2.36627400
H	–1.42202700	0.81455700	3.95662000
H	–2.54840000	–0.00488800	2.87602000
C	3.49168000	2.71473100	1.16115700
H	2.68617300	3.32875900	0.76189200
H	3.27154700	2.45657000	2.20180400
H	4.43348900	3.27028100	1.11140300
C	4.59015900	0.66828400	0.81471500
H	4.40221200	0.35834600	1.84820600
H	4.58142000	–0.20575400	0.16555200
H	5.56725000	1.15832400	0.75483600
O	3.56848500	1.54241000	0.36440900

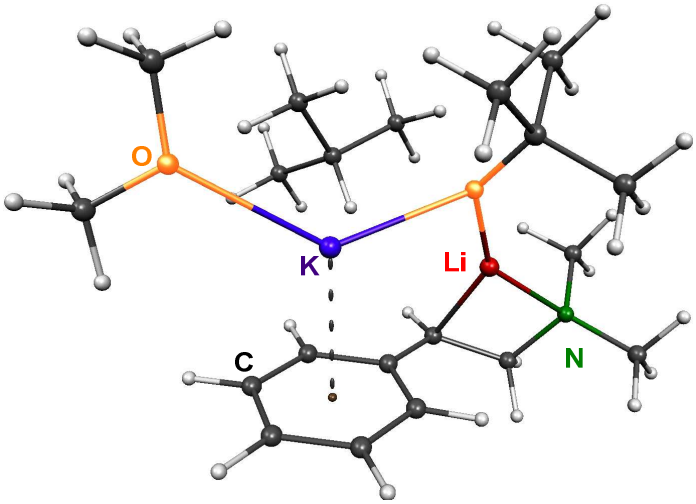


Fig. 26 Molekel plot of [**1**·*t*-BuLi·*t*-BuOK·Me_2O] (product)

Table 41 Cartesian coordinates of [**1**·*t*-BuLi·*t*-BuOK·Me_2O] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	1.47464200	–3.07666300	–0.32422700
C	1.35275500	–3.01464200	–1.72674200
C	0.13060500	–2.56953900	–2.24363300
C	–0.92156000	–2.18307700	–1.41998700
C	–0.83966000	–2.26239800	0.01691700
C	0.44259900	–2.69866600	0.51352100
C	–1.89546800	–1.92795500	0.88001300
C	–3.30305400	–1.81005900	0.37834100
N	–3.68621200	–0.41671400	–0.02032600
C	–4.02988300	0.36136600	1.16806900
C	–4.80077300	–0.41507000	–0.95776900
Li	–1.72227900	0.08585400	–0.13987100
O	–0.61476800	1.40592800	–0.51551100
C	–0.87207100	2.66630400	–1.04350300
C	–2.06275100	2.60567700	–2.01362800
C	0.36528200	3.16983100	–1.80652800
C	–1.19370700	3.65859300	0.08330000
H	2.39458500	–3.44709800	0.11894800
H	2.15056800	–3.34871000	–2.37741000
H	–0.00983900	–2.52090000	–3.31896300
H	–1.84431700	–1.85070700	–1.88572000
H	0.56562500	–2.79374600	1.58732300
H	0.29601100	–0.29239400	1.83809800
H	–1.74102300	–2.08217100	1.94192200
H	–4.02111500	–2.16314500	1.13413500
H	–3.44958300	–2.42983300	–0.51381400
H	–4.21282800	1.40227100	0.89372500
H	–3.20070300	0.32598500	1.87882600
H	–4.92772400	–0.04137200	1.66339100
H	–5.05303300	0.61173300	–1.22805400
H	–5.69400000	–0.89420100	–0.52752900
H	–4.51957000	–0.95285300	–1.86468600
H	–2.28381400	3.57768500	–2.46611700
H	–2.95395700	2.26365000	–1.47728300
H	–1.85007400	1.88664800	–2.81058500
H	0.22168100	4.16919700	–2.22782500
H	0.59762200	2.48547900	–2.63049500
H	1.22282100	3.20726800	–1.12471100
H	–1.40528000	4.66288300	–0.29761700
H	–0.34946200	3.71673400	0.77605500

H	–2.06603500	3.30597300	0.64160300
C	0.71716800	0.28430900	2.66905600
C	1.24318800	–0.69600200	3.71665600
C	1.84877400	1.16577600	2.13825200
C	–0.40649500	1.14608800	3.24172700
K	1.39996900	–0.05269900	–0.93330100
H	0.44613600	–1.35336900	4.07412000
H	1.64469800	–0.15300900	4.57884800
H	2.04265800	–1.32240600	3.31010100
H	1.47580700	1.84424000	1.36497100
H	2.66251000	0.55995500	1.72258000
H	2.27180100	1.77148500	2.94678700
H	–0.81046200	1.80762500	2.47235900
H	–0.03632000	1.76024600	4.06999100
H	–1.21887700	0.52084200	3.62249300
C	4.65043500	1.63340800	–0.35283700
H	3.92719000	2.42488500	–0.54043400
H	4.91234400	1.62540500	0.71006100
H	5.55095700	1.81159200	–0.94902500
C	4.90597400	–0.69852700	–0.50492700
H	5.16639200	–0.77637200	0.55597900
H	4.37137300	–1.59500700	–0.81505500
H	5.82116900	–0.59540200	–1.09657400
O	4.04489200	0.40646100	–0.72551800

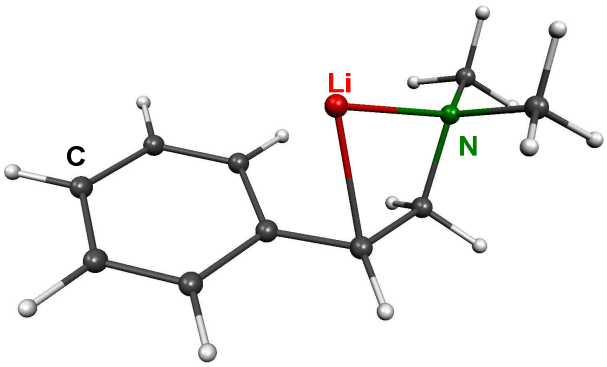


Fig. 27 Molekel plot of [**5**-Li] (starting material)

Table 42 Cartesian coordinates of [**5**-Li] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–2.24980700	1.50520900	0.04879000
C	–3.39730000	0.76468800	0.29986300
C	–3.30597100	–0.64592000	0.23524900
C	–2.11455700	–1.28232400	–0.04988300
C	–0.89733600	–0.55650900	–0.30336600
C	–1.02056700	0.87939900	–0.23228300
C	0.35375400	–1.21748800	–0.46331700
C	1.57663900	–0.48128300	–0.92240800
N	2.30864000	0.20998200	0.23487800
C	3.08012600	1.37425000	–0.21468400
C	3.19096400	–0.75012400	0.91475900
Li	0.52262500	0.11336800	1.14834100
H	–2.29197700	2.59333100	0.05694100
H	–4.34228600	1.25123100	0.52318300
H	–4.19722800	–1.24751500	0.40598400
H	–2.08159500	–2.36909700	–0.10242300
H	–0.18224700	1.51062900	–0.53379200
H	0.34791100	–2.30053600	–0.54712200

H	2.28927200	–1.15433000	–1.42343900
H	1.34088400	0.32457600	–1.63440400
H	3.55736900	1.85944200	0.64415100
H	3.86765500	1.09571000	–0.93623800
H	2.41450100	2.09822400	–0.69585000
H	3.62233500	–0.29856400	1.81581200
H	2.61321800	–1.63539800	1.20236200
H	4.01816000	–1.07707100	0.25934300

Table 43 Cartesian coordinates of [**5**-Li] (starting material) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	–2.24980700	1.50520900	0.04879000
C	–3.39730000	0.76468800	0.29986300
C	–3.30597100	–0.64592000	0.23524900
C	–2.11455700	–1.28232400	–0.04988300
C	–0.89733600	–0.55650900	–0.30336600
C	–1.02056700	0.87939900	–0.23228300
C	0.35375400	–1.21748800	–0.46331700
C	1.57663900	–0.48128300	–0.92240800
N	2.30864000	0.20998200	0.23487800
C	3.08012600	1.37425000	–0.21468400
C	3.19096400	–0.75012400	0.91475900
Li	0.52262500	0.11336800	1.14834100
H	–2.29197700	2.59333100	0.05694100
H	–4.34228600	1.25123100	0.52318300
H	–4.19722800	–1.24751500	0.40598400
H	–2.08159500	–2.36909700	–0.10242300
H	–0.18224700	1.51062900	–0.53379200
H	0.34791100	–2.30053600	–0.54712200
H	2.28927200	–1.15433000	–1.42343900
H	1.34088400	0.32457600	–1.63440400
H	3.55736900	1.85944200	0.64415100
H	3.86765500	1.09571000	–0.93623800
H	2.41450100	2.09822400	–0.69585000
H	3.62233500	–0.29856400	1.81581200
H	2.61321800	–1.63539800	1.20236200
H	4.01816000	–1.07707100	0.25934300

