Supporting Information

Base Induced Heterochiral Dimerization of an Oxiranyl Carbaldimine: Stereoselective Synthesis of a Highly Functionalized Aziridine

Dirk Alickmann, Roland Fröhlich, Ernst-Ulrich Würthwein*

Institut für Organische Chemie, Corrensstrasse 40 D-48149 Münster Germany wurthwe@uni-muenster.de

Experimental

IR: Perkin Elmer PE 298 or Nicolet 5DXC FT-IR. – MS: Finnigan MAT C 312. – ^{1}H NMR: Bruker WM 300 (300 MHz) and Varian (600 MHz), internal reference tetramethylsilane. – ^{13}C NMR: Bruker WM 300 (75 MHz) and Varian (151 MHz), internal reference deuterochloroforme. – CHN: Perkin-Elmer CHN-Analysator 240. - melting points are uncorrected. – Anhydrous conditions requiring reactions are performed in glass ware, which is thoroughly dried by repeated heating under argon and subsequent evacuation. – THF is distilled from potassium and benzophenone. Diisopropylamine is distilled from potassium hydroxide and stored over potassium hydroxide. *tert*.-Butyl hydroperoxide (ca. 4.8 m in toluene): *tert*.-Butyl hydroperoxide (100ml, 70% in water) is extracted with toluene (100 ml). The organic layer is dried over molecular sieves (4 Å). The concentration is determined by ^{1}H NMR spectroscopy. DMSO is dried using molecular sieves (4 Å).

***N*-Isopropyl-3,4-epoxy-1-aza-pent-1-ene (*rac*-3)**

2,3-Epoxybutanal[1] (trans/cis-ratio 92:8, 5.00 g, 58.1 mmol) (**2**), dissolved in dry dichloromethane (20 ml), is treated with 6 g of molecular sieves (4 Å). At -10 °C isopropylamine (3.77 g, 63.9 mmol) is added dropwise to the slowly stirred reaction mixture. After stirring at room temperature (12h), the molecular sieves are filtered off and washed with dichloromethane. The solvent is removed at reduced pressure; the residue is distilled using a vigreux column. Yield.: 4.81 g (37.8 mmol, 65.1%); colorless liquid, bp.: 59 °C / 70 mbar. (trans/cis-ratio: 92:8).- **IR** (neat): $\tilde{\nu}$ = 2969 (vs) cm^{-1}, 2930 (m), 2867 (m), 1696 (s), 1467 (m), 1456 (m), 1429 (m), 1380 (s), 1363 (s), 1322 (w), 1284 (m), 1232 (w), 1162 (m), 1136 (w), 1120 (w), 1009 (m), 959 (m), 945 (w), 936 (w), 851 (s), 828 (m), 809 (w), 755 (w).- **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 1.17 [d, ^{3}J = 6.2 Hz, 6H, (CH_3)$_2$-CH], 1.38 (d, ^{3}J = 5.2 Hz, 6H, CH_3CHCH), 3.09 (dq, ^{3}J = 5.2 Hz, ^{3}J = 1.9 Hz, 1H, CH_3CHCH), 3.18 (dd, ^{3}J = 7.1 Hz, ^{3}J = 1.9 Hz, 1H, CH_3CHCH), 3.38 [sept, ^{3}J = 6.2 Hz, 1H, (CH_3)$_2$-C*H*], 7.15 (d, ^{3}J = 7.1 Hz, 1H, CHN).- **^{13}C NMR** (75 MHz, $CDCl_3$): δ = 16.8 (CH_3CHCH), 23.5 [(CH_3)$_2$CH], 53.5, 58.6 (CHCH), 60.8 [(CH_3)$_2C$H], 160.3 (CH=N).- **GC-MS** (70 eV), *m/z* (%): 127 (3) [M$^+$], 112 (34), 94 (6), 84 (24) [M$^+$-CH(CH_3)$_2$], 70 (46), 57 (17), 56 (18), 43 (100), 41 (53).

$C_7H_{13}NO$ (127.18) calcd.: C 66.11, H 10.30, N 11.01 found: C 66.16, H 9.89, N 11.42

---

[1] Ceroni, M.; Séquin, U. *Helv. Chim. Acta* **1982**, *65*, 302-316.

