SUPPORTING INFORMATION

for

"Synthesis of 1-Aza-8-thiabicyclo[4.2.1]nona-2,4-diene 8,8-Dioxide and its Conversion to a Strained Spirocycle *via* Photoinduced SO_2-N Bond Cleavage"

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General experimental details and $^{1}H/^{13}C$ NMR spectral data for all compounds, as well as the crystallographic details for **23**

(16 pages)

Chromyl Acetate Oxidation of 7. Chromium trioxide (342 mg, 3.42 mmol) was added to acetic acid (0.66 mL, 11.4 mmol) and acetic anhydride (0.54 mL, 5.70 mmol) and stirred for 30 min, at which time CH_2Cl_2 (3 mL) was introduced and the solution was cooled to 0 °C. Sultam **7** (200 mg, 1.14 mmol) was added in one portion and stirring was maintained for 1 h in an ice bath and for 26 h at rt. The reaction mixture was quenched with water and solid sodium carbonate, and the aqueous layer was extracted with CH_2Cl_2 (3x). The combined organic layers were washed with water, dried and evaporated to leave a residue that was chromatographed on silica gel (elution with 50% ethyl acetate in hexanes). There was isolated 62 mg (23%) of **8** and 150 mg (70%) of **9**. The ^{1}H and ^{13}C NMR spectra of both products were identical to those reported earlier.[6]

Flash Vacuum Pyrolysis of 8. A two-necked round-bottomed flask containing **8** (325 mg, 1.39 mmol) was attached to a quartz tube (ID = 13mm, length 280 mm) packed with quartz chips and heated to 500 °C in a horizontal furnace. The tube was attached to a U-shaped adaptor that was cooled in a dry ice/acetone bath. A gentle flow of N_2 was initiated through the second neck of the flask and the sample of **8** was slowly volatilized into the hot zone. The material that collected in the cold trap was purified chromatographically on silica gel. Elution with 3.2 hexanes/ethyl acetate afforded 19 mg (8%) of **10** as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.16-6.12 (m, 1 H), 5.78-5.72 (m, 1 H), 3.71 (dd, *J* = 5.5, 13.4 Hz, 1 H), 3.45 (dd, *J* = 8.2, 13.4 Hz, 1 H), 3.37-3.32 (m, 1 H), 3.12-3.10 (m, 1 H), 2.95-2.89 (m, 1 H), 2.43-2.32 (m, 2 H), 1.85-1.78 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 133.9, 130.1, 56.6, 54.2, 39.5, 30.5, 23.6; ES HRMS *m/z* $(M + Na)^+$ calcd 196.0403, obsd 196.0402.

Pd(II)-Catalyzed Cyclization of 6. Tri-2-furylphosphine (37 mg, 0.16 mmol) and K_2CO_3 (330 mg, 2.36 mmol) was added to a solution of **6** (200 mg, 0.79 mmol) in DMF (8 mL) and the reaction vessel was deoxygenated with a stream of N_2 for 15 min. Palladium acetate (19 mg, 0.08 mmol) was introduced and deoxygenation was continued for a further 5 min. The reaction mixture was stirred vigorously at 100 °C for 72 h, cooled to rt, and filtered through Celite. The pad was rinsed with ethyl acetate, and the combined organic phrases were washed with water and brine, dried, and evaporated. The dark-colored residue was chromatographed on silica gel (elution with 4:1 hexanes/ethyl acetate) to furnish 92 mg (67%) of **11**, 6.3 mg (5%) of reduced (debrominated) product, and 7 mg (5%) of **12**.

For **11**: colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.97-5.91 (m, 1 H), 5.83-5.75 (m, 1 H), 3.86-3.78 (m 1 H), 3.55 (s, 1 H), 3.54 (s, 1 H), 3.43 (dd, *J* = 8.3, 13.2Hz, 1 H), 3.32-3.16 (m, 2 H), 2.97 (dd, *J* = 1.0, 13.1 Hz, 1 H), 2.81-2.71 (m, 1 H), 2.39-2.29 (m, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 133.5, 128.9, 55.9, 52.9, 49.7, 41.5, 26.5; ES HRMS *m/z* $(M + Na)^+$ calcd 196.0403, obsd 196.0413.