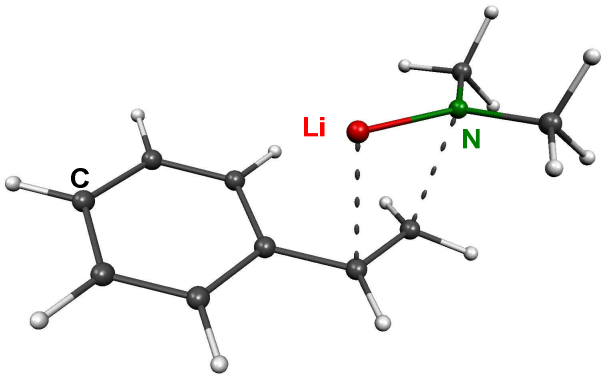


Fig. 28 Molekel plot of [**5**-Li] (transition state)

Table 44 Cartesian coordinates of [**5**-Li] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	2.24192700	1.52773500	0.14614600
C	3.39628100	0.89826400	–0.30859100
C	3.39425000	–0.48936500	–0.47236800
C	2.25701200	–1.23147200	–0.18792200
C	1.08137500	–0.61596600	0.28487700

C	1.09684600	0.78637400	0.43598900
C	–0.12491000	–1.41531100	0.52537100
C	–1.27956000	–0.90997000	1.05440300
Li	–0.86229600	–0.05669100	–1.01700200
N	–2.56710100	0.33626800	–0.53522200
C	–3.66205400	–0.57995200	–0.73212000
C	–3.02961100	1.49147600	0.18626700
H	2.22572400	2.60284900	0.27885900
H	4.28382600	1.47541800	–0.53412800
H	4.28622300	–0.99314900	–0.82505900
H	2.26707800	–2.30816300	–0.31691700
H	0.21694800	1.30423500	0.80540300
H	–0.10167700	–2.44401500	0.18039900
H	–2.13541100	–1.55538100	1.20037500
H	–1.30060700	0.02404800	1.60262100
H	–4.43801800	–0.16800600	–1.39868200
H	–4.17418600	–0.84266900	0.21495700
H	–3.31099600	–1.51484900	–1.18467900
H	–3.84533400	2.01697100	–0.33780700
H	–3.42568400	1.23198100	1.18951600
H	–2.22062200	2.21605300	0.33040000

Table 45 Cartesian coordinates of [**5**-Li] (transition state) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	2.32994600	1.51546100	0.06130700
C	3.44912200	0.79845600	–0.36244600
C	3.36303300	–0.60136500	–0.43887800
C	2.18785600	–1.26351900	–0.10693800
C	1.03206600	–0.56141000	0.33362600
C	1.14118700	0.85736100	0.39796700
C	–0.20549400	–1.27246500	0.62033400
C	–1.37296700	–0.66810400	1.08870300
Li	–0.75614300	0.06445700	–0.98023200
N	–2.51822400	0.28728900	–0.46166900
C	–3.17219800	1.43341400	0.13271100
C	–3.48916500	–0.72425900	–0.83314300
H	2.37482700	2.59970100	0.13809300
H	4.36968000	1.31157800	–0.62561500
H	4.22665700	–1.17892100	–0.76139000
H	2.14455200	–2.34905400	–0.16920400
H	0.30542100	1.45138700	0.76684100
H	–0.22231000	–2.33565700	0.38783400
H	–2.20790200	–1.30199500	1.37162900
H	–1.32708900	0.27262600	1.63448900
H	–3.86728000	1.92530000	–0.57171100
H	–3.76864000	1.16630500	1.02967600
H	–2.43370600	2.18689700	0.43850600
H	–4.13969300	–0.38821300	–1.66044400
H	–2.97976700	–1.63850300	–1.17112900
H	–4.15907500	–1.00726500	0.00534800

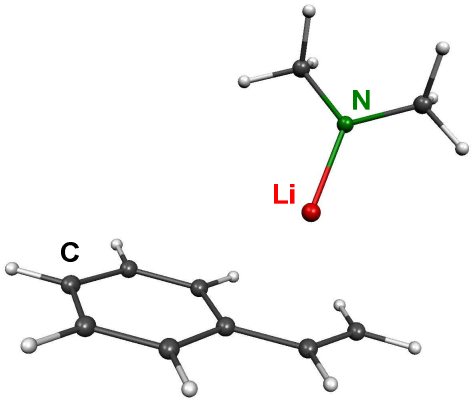


Fig. 29 Molekel plot of [**5**-Li] (product)

Table 46 Cartesian coordinates of [**5**-Li] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	1.42685800	–1.24286500	–1.08094700
C	2.20145200	–1.59730800	0.02829700
C	2.44559900	–0.65214100	1.02738400
C	1.91088700	0.63430100	0.92160400
C	1.10564800	0.99103500	–0.17003500
C	0.88531100	0.03895200	–1.17812100
C	0.42561700	2.30294100	–0.20673800
C	–0.86698400	2.41717500	–0.52176100
Li	–0.16268700	–0.88145000	0.73197700
N	–1.92218300	–0.79684400	0.40551100
C	–2.95969300	–0.25986500	1.24398400
C	–2.51136000	–1.23924500	–0.82874500
H	1.22640900	–1.96974500	–1.85784000
H	2.60893400	–2.59659600	0.11135100
H	3.04306100	–0.91727900	1.89062300
H	2.08361600	1.35766000	1.70996700
H	0.25928900	0.30301600	–2.02048100
H	1.00943000	3.17055500	0.08538600
H	–1.35387500	3.38450800	–0.52440000
H	–1.46878200	1.53360600	–0.71810500
H	–3.75088900	–0.99774600	1.48294000
H	–3.48585300	0.60055800	0.77680700
H	–2.55327000	0.09593900	2.19761700
H	–3.27836600	–2.02664500	–0.69139200
H	–3.02460300	–0.42049700	–1.38110500
H	–1.75176500	–1.65294900	–1.50540800

Table 47 Cartesian coordinates of [**5**-Li] (product) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	–1.95714400	–1.26176500	1.06042400
C	–2.88036300	–1.49192800	0.03649800
C	–3.01123800	–0.56062000	–0.99990600
C	–2.21860900	0.58506000	–1.01361700
C	–1.28415000	0.83649300	0.01295500
C	–1.16916900	–0.10966700	1.05583300
C	–0.44820900	2.04957900	–0.06054700
C	0.51584700	2.42520700	0.80737700
H	–1.85030200	–1.97905000	1.86961200
H	–3.49278100	–2.38933300	0.04549100
H	–3.72678000	–0.73108100	–1.79977900
H	–2.31949300	1.30220000	–1.82538300
H	–0.47408600	0.05580200	1.87506700

H	–0.62664900	2.67742900	–0.93366500
H	1.09503900	3.32682700	0.63387000
H	0.74907200	1.87606500	1.71642500
N	2.69567100	–0.49967600	–0.28589200
C	2.89327900	–1.90623100	–0.02587700
C	3.97693200	0.15251200	–0.42326500
Li	1.12269500	0.32338900	–0.34271100
H	3.45292600	–2.42037000	–0.83887100
H	3.47059500	–2.10296000	0.90561600
H	1.92937800	–2.42776100	0.07719800
H	4.58687600	–0.26706100	–1.25409200
H	3.85298200	1.22692500	–0.62837800
H	4.61237900	0.06810100	0.48700800

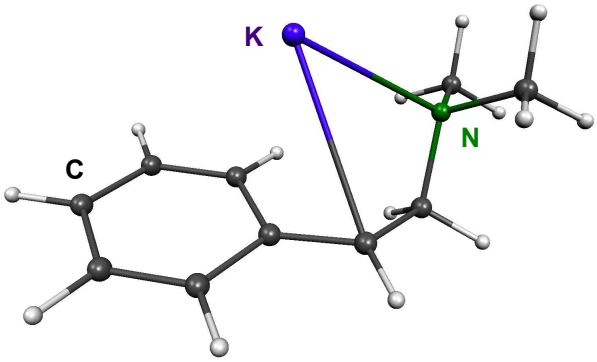


Fig. 30 Molekel plot of [**5**-K] (starting material)