(2-(1-Hydroxyethyl)-3-(1-hydroxy-2-propenyl)-1-isopropyl-aziridin-2-yl)-methyliden-isopropylamine (*rac*-4):

A solution of *n*-butyllithium (10 ml, 16.0 mmol, 1.6 m in *n*-hexane) is added to a carefully dried (heat, vacuum) Schlenk-flask under argon. After removal of the solvent under reduced pressure (ca. 0.1 mbar) the residue is dissolved at -78 °C in THF (16 ml) and treated with diisopropylamine (1.61 g, 16 mmol) and potassium *tert*.-butylat (1.79 g, 16.0 mmol). After stirring for ca. 40 min the alkoxide is dissolved almost completely. To this orange reaction mixture a solution of ***rac*-3** (2.03 g, 16.0 mmol) in THF (10 ml) is added dropwise at -78 °C. The reaction mixture is allowed to warm up to 0 °C and stirred at this temperature for 60 min; a brown solution is formed. The reaction mixture is quenched with water (20 ml) and extracted with five portions of dichloromethane (30 ml). The dichloromethane layer is dried with magnesium sulfate; after filtration, the solvent is removed under reduced pressure. The resulting orange oil is treated with some petrol ether; yellow-orange crystals are formed. After recrystallization from dichloromethane / petrol ether colorless cuboid crystals are obtained. Yield of crude product: 2.2 g; Yield of pure product: 1.09 g (4.28 mmol, 53.4%). mp.: 128 °C. **IR** (KBr): $\tilde{\nu}$ = 3350 (sh) cm^{-1}, 3180 (br), 2910 (br), 1640 (m), 1450 (m), 1410 (s), 1370 (s), 1320 (m), 1270 (m), 1130 (s), 1080 (s), 1030 (m), 1000 (s), 930 (s), 910 (m), 880 (m), 850 (w), 790 (m), 760 (m), 680 (m).- **^{1}H NMR** (600 MHz, $CDCl_3$): δ = 1.04 (d, ^3J = 6.2 Hz, 3H, C*H*$_3$CH-NR$_2$), 1.17 (d, ^3J = 6.2 Hz, 3H, C*H*$_3$CH-NR$_2$), 1.19 (d, ^3J = 6.2 Hz, 3H, C*H*$_3$CH-N=C), 1.20 (d, ^3J = 6.2 Hz, 3H, C*H*$_3$CH-N=C), 1.42 (d, ^3J = 6.5 Hz, 3H, C*H*$_3$CH-OH), 2.12 [d, ^3J = 6.8 Hz, 1H, HC(OH)-C*H*-N], 2.56 (sept, ^3J = 6.2 Hz, 1H, R$_2$C$_2$-N-CH), 3.06 (br, 1H, CH$_3$-CHO*H*), 3.32 (sept, ^3J = 6.2 Hz, 1H, CH=N-C*H*), 3.66 [m, 1H, CH$_3$C*H*(OH)], 4.20 (m, 1H, CH$_2$=CH-C*H*), 4.70 (br, 1H, CH$_2$=CH-CH-CHO*H*), 5.19 (dd, ^2J = 1.5 Hz, $^3J_{cis}$ = 10.6 Hz, 1H, HC*H*$_{cis}$=CH), 5.41 (dd, ^2J = 1.7 Hz, $^3J_{trans}$ = 17.3 Hz, 1H, HC*H*$_{trans}$=CH), 6.05 (ddd, ^3J = 4.7 Hz, ^3J = 10.6 Hz, ^3J = 17.3 Hz, 1H, CH$_2$=C*H*), 7.48 (d, ^3J = 1.2 Hz, 1H, CH=N).- **^{13}C NMR** (150 MHz, $CDCl_3$): δ = 19.8 [*C*H$_3$-CH(OH)], 21.8 (*C*H$_3$CH-N-R$_2$), 22.7 (*C*H$_3$CH-N=C), 23.7 (*C*H$_3$CH-N-R$_2$), 24.0 (*C*H$_3$CH-N=C), 49.8 (C$_q$), 52.0 (*C*H-N-R$_2$), 54.9 [CH-*C*H(OH)], 61.7 (*C*H-N=C), 68.9 [CH$_3$-*C*H(OH)], 69.0 [CH$_2$=CH-*C*H(OH)], 115.0 (*C*H$_2$=CH), 138.6 (CH$_2$=*C*H), 158.7 (CH=N).- **MS** (70 eV), *m/z* (%): 254 (0.33) [M$^+$], 228 (0.32), 197 (78.64), 179 (49.78), 162 (6.01), 155 (8.44), 138 (23.68), 137 (51.33), 122 (51.78), 120 (100), 95 (62.87), 70 (19.55). **$C_{14}H_{26}N_2O_2$ (254.37)** calcd.: C 66.11 H 10.30 N 11.01 found: C 65.93 H 10.41 N 10.85