For **12**: colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.44 (dd, *J* = 9.2, 10.6Hz, 1 H), 6.25 (dd, *J* = 0.6, 8.5Hz, 1 H), 5.98 (dd, *J* = 8.0, 10.6Hz, 1 H), 5.85 (ddd, *J* = 0.7, 8.0, 8.5 Hz, 1 H), 4.09 (dd, *J* = 5.2, 13.3 Hz, 1 H), 3.49-3.34 (m, 2 H), 2.96 (d, *J* = 12.9 Hz, 1 H), 2.83 (ddd, *J* = 0.9, 2.3, 12.9 Hz, 1

H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.3, 134.4, 123.2, 119.6, 61.0, 49.5, 38.1; ES HRMS *m/z* (M + CH_3OH + Na)$^+$ calcd 226.0508, obsd 226.0507.

Allylic Bromination of 11. A solution of **11** (450 mg, 2.60 mmol) in $CHCl_3$ (100 mL) was treated with *N*-bromosuccinimide (462 mg, 2.60 mmol), irradiated with a portable heating work light so as to maintain a gentle reflux for 3 h, allowed to cool with stirring for 30 min, and evaporated to dryness. The residue was chromatographed on silica gel (elution with 4:1 hexanes/ethyl acetate) to give 380 mg (58%) of **13** as an epimeric mixture; white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.87-5.80 (m, 1 H), 5.68-5.61 (m, 1 H), 4.81 (br m, 1 H), 4.25 (dd, *J* = 4.9, 19.7 Hz, 1 H), 3.87 (d, *J* 14.2 Hz, 1 H), 3.79-3.71 (m, 2 H), 3.53-3.44 (m, 2 H), 2.64 (d, *J* = 11.5 Hz, 1 H); ^{13}C NMR (75MHZ, $CDCl_3$) δ (major diastereomer) 131.0, 126.3, 52.7, 52.0, 50.7, 49.9, 46.3; ES HRMS *m/z* (M + Na)$^+$ calcd 273.9508, obsd 273.9498.

Dehydrobromination of 13. A. With Lithium Bromide/Lithium Carbonate. A stirred reaction mixture consisting of **13** (70 mg, 0.28 mmol), lithium carbonate (23 mg, 0.31 mmol), lithium bromide (27 mg, 0.31 mmol) and DMF (5.0 mL) was heated at 120 °C for 3 h, cooled to ambient temperature, and partitioned between ethyl acetate and water. The separated aqueous layer was extracted twice with ethyl acetate, and the combined organic layers were washed with water and brine, dried, and evaporated. Chromatography on silica gel (elution with 4:1 hexanes/ethyl acetate) gave 28 mg (59%) of **12** as a colorless oil having spectroscopic properties identical to those defined above.

B. With DBU in Acetonitrile. A solution of **13** (372 mg, 1.48 mmol) in acetonitrile (40 mL) was treated with DBU (2.21 mL, 14.8 mmol), warmed to 70 °C and stirred at this temperature under N_2 for 9 h. The reaction mixture was concentrated and purified by chromatography on silica gel as above to provide 202 mg (80%) of colorless **12.**

Photoisomerization of 12. A. In Neat Acetone. A solution of **12** (11.6 mg, 0.068 mmol) in acetone (15 mL) was deoxygenated and irradiated through Pyrex with a bank of 350 nm bulbs in a Rayonet reactor for 1 h and evaporated to dryness. the residue was purified by chromatography on basic alumina (elution with 1% methanol in CH_2Cl_2) to give **17** (6 mg, 52%); ^{1}H NMR (300 MHz, C_6D_6) δ 5.81 (d, *J* = 2.8 Hz, 1 H), 5.69 (d, *J* = 2.8 Hz 1 H), 4.53 (s, 1 H), 3.08 (dd, *J* = 9.0, 12.8 Hz, 1 H), 2.75-2.65 (m, 2 H), 2.41 (d, *J* = 12.9 Hz, 1 H), 1.97 (ddd, *J* = 4.8, 9.0, 9.0 Hz, 1 H); ^{13}C NMR (125 MHz, C_6D_6) δ 140.9, 132.9, 97.8, 70.5, 61.2, 50.9, 31.9; ES HRMS *m/z* (m + Na)$^+$ calcd 194.0246, obsd 194.0242.