Table 48 Cartesian coordinates of [**5**-K] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	2.18451500	0.03698200	1.52772700
C	3.22660200	0.32664300	0.63852600
C	3.10401000	–0.17489000	–0.67392600
C	1.97060000	–0.83868000	–1.09971900
C	0.81290100	–1.01078800	–0.25314300
C	1.02599500	–0.61287300	1.11999100
C	–0.43265600	–1.36636400	–0.76912900
C	–1.66827800	–1.32489800	0.06162200
K	0.14086200	1.61346900	–0.41036100
N	–2.24357100	0.05820800	0.20650000
C	–2.90851900	0.42921800	–1.03573700
C	–3.21145100	0.08858500	1.29550400
H	2.27672500	0.32671900	2.57048100
H	4.12669300	0.82864700	0.96696000
H	3.92445700	–0.04349600	–1.37270800
H	1.91228900	–1.19925000	–2.12222600
H	0.24551500	–0.78973400	1.85099200
H	–0.49638200	–1.71484700	–1.79385900
H	–2.45356800	–1.97594000	–0.35641600
H	–1.48948500	–1.67703600	1.08304600
H	–3.26302000	1.46363300	–0.98663300
H	–3.77670700	–0.21812200	–1.24608100
H	–2.20763100	0.32034700	–1.86768600
H	–3.64687800	1.08696900	1.38301700
H	–4.03166600	–0.63121800	1.13713500
H	–2.71404100	–0.15765700	2.23505600

Table 49 Cartesian coordinates of [**5**-K] (starting material) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	–2.80719400	–1.36608000	–0.70078500
C	–3.84979500	–0.46106200	–0.47640300
C	–3.56632200	0.69039000	0.27750700
C	–2.28925200	0.92935200	0.76763400
C	–1.19368300	0.03891100	0.53556900
C	–1.51974500	–1.13049700	–0.21502700
C	0.11928000	0.36028500	1.03854200
C	1.24811600	–0.62546400	1.14417100
K	1.56903400	2.03631600	–0.66514200
N	2.32890900	–0.55887100	0.06762700
C	3.54604300	–1.23512100	0.52396100
C	1.86607800	–1.18078000	–1.17696800
H	–2.99732500	–2.28040800	–1.26186700
H	–4.84899800	–0.64813400	–0.86056000
H	–4.35922100	1.40624900	0.49103800
H	–2.10685800	1.82742000	1.35919000
H	–0.75512700	–1.87966900	–0.40220300
H	0.09759300	1.07631700	1.86553700
H	1.79323800	–0.44645300	2.08012600
H	0.90001200	–1.67884100	1.17769900
H	4.31873700	–1.18360200	–0.25256400
H	3.37396400	–2.30196600	0.76286400
H	3.92930400	–0.74341000	1.42491700
H	2.63053100	–1.08045200	–1.95872000
H	1.64962900	–2.25889300	–1.05290800
H	0.93935500	–0.70567100	–1.51744800

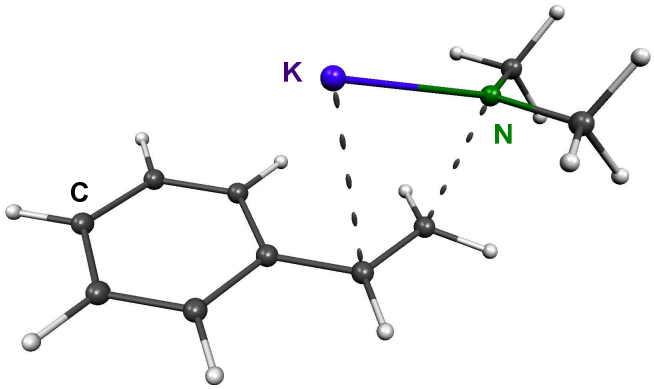


Fig. 31 Molekel plot of [**5**-K] (transition state)

Table 50 Cartesian coordinates of [**5**-K] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–2.42092300	1.47804700	–0.59804600
C	–3.57709100	0.94146600	–0.03119300
C	–3.59970600	–0.41091600	0.30863200
C	–2.48299800	–1.21056100	0.08754100
C	–1.30997200	–0.68978700	–0.48771600
C	–1.30121600	0.68053200	–0.81738200
C	–0.13332400	–1.55021800	–0.65309600
C	1.03888700	–1.16593300	–1.20785200
K	0.71571200	0.15378800	1.65487600
N	2.73141400	0.31200900	0.15667000
C	3.89153000	–0.49942300	–0.08218700
C	2.81462600	1.46418500	–0.69458900
H	–2.38910500	2.52580700	–0.87341800

H	–4.44570000	1.56529300	0.13825800
H	–4.49132300	–0.84568200	0.74452400
H	–2.51521700	–2.26361900	0.34721700
H	–0.41604100	1.12107200	–1.26275800
H	–0.22027100	–2.55080200	–0.23757200
H	1.86851300	–1.85603200	–1.27431000
H	1.15772300	–0.23634400	–1.74598400
H	4.84124300	0.02060400	0.15413400
H	3.99027600	–0.81763800	–1.14565100
H	3.86467300	–1.41285000	0.52422800
H	3.73393000	2.06228500	–0.53570200
H	2.81953700	1.21253200	–1.78230200
H	1.96446500	2.14499000	–0.53466600

Table 51 Cartesian coordinates of [**5**-K] (transition state) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	2.67859700	–1.14620900	–0.95070100
C	3.71815600	–0.65594100	–0.15098100
C	3.51564400	0.54326800	0.54661600
C	2.30442400	1.22537000	0.45558200
C	1.22940600	0.74887700	–0.34328000
C	1.46157100	–0.46865300	–1.04367600
C	–0.03238400	1.47008700	–0.37893500
C	–1.17106800	1.08764800	–1.05880700
K	–0.58845600	–0.90946200	1.36454600
N	–2.68529600	–0.27848900	–0.00694600
C	–3.52628600	0.67917200	0.67481100
C	–3.40145900	–0.83908600	–1.12707600
H	2.81854200	–2.06458000	–1.51787400
H	4.66403100	–1.18606600	–0.08259100
H	4.31253700	0.95228300	1.16447100
H	2.17479800	2.16059600	0.99817700
H	0.68772200	–0.86751000	–1.69632500
H	–0.07247500	2.37859700	0.22295700
H	–1.99908100	1.78378700	–1.14502600
H	–1.13516800	0.32903400	–1.83540900
H	–4.40514600	0.21120000	1.16482900
H	–3.93986100	1.46690700	0.00293600
H	–2.96132800	1.20577500	1.46288200
H	–4.33043700	–1.36438400	–0.82419800
H	–3.71803100	–0.07224200	–1.87258000
H	–2.77798200	–1.57139000	–1.66132900

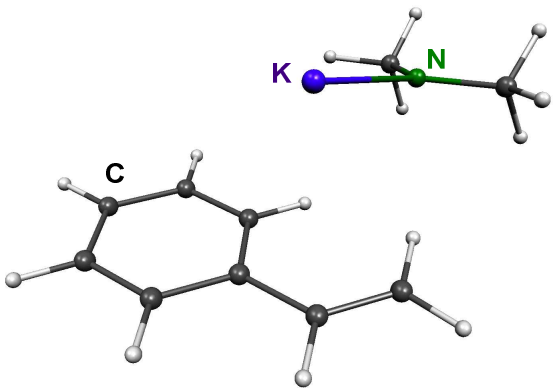


Fig. 32 Molekel plot of [**5**-K] (product)

Table 52 Cartesian coordinates of [**5**-K] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	1.42126400	–1.21356600	–1.21772200
C	2.56350400	–1.43316600	–0.44527400
C	3.07141000	–0.39918400	0.34302400
C	2.42729000	0.83723300	0.36732500
C	1.26045700	1.05858700	–0.37899200
C	0.77498000	0.02076900	–1.19052000
C	0.52744800	2.33201800	–0.23798800
C	–0.80083000	2.43084900	–0.37039200
K	–0.30407300	–0.72838500	1.58510800
N	–2.28927700	–0.57533900	0.05149700
C	–3.46374500	0.19668000	0.34744900
C	–2.49337000	–1.20593300	–1.21970200
H	1.02934800	–2.00424200	–1.84581700
H	3.06543600	–2.39253300	–0.47524700
H	3.97047000	–0.55174900	0.92809200
H	2.82210100	1.63974500	0.98158500
H	–0.11740700	0.17708200	–1.78185000
H	1.12127000	3.20160100	0.03033600
H	–1.29451000	3.38586400	–0.23666000
H	–1.41641500	1.55109200	–0.55794200
H	–4.39122200	–0.41142900	0.40770800
H	–3.68514900	0.98127000	–0.41596100
H	–3.36614300	0.72038100	1.30953300
H	–3.39758000	–1.85011700	–1.25669700
H	–2.62568100	–0.47880100	–2.05903500
H	–1.64263500	–1.84720100	–1.48880600