X-ray crystal structure analysis of ***rac*-4**: formula $C_{14}H_{26}N_2O_2$, M = 254.37, colorless crystal 0.70 x 0.40 x 0.20 mm, a = 8.343(1), b = 8.915(1), c = 11.437(1) Å, α = 76.96(1), β =

75.84(1), γ = 73.47(1)°, V = 779.5(1) Å^3, ρ_{calc} = 1.084 g cm^{-3}, μ = 5.72 cm^{-1}, empirical absorption correction via ψ scan data (0.690 ≤ T ≤ 0.894), Z = 2, triclinic, space group P1bar (No. 2), λ = 1.54178 Å, T = 223 K, ω/θ scans, 3395 reflections collected (-h, ±k, ±l), [(sinθ)/λ] = 0.62 Å^{-1}, 3170 independent (R_{int} = 0.018) and 2960 observed reflections [$I \geq 2\ \sigma(I)$], 171 refined parameters, R = 0.039, wR^2 = 0.111, max. residual electron density 0.29 (-0.14) e Å^{-3}, hydrogens calculated and refined as riding atoms. Data set was collected with an Enraf Nonius CAD4 diffractometer.[2,3]

(2*S-trans*)-3-Methyloxirane methanol

This procedure is adapted from work by *Sharpless et al*.[4] Molecular sieves (10 g, 4 Å) in a Schlenk flask are carefully dried under reduced pressure (ca. 0.1mbar). In an argon atmosphere dichloromethane (400 ml) is cooled to –20 °C. *L*(+) diisopropyl tartrate (2.82 g, 12 mmol), *E*-2-buten-1ol (14.4 g, 200 mmol) and titanium(IV)-isopropoxide (2.84 g, 10 mmol) are added. After stirring for 15 min at –20 °C *tert*.-butyl hydroperoxide (83 ml, 400 mmol, 4.8 m in toluene) is added dropwise. The mixture is stirred for 2 h at -20 °C. Then, triphenylphosphine is added to the reaction mixture until no peroxides are detected. The solvent is removed under reduced pressure; the residue is distilled using a Vigreux column (20 mbar, 60 °C). The ee is determined by chiral GC after silylation using

---

[2] Programs used: data collection EXPRESS (Nonius B.V., 1994), data reduction MolEN (K. Fair, Nonius B.V., 1990), structure solution SHELXS-93 (G.M. Sheldrick, *Acta Cryst.* **1990**, *A46*, 467-473), structure refinement SHELXL-97 (G.M. Sheldrick, Universität Göttingen, 1997), graphics SCHAKAL (E. Keller, Universität Freiburg, 1997).

[3] Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication CCDC 156107. Copies of the data can be obtained free of charge on application to The Director, CCDC, 12 Union Road, CambridgeCB2 1EZ, UK [fax: int. code +44(1223)336-033, e-mail: deposit@ccdc.cam.ac.uk].

[4] Gao, Y.; Hanson, R. M.; Klunder, J. M.; Ko, S. Y.; Masamune, H.; Sharpless, K. B. *J. Am. Chem. Soc*. **1987,** *109,* 5765.

bistrimethylsilylacetamide (BSA). Yield: 9.20 g (105 mmol, 52.2 %, Lit.:[4] 70%), colorless liquid. ee: 86%, Lit.:[4] 90-92%