B. In Acetone/Acetonitrile. A solution of **12** (320 mg, 1.87 mmol) in acetone/acetonitrile (3:2, 250 mL) was deoxygenated and irradiated through Pyrex for 2 h as detailed above. The solvent was evaporated, and the residue was purified by chromatography on basic alumina (elution with 1% methanol in CH_2Cl_2) to give 88 mg of **17** having spectroscopic properties identical to those defined

above, 6 mg of an unknown isomer, and unreacted **12** (215 mg, 67%). The corrected yield of **17** is 42%.

For the unstable unknown compound: ^{1}H NMR (300 MHz, C_6D_6) δ 6.36 (ddd, *J* = 0.7, 2.6, 7.6 Hz, 1 H), 5.66-5.60 (m, 1 H), 4.34-4.28 (m, 2 H), 3.41 (d, *J* = 9.2, 12.4 Hz, 1 H), 2.94 (dd, *J* = 6.9, 12.4 Hz, 1 H), 2.59-2.49 (m, 1 H), 2.41-2.30 (m, 1 H), 2.00-1.91 (m, 1 H); ^{13}C NMR (75 MHz, C_6D_6) δ 148.4, 125.7, 91.8, 64.0, 48.9, 35.8, 29.9; ES HRMS *m/z* $(m + Na)^+$ calcd 194.0246, obsd 194.0242.

Hydrogenation of 17. A solution of **17** (13 mg, 0.075 mmol) in ethyl acetate/ethanol (3:4, 3.5 mL) was treated with 10% Pd/C (4 mg), purged with N_2, and hydrogenated at rt and 1 Torr for 22 h. The reaction mixture was filtered through Celite and freed of solvent to furnish 11 mg (85%) of **18**; ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.55-4.52 (m, 1 H), 4.06 (dd, *J* = 9.8, 13.3 Hz, 1 H), 3.45 (dd, *J* = 5.3, 12.8 Hz, 1 H), 3.39 (dd, *J* = 7.9, 13.3 Hz, 1 H), 3.31 (d, *J* = 12.8 Hz, 1 H), 2.86-2.82 (m, 1 H), 2.54-2.47 (m, 1 H), 2.27-2.20 (m, 1 H), 2.08-2.01 (m, 1 H), 1.86-1.78 (m, 1 H);^{13}C NMR (75 MHz, $CDCL_3$) δ 92.9, 64.3, 63.2, 51.8, 34.5, 20.5, 19.1; ES HRMS *m/z* $(m + Na)^+$ calcd 196.0403, obsd 196.0402.

Cycloaddition of 19 to 17. A solution of **17** (40 mg, 0.24 mmol) in CH_2Cl_2 (1 mL) was added at 0 °C to **19** (47 mg, 0.24 mmol) dissolved in CH_2Cl_2 (1 mL). The reaction mixture was stirred at rt for 2 h and concentrated. Purification of the adduct was achieved on basic alumina (elution with 1% methanol in CH_2Cl_2) to furnish 54 mg (63%) of **21**; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.58 (br s, 1 H), 7.56 (m, 1 H), 6.07 (dd, *J* = 2.4, 6.5 Hz, 1 H), 4.81 (d, *J* = 6.5 Hz, 1 H), 4.18 (dd, *J* = 10.3, 13.4 Hz, 1 H), 4.10 (d, *J* = 17.2 Hz, 1 H), 4.05-3.99 (m, 1 H), 3.90 (s, 3 H), 3.89 (s, 3 H), 3.58 (dd, *J* = 6.7, 13.5 Hz, 1 H), 2.74-2.69 (m, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.1, 161.0, 159.8, 131.8, 127.6, 103.8, 70.0, 68.0, 53.2, 53.1, 32.2, 26.4 ES HRMS *m/z* $(m + Na)^+$ calcd 364.0574, obsd 364.0563.