Table 53 Cartesian coordinates of [**5**-K] (product) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	1.69908100	–1.63300300	–0.65058800
C	2.96502400	–1.57799500	–0.05536700
C	3.49273500	–0.33985500	0.32649700
C	2.75479300	0.82727400	0.12064600
C	1.47587700	0.78979200	–0.47178500
C	0.96183700	–0.46656500	–0.86549600
C	0.72269000	2.04595500	–0.63969000
C	–0.56375900	2.16697900	–1.02183700
K	–0.85477800	0.20579800	1.72702600
N	–2.58268500	–0.52013700	0.04127000
C	–3.73124300	0.24539000	–0.36817200
C	–2.62274900	–1.80028100	–0.61531700
H	1.28484500	–2.58836800	–0.96270900
H	3.53832600	–2.48866300	0.09760800
H	4.47971500	–0.28232600	0.77883900
H	3.17357200	1.78757300	0.41634000
H	–0.01940700	–0.53168800	–1.32669200
H	1.28886600	2.95112200	–0.41400200
H	–1.01614200	3.15187800	–1.10603600
H	–1.20810200	1.31108700	–1.22257100
H	–4.70697500	–0.24353800	–0.12942600
H	–3.77222000	0.44226100	–1.47072200
H	–3.74782500	1.23307800	0.12415100
H	–3.54303200	–2.39336000	–0.39199600
H	–2.59043000	–1.73470800	–1.73397600
H	–1.76733700	–2.42970000	–0.31453100

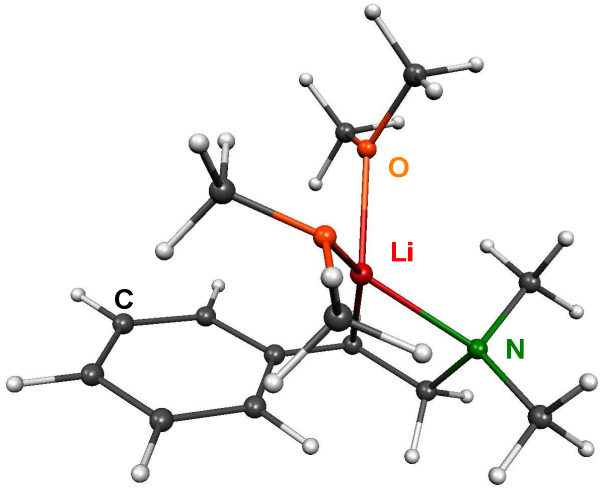


Fig. 33 Molekel plot of [**5**-Li·$(Me_2O)_2$] (starting material)

Table 54 Cartesian coordinates of [**5**-Li·$(Me_2O)_2$] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–3.35080000	0.11832500	–1.19366200
C	–3.69582600	–0.25687500	0.11813700
C	–2.75779700	–0.98380800	0.84465000
C	–1.51260700	–1.31836600	0.31389100
C	–1.14612500	–0.98353300	–1.03416200
C	–2.13605500	–0.22472700	–1.74956400
C	0.10231700	–1.30966300	–1.59997200
C	1.06772400	–2.17854800	–0.86877200
N	1.90403200	–1.40491200	0.12232000
C	3.03530600	–0.79897600	–0.57553000
C	2.39400400	–2.26639600	1.19070700
Li	0.51061400	0.15409200	0.06859000
C	2.00651300	2.76596600	–0.15129900
O	1.09929700	1.85984500	–0.75619500
C	0.90822000	2.12299800	–2.13988800
C	–0.97011600	1.98760500	1.67957700
O	0.13734800	1.09287600	1.79861800
C	0.04936300	0.31151800	2.98169600
H	–4.06221000	0.67573100	–1.79457800
H	–4.66036700	–0.00320900	0.53828200
H	–2.99654900	–1.30748100	1.85417400
H	–0.83238000	–1.90553600	0.92401200
H	–1.92437800	0.04700100	–2.77972500
H	0.25770300	–1.12312600	–2.65577000
H	1.74781400	–2.69845100	–1.55913500
H	0.55629300	–2.95378500	–0.28418500
H	2.66197100	–0.23605200	–1.43274800
H	3.73766600	–1.56606600	–0.93850800
H	3.57203700	–0.11952600	0.09163900
H	2.99904100	–1.68423400	1.88988500
H	3.01277500	–3.08893300	0.79954600
H	1.54988700	–2.69830900	1.73210900
H	2.99404900	2.68151700	–0.61657700
H	1.64381400	3.79354700	–0.25815700
H	2.06482700	2.50452400	0.90265800
H	0.20580900	1.38125400	–2.50907500
H	1.85870000	2.03527400	–2.67602200
H	0.50330600	3.13065200	–2.27475600
H	–1.90242800	1.42345100	1.60440000
H	–0.99586700	2.65842300	2.54396400

H	–0.81858700	2.55992700	0.76721900
H	0.89199500	–0.37712900	2.97820700
H	–0.88750100	–0.25145000	2.99471800
H	0.10463000	0.95919400	3.86216800

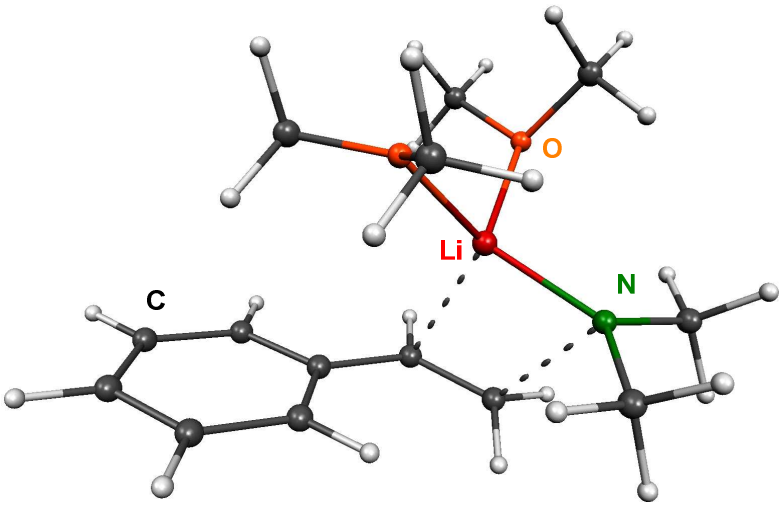


Fig. 34 Molekel plot of [**5**-Li·(Me_2O)$_2$] (transition state)

Table 55 Cartesian coordinates of [**5**-Li·(Me_2O)$_2$] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–3.77922700	0.72971900	–0.79015100
C	–4.13578200	–0.06883100	0.29803500
C	–3.25043800	–1.06102300	0.72069000
C	–2.03016500	–1.24757300	0.07875900
C	–1.65869900	–0.45941300	–1.02983000
C	–2.56620300	0.53650200	–1.44021900
C	–0.39270300	–0.63442900	–1.73287500
C	0.47323800	–1.68489500	–1.53432200
N	1.96936500	–1.52753500	0.13713800
C	3.19306000	–1.80165600	–0.57305400
C	1.65098600	–2.65536000	0.97103400
Li	1.01264000	0.07462700	–0.11003400
C	1.66685900	2.74398600	–1.19985900
O	2.19921900	1.51040300	–0.75024900
C	3.22761600	1.69583400	0.21659200
C	–0.93465100	1.81376200	1.41651900
O	0.23886700	1.00826600	1.43483800
C	0.39081100	0.31546900	2.66766600
H	–4.45525200	1.50191900	–1.13919600
H	–5.08351600	0.07601400	0.80124400
H	–3.50906200	–1.69247900	1.56341100
H	–1.35297000	–2.01274100	0.44015100
H	–2.31018400	1.15515600	–2.29471000
H	–0.14802600	0.11109500	–2.48469400
H	1.30529900	–1.80957100	–2.21559100
H	0.14508300	–2.58686700	–1.03046000
H	3.43331700	–0.98327000	–1.26022000
H	3.13847500	–2.73166400	–1.17489200
H	4.05290800	–1.93133000	0.10798100
H	2.44384300	–2.86575000	1.71010100
H	1.51914000	–3.59419400	0.39362000
H	0.72363100	–2.48417000	1.52778000
H	1.25878400	3.31320100	–0.35765100
H	2.44321500	3.33490800	–1.69515800

H	0.87310700	2.51660500	–1.90950300
H	3.52954100	0.70499700	0.54897000
H	2.84322400	2.26865600	1.06651200
H	4.07395700	2.22204000	–0.23460300
H	–1.82432100	1.19731500	1.56663800
H	–0.86888500	2.57978800	2.19593800
H	–0.99314000	2.28350400	0.43754200
H	1.29246200	–0.28771900	2.58221000
H	–0.47490000	–0.33051000	2.84473700
H	0.48788600	1.03200900	3.48933900