(2*S*-*trans*)-3-Methyloxirane carbaldehyde

This procedure is adapted from work of *Lindström and Somfai*.[5] To a solution of dimethyl-sulfoxide (DMSO, 21.8 g, 280 mmol) in dichloromethane (400 ml) oxalic dichloride (17.4 g, 140 mmol) is added dropwise at –78 °C. After ceasing of the gas evolution (ca. 15 min) a solution of (2*S*-*trans*)-3-methyloxirane methanol (8.0 g, 90 mmol) in dichloromethane (50 ml) is added; a white clouding of the mixture is observed. After 90 min stirring at –78 °C triethyl-amine (38.4 g, 380 mmol) is added dropwise. After additional 20 min the mixture is allowed to warm to room temp. The precipitate (triethylamine hydrochloride) is filtered off. The filtrate is freed from the solvent at reduced pressure. The residue obtained is purified by column chromatography (eluent petrol ether : diethyl ether = 1 : 1). Yield: 1.94 g (22.5 mmol, 25.0 %), yellow liquid.

For the preparation of **(2*S*-*trans*)-*N*-isopropyl-3,4-epoxy-1-aza-pent-1-ene**, see above (***rac*-3**).

Treatment of (2*S*-*trans*)-*N*-Isopropyl-3,4-epoxy-1-aza-pent-1-ene with LDA/KOtBu

As above (2*S*-*trans*)-*N*-isopropyl-3,4-epoxy-1-aza-pent-1-ene (86% ee, 298 mg, 3.46 mmol, obtained from (2*S*-*trans*)-3-methyloxirane carbaldehyde and isopropylamine as above) is added to an equimolar amount of LDA/KOtBu at –78°C. During the addition the reaction mixture turns brown. After aqueous work up 300 mg of a brown oil are obtained.

In the **^{1}H NMR-Spectrum** of the crude product about 10 signals are found between 7.2 –7.6 ppm (imine protons), among them one (<10%) with the shift of **4**. Additional olefin signals prove the formation of **4** in low yield. The **GC** of the silylated crude product (BSA) also shows a retention time identical with that of **4**; however tailing due to decomposition prevents a detailed analysis. The **Quadrupol-MS** of the BSA derivatised crude product shows a base peak at m/z = 327 (M+1, monosilylation of **4**) and 399 (12%)(M+1 of bissilylated **4**). The fragmentation scheme is very similar to that of **4**.

---

[5] U. M. Lindström, P. Somfai, *Synthesis* **1998,** 109.

Quantum mechanical calculations: GAUSSIAN 98 Archive entries:

1|1|UNPC-UNK|FOpt|RB3LYP|6-31+G(d,p)|C7H12N1O1(1-)|PCUSER|26-Jan-2001|0||#
B3LYP/6-31+G** OPT=READFC GEOM=CHECK GUESS=READ PUNCH=ARC||iminooxiran-
anion||-1,1|C,-2.095564903,0.667742555,-1.4073230038|O,-2.0064144227,-
0.7147465129,-0.9931593475|C,-1.4081238787,0.3489866463,-0.1636748943|C,-
3.4862727927,1.2660403201,-1.4448417321|C,-0.0305411374,0.4213677052,
0.1329058091|N,0.8209740647,-0.545550704,0.3862131706|C,2.1083234065,-
0.1612363944,0.9145845357|C,3.2389272837,-0.7763010488,0.0677886654
|C,2.2464661231,-0.6052259517,2.3870862333|H,-1.5139211496,0.8649470686,-
2.3216142737|H,-4.0179066975,1.0077118685,-0.5239104833|H,-4.0586730331,
0.8941945705,-2.3081484884|H,-3.4332118477,2.3619896338,-1.5203266484|
H,0.2944450419,1.4740629489,0.2903723905|H,2.240263959,0.9448825253,0.89350
60411|H,3.1742558971,-0.4211690015,-0.9667247511|H,4.2323230401,-
0.5228846718,0.4663952585|H,3.135538664,-1.8682301869,0.0502491648
|H,2.121874669,-1.6928602494,2.4586787454|H,3.226649404,-0.3340515866,
2.808184683|H,1.4635743724,-0.1400088775,2.9959672687||Version=x86-Win32-
G98RevA.7|HF=-403.9096923|RMSD=1.633e-009|RMSF=2.503e-006|Dipole=1.2072172,
0.9114987,-0.1310759|PG=C01 [X(C7H12N1O1)]||@
1|1|UNPC-UNK|FOpt|RB3LYP|6-31+G(d,p)|C7H12Li1N1O1|PCUSER|30-Jan-2001|0||#
B3LYP/6-31+G** OPT PUNCH=ARC||Lithiated Iminooxirane||0,1|C,2.5716489209,
0.2307893163,-0.2342354826|O,1.8506535201,-0.68147237,0.6607154196|
C,1.2921878024,-0.2716748128,-0.7023833173|C,3.8857459879,-0.2911361657,-
0.753952725| C,0.0089864803,0.2817665089,-0.7055791284|N,-0.8907570032,
0.0700604193, 0.251596565|C,-2.2760939525,0.4491569979,-0.0114288543
|Li,0.2610223693,-0.6724027223,1.5438326055|C,-2.8822522406,1.1074986538,
1.2344233254|C,-3.1032057723,-0.772086425,-0.4494709466|H,2.6270917849,
1.240485708, 0.1900949085|H,3.767987455,-1.3189913984,-1.1050031757|
H,4.2204212269, 0.3291902615, -1.5940460396|H,4.657482163,-0.2555735364,
0.0238135585|H,-0.2692835596,0.8330875746,-1.6140284583|H,-2.3055043704,
1.1862221518,-0.8333178993|H,-2.8809868707,0.4048930837,2.0779526853|H,-
3.9193387547, 1.4132149127,1.0563473316|H,-2.3063004887,1.9917725739,
1.5267095645|H,-3.1131982542,-1.530142747,0.3433493|H,-2.6725847082,-
1.2292961872,-1.3460452018|H,-4.1408852263,-0.492182646,-0.6684609293||
Version=x86-Win32-G98RevA.7|HF=-411.4714587|RMSD=2.753e-009|RMSF=7.653e-
006|Dipole=-0.1375919,0.2940865,1.0950191|PG=C01 [X(C7H12Li1N1O1)]||@
1|1|UNPC-UNK|FTS|RB3LYP|6-31+G(d,p)|C7H12N1O1(1-)|PCUSER|25-Jan-2001|0||#
B3LYP/6-31+G** OPT=(TS,NOEIGENTEST,READFC) PUNCH=ARC GEOM=CHECK
GUESS=READ||Iminooxiran, TS||-1,1|C,-2.5070253431,-0.2264474867,-
1.2605396752| O,-2.4833614924,-0.3587048886,0.2078093221|C,-1.2701534031,-
0.3471593269,-0.5589742439|C,-3.0563288863,1.0874475146,-1.7806163741|