Cycloaddition of 22 to 17. A solution of **17** (24 mg, 0.14 mmol) and **22** (189 mg, 0.20 mmol) in benzene (1 mL) was stirred at 75 °C for 1.5 h and concentrated. The residue was chromatographed on basic alumina (elution with 1% methanol in CH_2Cl_2) to give a 1.25:1 mixture of **23** and its *exo* isomer (41 mg, 66%). Crystallization of the mixture from ethyl acetate afforded pure **23** as small, colorless prisms, mp 229-232 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.5 Hz, 2 H), 7.63-7.43 (m, 8 H), 7.33-7.26 (m, 4 H), 3.90 (dd, *J* = 9.9, 13.3 Hz, 1 H), 3.62 (d, *J* = 3.4 Hz, 1 H), 3.38-3.27 (m, 2 H), 3.21-3.17 (m, 2 H), 3.13 (dd, *J* = 8.6, 13.4 Hz, 1 H), 2.87-2.81 (m, 1 H), 2.50 (br s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.9, 138.2, 138.0, 128.6, 128.4, 128.22, 128.20, 128.1, 127.6, 126.9, 126.3, 122.3, 120.6, 91.4, 91.3, 90.7, 66.3, 63.0, 52.1, 50.8, 48.2, 35.5; ES HRMS *m/z* $(M + Na)^+$ calcd 464.1291, obsd 464.1266.

Crystallographic Details for 23

Empirical formula	$C_{27}H_{23}NO_3S$
Formula weight	441.52
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 11.708(1) Å alpha = 70.286(5) deg.
	b = 11.755(1) Å beta = 87.739(5) deg.
	c = 17.101(2) Å gamma = 86.048(5) deg.
Volume	2210.0(4) $Å^3$
Z	4
Density (calculated)	1.327 Mg/m^3
Absorption coefficient	0.176 mm^{-1}
F(000)	928
Crystal size	0.12 x 0.12 x 0.23 mm
Theta range for data collection	2.14 to 25.05 deg.
Index ranges	-13<=h<=13, -13<=k<=14, -19<=l<=20
Reflections collected	42603
Independent reflections	7787 [R(int) = 0.040]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7787 / 0 / 585
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0408, wR2 = 0.0946
R indices (all data)	R1 = 0.0585, wR2 = 0.1041
Largest diff. peak and hole	0.262 and -0.396 e/A^3

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **23**.

	x	y	z	U(eq)
S(1A)	4478(1)	3306(1)	6199(1)	31(1)
O(1A)	8017(1)	651(1)	6594(1)	31(1)
O(2A)	4372(1)	3697(1)	5311(1)	39(1)
O(3A)	3786(1)	2341(1)	6689(1)	39(1)