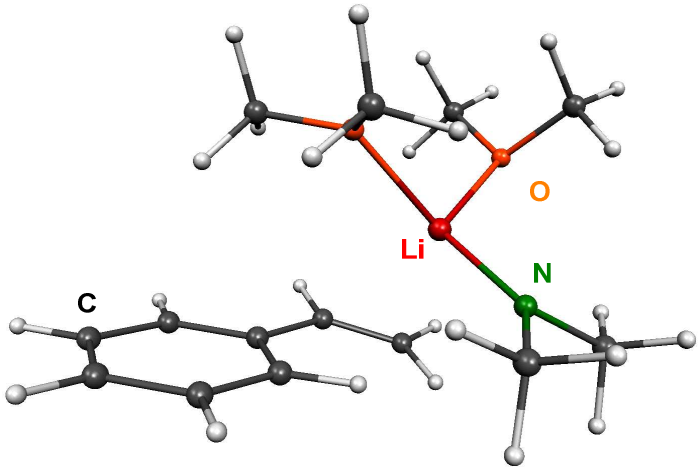


Fig. 35 Molekel plot of [**5**-Li·$(Me_2O)_2$] (product)

Table 56 Cartesian coordinates of [**5**-Li·$(Me_2O)_2$] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	4.02847400	–0.67841500	–0.08270700
C	3.92317800	0.54401300	0.57895200
C	2.79203100	1.33811200	0.38620100
C	1.77180600	0.92220900	–0.46415300
C	1.86780700	–0.30941500	–1.12892600
C	3.00368800	–1.10198500	–0.92446500
C	0.79314700	–0.81057100	–2.00751300
C	–0.22381900	–0.09180900	–2.50286400
N	–1.49630200	1.83775000	–0.03906800
C	–2.41392700	2.31704400	–1.03939900
C	–0.90571800	2.97599300	0.60644100
Li	–1.11681100	0.02290100	–0.07812800
C	–2.55193900	–2.51186600	–0.46600800
O	–2.68547300	–1.10355600	–0.41993800
C	–3.72533600	–0.69018800	0.46333200
C	0.65689000	–1.77859500	1.68175600
O	–0.41776600	–0.86275500	1.53697000
C	–0.47852500	0.06129000	2.62228800
H	4.90434600	–1.30040200	0.05770800
H	4.71609000	0.87606000	1.23804800
H	2.69994900	2.28840100	0.89880400
H	0.87926700	1.53080300	–0.57943200
H	3.08311400	–2.05707400	–1.43340400
H	0.86876800	–1.86278800	–2.27339400
H	–0.97097600	–0.55887800	–3.13314500
H	–0.34682100	0.96515800	–2.29400400
H	–2.89557900	1.48336200	–1.56728900
H	–1.92766200	2.94719400	–1.81753900
H	–3.22591300	2.94856600	–0.62096900

H	–1.65160600	3.63915300	1.09138800
H	–0.34246800	3.63542200	–0.09263100
H	–0.19702600	2.67039900	1.38642700
H	–2.29826500	–2.90435500	0.52456000
H	–3.48216900	–2.97139500	–0.81399600
H	–1.75047800	–2.73935400	–1.16780600
H	–3.68606300	0.39635200	0.50213400
H	–3.54950500	–1.10143300	1.46310700
H	–4.69207200	–1.03659300	0.08644900
H	1.61388200	–1.24892500	1.68265500
H	0.54236000	–2.34424400	2.61213500
H	0.62335100	–2.45988000	0.83320400
H	–1.26638600	0.77336000	2.38306700
H	0.47590300	0.58763200	2.71708500
H	–0.70012900	–0.47391200	3.55083300

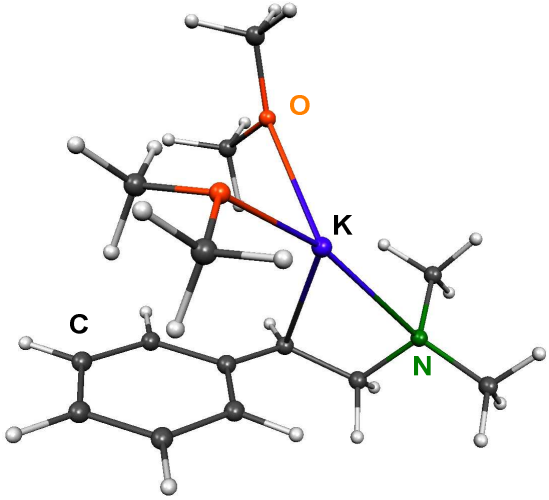


Fig. 36 Molekel plot of [**5**-K·$(Me_2O)_2$] (starting material)

Table 57 Cartesian coordinates of [**5**-K·$(Me_2O)_2$] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–1.88492100	–2.10160700	–1.90645000
C	–2.16910200	–2.82287900	–0.73205500
C	–1.18602400	–2.84455900	0.25685200
C	0.02873300	–2.18108400	0.10447700
C	0.37269500	–1.48043400	–1.10516400
C	–0.68214900	–1.44769600	–2.08418200
C	1.60543400	–0.84076400	–1.32057300
C	2.78691000	–1.08694700	–0.44168000
N	2.98584300	–0.10765600	0.67814900
C	3.42041600	1.16881500	0.12603600
C	4.00147300	–0.60479400	1.59533600
K	0.28706200	0.70350100	0.86720100
C	–1.24073800	3.94287800	–0.56369000
O	–0.48080300	2.75532500	–0.68762700
C	–0.35449500	2.34221900	–2.04462300
C	–2.96985800	0.56765800	0.56476900
O	–2.26452900	0.66860200	1.80011500
C	–2.72781000	–0.29966700	2.72858700
H	–2.62130900	–2.06584200	–2.70361500
H	–3.10566100	–3.35136600	–0.60907100
H	–1.36042700	–3.40041700	1.17411600
H	0.76564500	–2.26314700	0.89921400
H	–0.48844900	–0.93725200	–3.02333100
H	1.79755500	–0.46054000	–2.31884700

H	3.71634900	–1.09259900	–1.03821200
H	2.71930300	–2.06970100	0.04064400
H	2.69773600	1.50560200	–0.62098600
H	4.40069200	1.08248500	–0.37365900
H	3.50464500	1.91890000	0.91767300
H	4.16785600	0.11648600	2.39883000
H	4.96353100	–0.78064700	1.08484200
H	3.67090500	–1.54735900	2.03582100
H	–0.74560000	4.77140800	–1.08012600
H	–2.24228100	3.80555800	–0.98571100
H	–1.32413000	4.17068600	0.49724000
H	0.23781800	1.42706500	–2.05055500
H	0.15177600	3.11682100	–2.62944900
H	–1.34200800	2.14469700	–2.47410100
H	–2.81832800	–0.41732600	0.11375800
H	–4.03889700	0.74131900	0.72777000
H	–2.57502700	1.33929900	–0.09400900
H	–2.14834500	–0.18024100	3.64284700
H	–2.59139700	–1.30885400	2.32907800
H	–3.78775100	–0.13621300	2.95023200

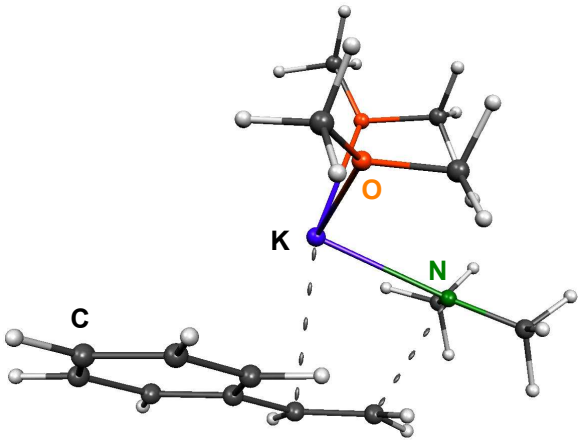


Fig. 37 Molekel plot of [**5**-K·$(Me_2O)_2$] (transition state)

Table 58 Cartesian coordinates of [**5**-K·$(Me_2O)_2$] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	4.09413000	–0.32528000	–1.55094700
C	4.19482700	–1.17037200	–0.44572300
C	3.40628100	–0.90798600	0.67451400
C	2.53163700	0.17389700	0.69446700
C	2.42546100	1.04758300	–0.40722600
C	3.22440700	0.75937300	–1.53131800
C	1.51488700	2.19216500	–0.44137000
C	0.68376000	2.57279700	0.56499100
N	–1.57400700	1.70782900	0.71153800
C	–2.19794300	2.50988400	–0.30478700
C	–1.89317300	2.27120800	1.99035600
K	–0.39589800	–0.11729700	–0.71980300
C	–3.42622200	–1.86454200	–2.45679200
O	–2.83782100	–0.99454100	–1.51108100
C	–3.74738600	–0.65864700	–0.46634400
C	0.46620200	–3.00038000	1.72304600
O	–0.31304700	–1.90599600	1.28461300
C	–1.12322000	–1.37559700	2.32624200
H	4.70012700	–0.50860700	–2.43070500
H	4.87591900	–2.01209900	–0.45520100
H	3.47480300	–1.55072400	1.54511800