C,0.0764312665,-0.3019269739,-0.3770586059|N,0.7952397336,-0.4071632319,
0.7532764055|C,2.2019245507,-0.1673437027,0.6021211705| C,2.9975536358,-
1.0481418318,1.585258846|C,2.5795118064, 1.3232677432, 0.8210534306|H,-
2.9541310509,-1.1041277789,-1.7520199994|H,-2.6525322839, 1.9150602525,-
1.1898785756|H,-4.1557933351,1.1068589315,-1.7299457909|H,-2.766284468,
1.2340332661,-2.8301271191|H,0.6122055611,-0.2058763969,-1.3457632469|
H,2.5550883911,-0.4242821547,-0.4287567939|H,2.8008845818,-2.1072592861,
1.3844539787|H,4.0812988137,-0.868286442,1.5216200725|H,2.6672739114,-
0.8395199009,2.610870878|H,2.2815867538,1.6337113589,1.8311304729|H,3.66044
67672,1.5062116643,0.6984293465|H,2.0386884008,1.955082604,0.1071100741||Ve
rsion=x86-Win32-G98RevA.7|HF=-403.9026253|RMSD=9.067e-009|RMSF=2.029e-
006|Dipole=0.1933446,0.6078046,-1.2170724|PG=C01 [X(C7H12N1O1)]||@
1|1|UNPC-UNK|FOpt|RB3LYP|6-31+G(d,p)|C7H12Li1N1O1|PCUSER|28-Feb-2001|0||#
B3LYP/6-31+G** OPT PUNCH=ARC||Iminooxiran lith. cis||0,1|C,-1.777551365,
1.4164216098,-1.5333619127|O,-1.7912797067,1.3483140465,-0.0682480815|C,-
0.4908258173,1.3821680979,-0.863876521|C,-2.4014697813,0.2419884509,-
2.2489611714|C,0.4395936053,0.3813278436,-0.5964080261|N,0.4856770029,-
0.2990319411,0.550899496|C,1.6867205394,-1.0785302725,0.8339660014|Li,-
1.1921250269,0.2119068533,1.2261504693|C,1.3010837355,-2.4035409452,
1.5035574947| C,2.6678512045,-0.2814919711,1.7118874731|H,-2.137788062,
2.3876889496,-1.880613088|H,-3.4957337078,0.2795001157,-2.1860335077|H,-
2.1277163617,0.2710152987,-3.3103899386|H,-2.0471030855,-0.7039452484,-
1.8289681325|H,1.2247808675,0.2446782515,-1.3522052602|H,2.2031891532,-
1.3152210291,-0.1135031526|H,0.7858770876,-2.2155589853,2.4546690244|
H,2.1861348538, -3.0129787632,1.7181025893|H,0.6293157996,-2.982998783,
0.8615275974|H,2.2034329394,-0.0344599168,2.6745376261|H,2.9477977199,
0.6575125043,1.2236778464|H,3.5822737829,-0.8542986181,1.9096151395||
Version=x86-Win32-G98RevA.7|HF=-411.4698861|RMSD=5.426e-009|RMSF=7.957e-
006|Dipole=-0.7528468,-0.7853422,0.4257933|PG=C01 [X(C7H12Li1N1O1)]|
|@
1|1|UNPC-UNK|FTS|RB3LYP|6-31G(d)|C14H25Li2N2O2(1+)|PCUSER|12-Feb-2001|0||#
B3LYP/6-31G* OPT=(TS,NOEIGENTEST,READFC) PUNCH=ARC GEOM=CHECK GUESS=READ||
Dimer TS R,S, cis, Ret||1,1|C,-0.7784502016,0.5263581895, 0.9659107268|
C,0.0889971195,-0.8796499691,-0.3554377194|N,0.7539056684,-0.2234575989,-
1.3041119558|Li,1.9686712977,1.0060967037,-0.5007062599|C,0.1050739088,
0.1361566645, -2.5743669977|N,1.4817087616,1.3802444112,1.3769075984|
C,0.6197625221,1.5146601889,-3.0130961671|C,0.39107486,-0.9163851443,-
3.6575679597|C,0.3035276059,1.0728129237,1.7981646875|C,2.4701722144,1.8651
531052,2.3595290913|C,3.7184613961,0.9764721696,2.302360576|C,2.8010747679,
3.3328807848,2.0632625357|C,-1.9502489725,1.3867390282,0.6855654304|O,-
2.0601813362,0.471716497,1.8061651299|C,-1.0193936199,-1.8488641894,-
0.6738129839|C,-2.919950902,1.1998426165,-0.4529279595|C,-0.89553409,-