N(1A)	7065(2)	4894(2)	6154(1)	35(1)
C(1A)	7723(2)	2677(2)	6449(1)	28(1)
C(2A)	8252(2)	1833(2)	5983(1)	30(1)
C(3A)	7429(2)	1870(2)	5306(1)	30(1)
C(4A)	7455(2)	2404(2)	4456(1)	36(1)
C(5A)	6511(2)	2280(2)	4020(1)	41(1)
C(6A)	5580(2)	1675(2)	4431(1)	41(1)
C(7A)	5546(2)	1159(2)	5296(1)	36(1)
C(8A)	6490(2)	1258(2)	5722(1)	30(1)
C(9A)	6772(2)	835(2)	6643(1)	29(1)
C(10A)	6708(2)	1957(2)	6939(1)	28(1)
C(11A)	5913(2)	3100(2)	6569(1)	28(1)
C(12A)	5567(2)	3917(2)	7097(1)	35(1)
C(13A)	6562(2)	4739(2)	6982(1)	40(1)
C(14A)	6906(2)	3779(2)	5993(1)	29(1)
C(15A)	4457(2)	4506(2)	6619(1)	38(1)
C(16A)	9507(2)	1908(2)	5766(1)	32(1)
C(17A)	10044(2)	2978(2)	5625(1)	41(1)
C(18A)	11206(2)	3035(2)	5439(1)	49(1)
C(19A)	11843(2)	2024(2)	5392(1)	49(1)
C(20A)	11315(2)	966(2)	5522(1)	47(1)
C(21A)	10150(2)	908(2)	5703(1)	40(1)
C(22A)	6254(2)	-294(2)	7205(1)	32(1)
C(23A)	6746(2)	-1423(2)	7260(1)	39(1)
C(24A)	6263(2)	-2467(2)	7774(1)	47(1)
C(25A)	5283(2)	-2387(2)	8226(1)	50(1)
C(26A)	4783(2)	-1276(2)	8181(2)	57(1)
C(27A)	5272(2)	-226(2)	7669(1)	49(1)
S(1B)	577(1)	8379(1)	1251(1)	32(1)
O(1B)	-2674(1)	5756(1)	1676(1)	32(1)
O(2B)	745(1)	8748(1)	363(1)	40(1)
O(3B)	1331(1)	7412(1)	1756(1)	40(1)
N(1B)	-2207(2)	10009(2)	1164(1)	35(1)
C(1B)	-2622(2)	7793(2)	1495(1)	30(1)
C(2B)	-2985(2)	6923(2)	1047(1)	32(1)
C(3B)	-2084(2)	6923(2)	381(1)	31(1)
C(4B)	-2076(2)	7404(2)	-474(1)	37(1)
C(5B)	-1058(2)	7257(2)	-893(1)	42(1)
C(6B)	-89(2)	6677(2)	-462(1)	42(1)
C(7B)	-100(2)	6202(2)	402(1)	36(1)
C(8B)	-1114(2)	6321(2)	813(1)	31(1)
C(9B)	-1462(2)	5931(2)	1728(1)	30(1)
C(10B)	-1573(2)	7069(2)	2003(1)	29(1)
C(11B)	-878(2)	8198(2)	1617(1)	29(1)
C(12B)	-700(2)	9041(2)	2128(1)	36(1)
C(13B)	-1793(2)	9872(2)	1993(1)	41(1)
C(14B)	-1887(2)	8877(2)	1026(1)	30(1)
C(15B)	392(2)	9601(2)	1651(1)	40(1)
C(16B)	-4221(2)	7000(2)	822(1)	35(1)
C(17B)	-4721(2)	5990(2)	780(1)	43(1)
C(18B)	-5872(2)	6047(2)	591(1)	49(1)
C(19B)	-6521(2)	7114(2)	428(1)	51(1)
C(20B)	-6030(2)	8134(2)	458(2)	54(1)

C(21B)	-4886(2)	8075(2)	652(1)	46(1)
C(22B)	-861(2)	4795(2)	2296(1)	31(1)
C(23B)	68(2)	4853(2)	2755(1)	43(1)
C(24B)	653(2)	3799(2)	3247(1)	47(1)
C(25B)	301(2)	2691(2)	3288(1)	41(1)
C(26B)	-627(2)	2621(2)	2835(1)	40(1)
C(27B)	-1209(2)	3670(2)	2341(1)	35(1)

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

Bond lengths [Å] and angles [deg] for **23**.

S(1A)-O(2A)	1.4381(14)
S(1A)-O(3A)	1.4416(14)
S(1A)-C(15A)	1.784(2)
S(1A)-C(11A)	1.791(2)
O(1A)-C(9A)	1.461(2)
O(1A)-C(2A)	1.465(2)
N(1A)-C(14A)	1.452(2)
N(1A)-C(13A)	1.469(3)
N(1A)-H(1NA)	0.87(2)
C(1A)-C(14A)	1.553(3)
C(1A)-C(10A)	1.553(2)
C(1A)-C(2A)	1.554(3)
C(1A)-H(1A)	1.00
C(2A)-C(16A)	1.503(3)
C(2A)-C(3A)	1.523(3)
C(3A)-C(4A)	1.376(3)
C(3A)-C(8A)	1.391(3)
C(4A)-C(5A)	1.399(3)
C(4A)-H(4A)	0.95
C(5A)-C(6A)	1.378(3)
C(5A)-H(5A)	0.95
C(6A)-C(7A)	1.397(3)
C(6A)-H(6A)	0.95
C(7A)-C(8A)	1.379(3)
C(7A)-H(7A)	0.95
C(8A)-C(9A)	1.525(3)
C(9A)-C(22A)	1.503(3)
C(9A)-C(10A)	1.561(3)
C(10A)-C(11A)	1.540(2)
C(10A)-H(10A)	1.00
C(11A)-C(12A)	1.550(3)
C(11A)-C(14A)	1.571(2)
C(12A)-C(13A)	1.528(3)
C(12A)-C(15A)	1.554(3)
C(12A)-H(12A)	1.00
C(13A)-H(13A)	0.99
C(13A)-H(13B)	0.99
C(14A)-H(14A)	1.00
C(15A)-H(15A)	0.99
C(15A)-H(15B)	0.99
C(16A)-C(21A)	1.385(3)
C(16A)-C(17A)	1.389(3)
C(17A)-C(18A)	1.385(3)
C(17A)-H(17A)	0.95
C(18A)-C(19A)	1.383(3)
C(18A)-H(18A)	0.95
C(19A)-C(20A)	1.374(3)
C(19A)-H(19A)	0.95
C(20A)-C(21A)	1.388(3)
C(20A)-H(20A)	0.95