H	1.92963900	0.34873700	1.57882800
H	3.16545200	1.41583500	–2.39332900
H	1.49700600	2.75008300	–1.37343800
H	0.11824200	3.49111200	0.48317600
H	0.75465000	2.15262900	1.55992600
H	–1.89102600	2.19106600	–1.31321100
H	–1.94718300	3.59064600	–0.23021800
H	–3.30667500	2.46747000	–0.28665600
H	–2.98251500	2.30897700	2.19386000
H	–1.53872000	3.32128000	2.10613300
H	–1.43379000	1.69228200	2.80128300
H	–3.70147800	–2.81726400	–1.99097300
H	–4.32080700	–1.40801100	–2.89327500
H	–2.69439700	–2.04429100	–3.24259800
H	–3.24849100	0.08026200	0.16444300
H	–4.00071700	–1.55292600	0.11402300
H	–4.66141000	–0.23252600	–0.89245700
H	1.12327900	–2.69912300	2.54654200
H	–0.17654300	–3.82157300	2.05890300
H	1.07307100	–3.33077000	0.88222200
H	–1.63112100	–0.49798200	1.92589500
H	–0.50042000	–1.07708000	3.17669300
H	–1.85173500	–2.12389200	2.65761000

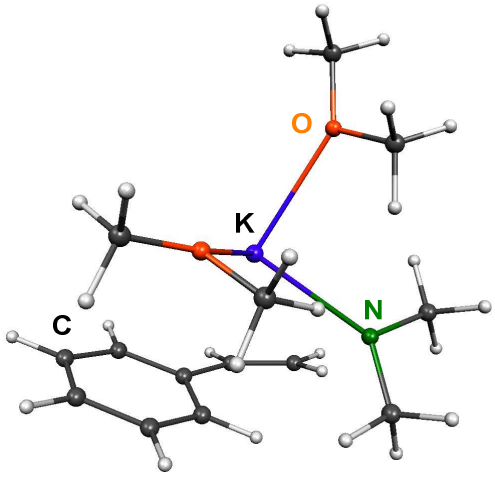


Fig. 38 Molekel plot of [**5**-K·$(Me_2O)_2$] (product)

Table 59 Cartesian coordinates of [**5**-K·$(Me_2O)_2$] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–3.41150200	1.23827100	–1.20361900
C	–3.17253100	1.64547200	0.10775500
C	–2.64060400	0.73840900	1.02489200
C	–2.34342200	–0.56520000	0.63883900
C	–2.56162200	–0.98070600	–0.68388900
C	–3.11066900	–0.06564900	–1.59279300
C	–2.17556500	–2.32892600	–1.14571000
C	–1.25021400	–3.09186900	–0.54998100
N	0.93406300	–1.40940700	1.39619400
C	1.78491100	–2.53912000	1.14280700
C	0.41434600	–1.54658800	2.72444500
K	0.42710300	–0.06420400	–0.76519600
C	3.96528600	0.40424300	–2.37508500
O	3.05210300	0.09840700	–1.34131000
C	3.68666800	0.08234600	–0.06363600
C	0.13549000	3.63046400	0.39376900
O	0.56467600	2.29209600	0.52225200

C	0.93837100	1.97780900	1.86153000
H	–3.83636700	1.93066300	–1.92048800
H	–3.41030200	2.65672500	0.41524900
H	–2.45908100	1.04255900	2.04899600
H	–1.92534400	–1.25884000	1.35660000
H	–3.29811300	–0.38140000	–2.61384000
H	–2.66971000	–2.67879400	–2.04845200
H	–1.00666000	–4.06796700	–0.95194600
H	–0.68973900	–2.74162000	0.31681700
H	2.19733300	–2.50829000	0.12228900
H	1.26865500	–3.52343100	1.24041700
H	2.65538400	–2.60768500	1.83430100
H	1.20075900	–1.62783200	3.50751500
H	–0.21888000	–2.45734800	2.86434500
H	–0.21421100	–0.68701500	2.99805500
H	4.40961900	1.39332700	–2.21860400
H	4.76418500	–0.34394400	–2.41684200
H	3.41701500	0.39852300	–3.31580100
H	2.93579100	–0.21775900	0.67148900
H	4.07939900	1.07843700	0.16919900
H	4.50729400	–0.64244900	–0.06348200
H	–0.73577400	3.81773100	1.03188000
H	0.93769200	4.32358100	0.67088500
H	–0.14029500	3.79195800	–0.64718100
H	1.17483600	0.91131700	1.89097500
H	0.10706000	2.19257500	2.54246000
H	1.80817200	2.57492900	2.15705200

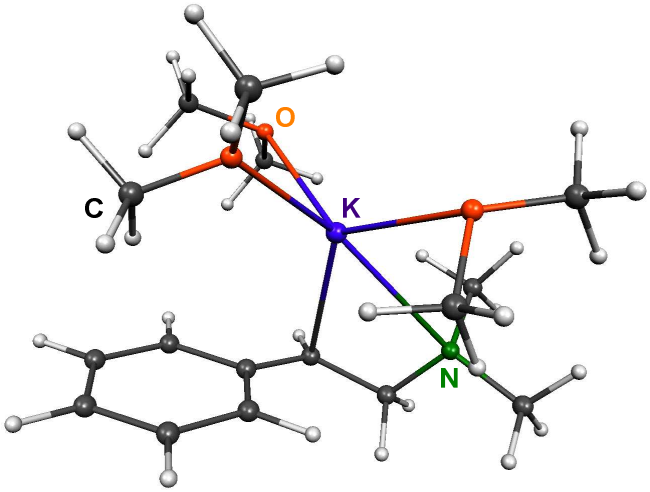


Fig. 39 Molekel plot of [**5**-K·$(Me_2O)_3$] (starting material)

Table 60 Cartesian coordinates of [**5**-K·$(Me_2O)_3$] (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	3.27070700	–1.36510900	–1.37334100
C	2.91315800	–0.60352900	–2.50044000
C	1.55098400	–0.45404800	–2.76308600
C	0.57662800	–1.03778000	–1.95889300
C	0.90979900	–1.89099800	–0.84626800
C	2.32079800	–1.96708600	–0.57029800
C	–0.04488000	–2.56254700	–0.06850100
C	–1.46057300	–2.68980900	–0.51761900
N	–2.39728400	–1.60834400	–0.05966200
C	–2.67578500	–1.77970000	1.35811800
C	–3.64327600	–1.69560800	–0.80550200
K	–0.33261300	0.33068700	0.61180000

C	1.43624300	–1.37948500	3.23783200
O	1.26937600	–0.04603600	2.78088600
C	2.52010800	0.60666500	2.62947900
C	2.27599800	2.28938800	–0.63090100
O	1.03525300	2.56344200	0.00825700
C	0.71546600	3.94118900	–0.01780000
C	–2.13886400	2.05028800	–1.47237900
O	–2.22077200	2.24480000	–0.06810400
C	–3.56469900	2.28901900	0.37436900
H	4.32071200	–1.50298600	–1.13248500
H	3.66427500	–0.15133000	–3.13531200
H	1.23208000	0.13655800	–3.61771000
H	–0.46821800	–0.89704600	–2.22155100
H	2.64468200	–2.59084100	0.25796000
H	0.31538500	–3.25726400	0.68302700
H	–1.88721300	–3.65364900	–0.18761100
H	–1.52368000	–2.67746900	–1.61340600
H	–1.73172800	–1.82983500	1.90722300
H	–3.22378400	–2.71690600	1.55843600
H	–3.27494500	–0.94488000	1.73538600
H	–4.34950700	–0.93822100	–0.45570800
H	–4.12183300	–2.68376200	–0.69387100
H	–3.45057600	–1.52923800	–1.86762700
H	2.02306200	–1.95892100	2.52001800
H	1.93263800	–1.38517500	4.21448700
H	0.44670000	–1.82193400	3.32779400
H	2.31752500	1.61579700	2.27509600
H	3.14160100	0.07820300	1.89832900
H	3.04423500	0.65387000	3.59027000
H	2.24645900	2.61409300	–1.67553300
H	3.09219500	2.80443000	–0.11155700
H	2.43748100	1.21311300	–0.60966700
H	–0.25892400	4.05703100	0.45092200
H	0.66876100	4.30439800	–1.05084600
H	1.46708700	4.52131600	0.52919300
H	–2.58287600	1.08882800	–1.75215800
H	–2.65241000	2.85970300	–2.00168600
H	–1.08269000	2.05468300	–1.73992200
H	–3.54843300	2.43649200	1.45266600
H	–4.08092000	1.35241600	0.13965200
H	–4.09825900	3.12113700	–0.09732600