3.2840455048,-0.3450530107|O,-1.7419957529,-2.4175900793,0.466668181|C,-
1.5966059322,-4.3690970914,-1.1122969133|H,0.7177910706,-1.2484000301,
0.4575064829| H,-0.9866411446,0.2216283001,-2.4521679581|H,0.0700306941,
1.1494738752,2.8715071406|H,2.0382796691,1.7996372321,3.3699808375|H,1.7098
754578,1.4892125553,-3.1593042177|H,0.3789629598,2.2865994279,-
2.2687742256| H,0.1769517762,1.8286813573,-3.9639712336|H,1.4710182841,-
1.0150896632,-3.8148200925|H,-0.0717664288,-0.6362157841,-4.6107230555|
H,0.0075304278,-1.9021141052,-3.3715071197|H,4.1977075767, 1.0257451489,
1.3141294028|H,3.4734130848,-0.0696398752,2.5146954917|H,4.4585418086,
1.309213423,3.0371400695|H,3.232929078,3.445976429,1.0600083824|H,3.5326110
275,3.7117296098,2.7843110258|H,1.9052203015,3.9592976063,2.1214102814|H,-
1.9051338492,2.4182553945,1.0428009792|H,-1.6865694238,-1.5948836318,-
1.4922914349|H,-2.604885277,1.7956387442,-1.3169634971|H,-3.9157795879,
1.5487230731,-0.1563033913|H,-2.9949117118,0.1541917554,-0.7634894362|
H,0.0059120876,-3.5809756044,0.1913297664|H,-2.4921513776,-3.9887707942,-
1.6121405671|H,-1.8872001761,-5.1863179611,-0.4438324986|H,-0.9192294733,-
4.7793929045,-1.8693993|Li,-2.359389701,-1.3230717826,1.799783648||
Version=x86-Win32-G98RevA.7|HF=-823.360109|RMSD=6.794e-009|RMSF=3.090e-
006|Dipole=-0.5603474,-0.7661985,0.8030051|PG=C01 [X(C14H25Li2N2O2)]||@
1\1\GINC-GOTLAND\FTS\RB3LYP\6-31G(d)\C14H25Li2N2O2(1+)\WURTHWE\10-Mar-
2001\0\\# B3LYP/6-31G* OPT=(TS,NOEIGENTEST,MNDOFC) PUNCH=ARC GEOM=CHECK
GUESS=READ\\Dimer S,S mit 2 Li+, cis, Ret.\\1,1\C,-0.5954310486,
0.3637319326, -0.8027989388\C,0.273249113,-1.2225847821, 0.2024592542\
C,0.0404191696, -2.1941047484,1.29901947\O,0.2501951925,-0.7657908231,
1.6198999079\C,-1.2636535438,-2.8051112669,1.7367458247\Li,-1.4451178051,
0.1199796362,1.329928937\O,-2.8297516095,-0.3565635151,0.0041973239\C,-
2.0336815413,0.0614061766,-1.1545002483\C,-2.6489990109,-1.2692547049,-
1.1351570729\N,-0.3193395502,1.3967967139,0.0397583637\C,1.6403076261,-
1.2371196028,-0.3722235047\N,2.488343403,-0.3135481466,-0.1202996664\
C,3.8160651388,-0.3431512626,-0.755461302\Li,1.3954242022,0.9975696697,
0.9327263096\C,-1.3494256202,2.3797166995,0.4537441627\C,-1.0136481446,
2.907320545,1.857831633\C,-1.4144357908,3.541100837,-0.5523622538\
C,3.9929738311, 0.922643397,-1.6021334064\C,4.8885061818,-0.4615460355,
0.3332450246\C,-3.8993346152,-1.5904879058,-1.9050868651\H,0.086656265,
0.2110594022,-1.6420246014\H,1.8576887027,-2.0486137047,-1.0814754719\
H,0.9061500486,-2.7919978499,1.595633439\H,-2.5283326524,0.8282198106,-
1.7527662305\H,-2.3656288224,1.9425519486,0.4949688366\H,-0.0233091054,
3.3809562572,1.8613715422\H,-1.0036777862,2.114494949,2.6238603697\H,-
1.7407568357,3.6578492443,2.1826805962\H,-0.4391671294,4.0358235296,-
0.6162189473\H,-2.163390356,4.2820611072,-0.2506467109\H,-1.6741977573,
3.1830250548,-1.5539894179\H,3.8798740317,-1.223499893,-1.413690062\
H,3.9374205092,1.8235013663,-0.9786715546\H,3.2243268612,0.9930484671,-

2.3790488554\H,4.9722375621,0.9136942828,-2.0912860104\H,4.8561861509,
0.4001556893,1.0108268027\H,5.8833078016,-0.4955579271,-0.1222006602\
H,4.7525753937,-1.3715547101,0.9266082767\H,-1.2610962419,-2.9502749498,
2.8229158862\ H,-1.3708254818,-3.7947212928,1.2771862848\H,-2.1387352818,-
2.2111378549,1.4577294489\H,-1.9982834463,-2.1071324707,-0.8973452635\H,-
4.4934534993,-0.6920592147,-2.0937313113\H,-4.5160534292,-2.3059425554,-
1.3515406502\H,-3.6344807964,-2.0458575414,-2.8660308743\\Version=IBM-
RS6000-G98RevA.7\HF=-823.3493077\RMSD=4.959e-09\RMSF=2.691e-06\Dipole=-
0.1782015,-0.689495,0.3666808\PG=C01 [X(C14H25Li2N2O2)]\\@