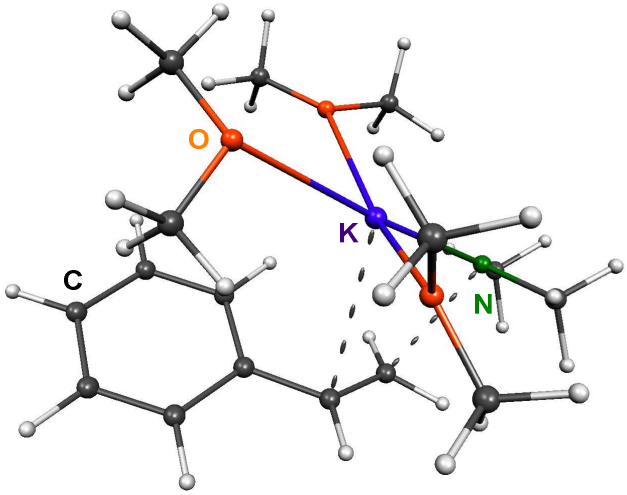


Fig. 40 Molekel plot of [**5**-K·(Me_2O)$_3$] (transition state)

Table 61 Cartesian coordinates of [**5**-K·(Me_2O)$_3$] (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–2.47011600	–1.86645900	1.11116400
C	–3.60110100	–1.16816600	1.53343000
C	–3.43144700	0.03702900	2.21789400
C	–2.15694000	0.52841000	2.47262900
C	–1.00176000	–0.17094800	2.07217400
C	–1.19193000	–1.37797700	1.37033700
C	0.32149200	0.36511900	2.39388000
C	1.48005600	–0.34533600	2.37768500
K	0.75675600	0.20869400	–0.65594900
N	2.98785600	–0.54964800	0.45284100
C	3.74710600	0.66690800	0.52001600
C	3.77276100	–1.59413500	1.03949500
C	1.22958500	3.75738600	0.33675000
O	0.65086800	2.96741700	–0.68919800
C	0.21128400	3.75759700	–1.77928200
C	–2.43065900	1.52109700	–1.06407800
O	–1.59570200	0.82976400	–1.98427000
C	–2.34321800	–0.05122800	–2.80006400
C	1.81302500	–2.92394600	–1.65420800
O	0.50868300	–2.34964900	–1.64885300
C	–0.48540400	–3.30852800	–1.94053100
H	–2.58215900	–2.80558700	0.58055200
H	–4.59320800	–1.55600700	1.33762800
H	–4.29754900	0.59339900	2.55779500
H	–2.03822100	1.46061500	3.01484600
H	–0.33119900	–1.94326400	1.02773400
H	0.34470200	1.40736200	2.70055200
H	2.39613700	0.09288100	2.75039100
H	1.48023200	–1.42126100	2.26105400
H	4.71513300	0.60732800	–0.01616600
H	4.00949300	0.97484700	1.56041900
H	3.19649400	1.50888300	0.07515600
H	4.74326900	–1.75005500	0.52774300
H	4.03380400	–1.40298400	2.10724400
H	3.23753800	–2.55169000	1.01475000
H	0.49450800	4.46687800	0.73174000
H	2.09637900	4.30698200	–0.04479600
H	1.54973700	3.08237100	1.12730800
H	–0.24142100	3.08441400	–2.50453700
H	–0.53292800	4.49053300	–1.44721500
H	1.05483500	4.28597400	–2.23591500
H	–2.96247100	0.81319900	–0.42212600
H	–3.15176700	2.14718700	–1.60242800
H	–1.78541700	2.14840000	–0.45167900
H	–1.63867000	–0.58749000	–3.43345100
H	–2.90089000	–0.76416300	–2.18243600
H	–3.04780600	0.50713500	–3.42655400
H	2.06813700	–3.26901600	–2.66233800
H	1.85118200	–3.77215500	–0.96211200
H	2.50440800	–2.15217300	–1.31369100
H	–1.45075600	–2.80779700	–1.89829700
H	–0.33552900	–3.73356300	–2.93970400
H	–0.46653800	–4.12002900	–1.20350300

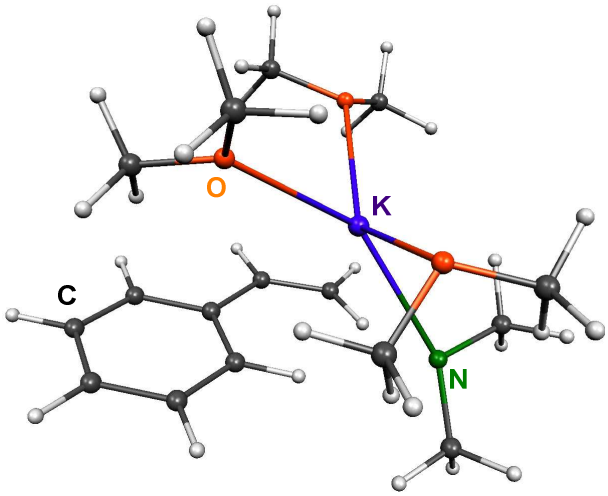


Fig. 41 Molekel plot of [**5**-K·$(Me_2O)_3$] (product)

Table 62 Cartesian coordinates of [**5**-K·$(Me_2O)_3$] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–3.70531700	–1.29658300	–1.38641200
C	–2.69647100	–2.10612600	–1.90284200
C	–1.43256900	–1.56203700	–2.13988600
C	–1.17351200	–0.22045100	–1.87546800
C	–2.18406400	0.60216100	–1.34808900
C	–3.44636500	0.04376500	–1.10687600
C	–1.96653700	2.03460500	–1.06260400
C	–0.83428500	2.71570600	–1.27985400
N	1.98611900	0.94326300	–1.60829100
C	2.67931000	2.13945000	–1.22936400
C	2.39338300	0.60630800	–2.94030500
K	0.78324400	0.29372900	0.59814800
C	–0.25098700	3.42222700	2.30954300
O	–0.29782000	2.00904900	2.40806000
C	–1.53847700	1.55856700	2.92066300
C	–1.72957600	–2.21749600	1.65827100
O	–0.37256000	–1.84005300	1.81476400
C	0.35949200	–2.78631700	2.57798600
C	2.33958100	–2.31703200	–0.46563800
O	2.82574800	–1.60945400	0.66749100
C	4.04191400	–0.93887900	0.34415800
H	–4.69278200	–1.70440000	–1.20529000
H	–2.89337500	–3.14781900	–2.12621400
H	–0.64348400	–2.18199800	–2.54985900
H	–0.18346900	0.19263700	–2.06915400
H	–4.23696000	0.67353600	–0.71207800
H	–2.83250400	2.55503100	–0.65853500
H	–0.79241900	3.77421200	–1.04886000
H	0.07022400	2.24510400	–1.67074000
H	2.40474900	2.46286200	–0.20877500
H	2.47165500	3.01336300	–1.89078800
H	3.79123600	2.04306000	–1.23024600
H	3.48473400	0.39096400	–3.03387500
H	2.19521800	1.40960200	–3.68537100
H	1.86807600	–0.28968100	–3.30140800
H	–1.06706700	3.79032800	1.67993500
H	–0.32244200	3.87622400	3.30342800
H	0.70154900	3.68663800	1.85435900
H	–1.48291800	0.47365100	2.99604400
H	–2.35669000	1.83976900	2.24800200

H	–1.72300600	1.98383000	3.91295900
H	–1.80283200	–3.18471300	1.15051200
H	–2.22502000	–2.28360200	2.63399800
H	–2.21541500	–1.46022400	1.04522900
H	1.40055200	–2.47171500	2.57055400
H	0.27885000	–3.78161500	2.12767000
H	–0.02076300	–2.82567200	3.60452400
H	2.19171900	–1.62084000	–1.29809400
H	3.04652700	–3.10310200	–0.75486600
H	1.38991100	–2.77240000	–0.18150100
H	4.35145400	–0.38812200	1.23168300
H	3.86831400	–0.25122100	–0.48933700
H	4.81583800	–1.67094800	0.08709000

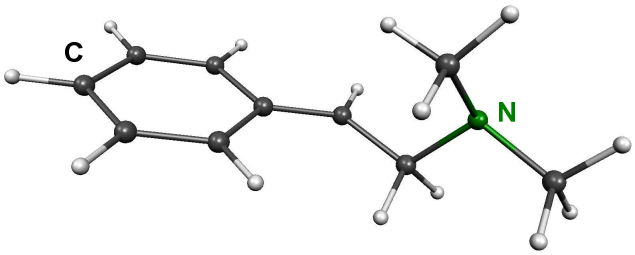


Fig. 42 Molekel plot of (*β*-anion) (starting material)

Table 63 Cartesian coordinates of (*β*-anion) (starting material) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–2.27313100	–1.42021600	–0.40943500
C	–3.41665400	–0.72544200	0.00644400
C	–3.23794600	0.62405400	0.36541500
C	–2.00513900	1.23950200	0.30176000
C	–0.80637500	0.56114100	–0.13613900
C	–1.02233800	–0.82621600	–0.47295500
C	0.41546500	1.22890800	–0.20706200
C	1.68962100	0.65277800	–0.70816200
N	2.66504100	0.20275600	0.32899700
C	3.86439800	–0.29761100	–0.30315900
C	2.08342000	–0.82258100	1.17260700
H	–2.35850100	–2.46920200	–0.68595700
H	–4.38675900	–1.20507900	0.06016100
H	–4.09334500	1.20611800	0.70216000
H	–1.91653500	2.28618000	0.58162800
H	–0.18059400	–1.43139900	–0.78928800
H	0.43852200	2.27119500	0.09901700
H	1.49435900	–0.20275300	–1.38652100
H	2.24297600	1.39640600	–1.29849300
H	4.59585400	–0.59400700	0.45513800
H	3.66591200	–1.17792100	–0.94888000
H	4.30844500	0.48343800	–0.92714300
H	2.76247600	–1.05252700	2.00035700
H	1.13474300	–0.45714000	1.56570700
H	1.88923900	–1.75850100	0.61325500

Table 64 Cartesian coordinates of (*β*-anion) (starting material) [B3LYP/6-31+G(d)]

atom	X	Y	Z
C	2.32864700	1.42383600	–0.40639700
C	3.46372900	0.70714900	0.01476800
C	3.26570800	–0.64476700	0.37285900
C	2.01890500	–1.24334600	0.30427700

C	0.82831400	–0.54372000	–0.13572800
C	1.06664600	0.84421700	–0.47426700
C	–0.41016100	–1.19755700	–0.21193800
C	–1.68212200	–0.62523400	–0.72442400
N	–2.69888500	–0.19509200	0.30492000
C	–3.91750600	0.26770100	–0.32807800
C	–2.16934400	0.80834300	1.21314300
H	2.43194100	2.47562800	–0.68270900
H	4.44464700	1.17429400	0.07253900
H	4.11585200	–1.24099800	0.71169900
H	1.91543500	–2.29295500	0.58395100
H	0.22981600	1.46152600	–0.79376700
H	–0.44122200	–2.24630100	0.08847300
H	–1.48893000	0.24087900	–1.39536800
H	–2.22741500	–1.36816400	–1.33220800
H	–4.67549500	0.50761700	0.43081000
H	–3.76754600	1.17902600	–0.95389800
H	–4.32147300	–0.51863100	–0.98007500
H	–2.87805700	0.98137600	2.03605500
H	–1.22103700	0.44841300	1.62190400
H	–1.98121300	1.78420300	0.71285600

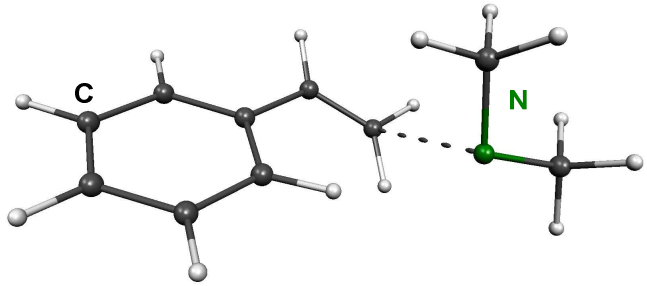


Fig. 43 Molekel plot of (*β*-anion) (transition state)

Table 65 Cartesian coordinates of (*β*-anion) (transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	–1.56900400	–1.60208300	–0.25308400
C	–2.90958000	–1.34063100	0.03901700
C	–3.30692800	–0.02900800	0.29920900
C	–2.37680500	1.00643700	0.25149100
C	–1.03363000	0.75911800	–0.06783700
C	–0.63810100	–0.56976700	–0.30090800
C	–0.03594300	1.83479100	–0.12516000
C	1.07259900	1.74485700	–0.88047300
N	2.92465100	0.00682900	–0.04378200
C	3.15445600	–1.30176900	–0.53873000
C	2.71980200	–0.06982000	1.35791400
H	–1.23969700	–2.62134900	–0.42196100
H	–3.63063300	–2.14949300	0.07981800
H	–4.34262700	0.18755400	0.53974600
H	–2.69083600	2.02616100	0.45239500
H	0.41816300	–0.76786600	–0.46152600
H	–0.18274800	2.68125000	0.54069800
H	1.22870500	0.94097100	–1.58199500
H	1.85308300	2.49240900	–0.83665900
H	4.08224000	–1.79201200	–0.13274000
H	2.33884600	–2.04461400	–0.29540300
H	3.26273100	–1.30283800	–1.63353300
H	3.61244500	–0.44104500	1.93177400
H	2.46686200	0.91537500	1.77486600
H	1.88970400	–0.76505300	1.66236300

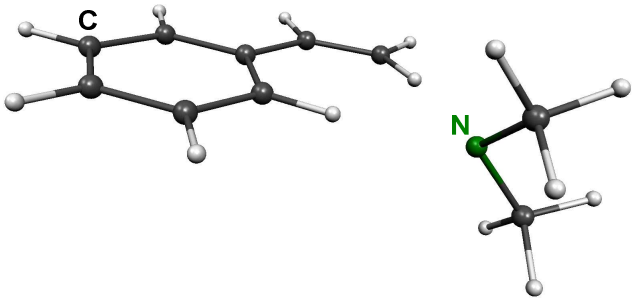


Fig. 44 Molekel plot of (*β*-anion) (product)

Table 66 Cartesian coordinates of (*β*-anion) (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	1.41866000	–1.61635400	–0.19374800
C	2.80779800	–1.51536200	–0.08131200
C	3.39295600	–0.25893400	0.05673500
C	2.58740400	0.87839700	0.08278000
C	1.19402600	0.78371400	–0.02706300
C	0.60668300	–0.48664500	–0.16872900
C	0.38648800	2.01871300	0.00837500
C	–0.94995400	2.07482400	–0.05796200
N	–2.54720200	–0.77156500	–0.16190200
C	–2.82480300	–0.67834600	1.22756200
C	–3.71313500	–0.38828000	–0.87407900
H	0.94982000	–2.58794000	–0.30251400
H	3.42611400	–2.40646000	–0.10140500
H	4.47001200	–0.16233800	0.14487000
H	3.04351000	1.85818800	0.19195200
H	–0.48227000	–0.59847200	–0.26506400
H	0.96175900	2.93942300	0.10045800
H	–1.44174000	3.04172400	–0.02119500
H	–1.56670300	1.17093200	–0.15452700
H	–3.65099800	–1.35022900	1.58123400
H	–3.15044800	0.35001000	1.56083100
H	–1.93775300	–0.93123100	1.82723000
H	–4.61635100	–1.01941500	–0.65716600
H	–4.06047400	0.66246300	–0.64734900
H	–3.55079900	–0.43606400	–1.95940200

Table 67 Cartesian coordinates of (*β*-anion) (transition state) [B3LYP /6-31+G(d)]

atom	X	Y	Z
C	1.27321000	–1.63321100	0.15220500
C	2.67449000	–1.67552400	0.15816300
C	3.39529900	–0.48101000	0.06417200
C	2.71289700	0.73455400	–0.03742400
C	1.30543300	0.78677000	–0.05006200
C	0.58309100	–0.42461300	0.05000200
C	0.63476000	2.09420200	–0.16641500
C	–0.69369900	2.30680000	–0.20154900
N	–2.64477100	–0.30330900	–0.00851100
C	–3.61390800	0.01469500	0.98207500
C	–3.19875500	–1.22497400	–0.93897500
H	0.70105300	–2.55591200	0.23215400
H	3.19751100	–2.62749100	0.23630100
H	4.48431100	–0.49360200	0.07056600
H	3.27880800	1.66352400	–0.11071000

H	–0.51939200	–0.42211900	0.06558800
H	1.31466300	2.94933100	–0.22632000
H	–1.06555500	3.32783100	–0.29200100
H	–1.43617100	1.49322800	–0.17579800
H	–3.96606700	–0.86806300	1.59583600
H	–4.57248300	0.45680200	0.57257400
H	–3.21651000	0.74954200	1.70496400
H	–3.55089100	–2.19825000	–0.48107200
H	–4.11069700	–0.84255000	–1.48960500
H	–2.46209100	–1.49523400	–1.71605300

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