C(21A)-H(21A)	0.95
C(22A)-C(27A)	1.383(3)
C(22A)-C(23A)	1.384(3)
C(23A)-C(24A)	1.388(3)
C(23A)-H(23A)	0.95
C(24A)-C(25A)	1.372(3)
C(24A)-H(24A)	0.95
C(25A)-C(26A)	1.374(3)
C(25A)-H(25A)	0.95
C(26A)-C(27A)	1.396(3)
C(26A)-H(26A)	0.95
C(27A)-H(27A)	0.95
S(1B)-O(3B)	1.4407(14)
S(1B)-O(2B)	1.4411(14)
S(1B)-C(15B)	1.785(2)
S(1B)-C(11B)	1.794(2)
O(1B)-C(9B)	1.459(2)
O(1B)-C(2B)	1.463(2)
N(1B)-C(14B)	1.451(2)
N(1B)-C(13B)	1.469(3)
N(1B)-H(1NB)	0.84(2)
C(1B)-C(14B)	1.554(3)
C(1B)-C(2B)	1.559(3)
C(1B)-C(10B)	1.559(2)
C(1B)-H(1B)	1.00
C(2B)-C(16B)	1.501(3)
C(2B)-C(3B)	1.521(3)
C(3B)-C(4B)	1.378(3)
C(3B)-C(8B)	1.393(3)
C(4B)-C(5B)	1.397(3)
C(4B)-H(4B)	0.95
C(5B)-C(6B)	1.384(3)
C(5B)-H(5B)	0.95
C(6B)-C(7B)	1.392(3)
C(6B)-H(6B)	0.95
C(7B)-C(8B)	1.379(3)
C(7B)-H(7B)	0.95
C(8B)-C(9B)	1.521(3)
C(9B)-C(22B)	1.507(3)
C(9B)-C(10B)	1.556(3)
C(10B)-C(11B)	1.541(3)
C(10B)-H(10B)	1.00
C(11B)-C(12B)	1.555(3)
C(11B)-C(14B)	1.572(2)
C(12B)-C(13B)	1.531(3)
C(12B)-C(15B)	1.551(3)
C(12B)-H(12B)	1.00
C(13B)-H(13C)	0.99
C(13B)-H(13D)	0.99
C(14B)-H(14B)	1.00
C(15B)-H(15C)	0.99
C(15B)-H(15D)	0.99
C(16B)-C(17B)	1.383(3)

C(16B)-C(21B)	1.387(3)
C(17B)-C(18B)	1.390(3)
C(17B)-H(17B)	0.95
C(18B)-C(19B)	1.371(3)
C(18B)-H(18B)	0.95
C(19B)-C(20B)	1.381(3)
C(19B)-H(19B)	0.95
C(20B)-C(21B)	1.385(3)
C(20B)-H(20B)	0.95
C(21B)-H(21B)	0.95
C(22B)-C(23B)	1.384(3)
C(22B)-C(27B)	1.387(3)
C(23B)-C(24B)	1.391(3)
C(23B)-H(23B)	0.95
C(24B)-C(25B)	1.372(3)
C(24B)-H(24B)	0.95
C(25B)-C(26B)	1.381(3)
C(25B)-H(25B)	0.95
C(26B)-C(27B)	1.388(3)
C(26B)-H(26B)	0.95
C(27B)-H(27B)	0.95

O(2A)-S(1A)-O(3A)	117.39(8)
O(2A)-S(1A)-C(15A)	114.56(9)
O(3A)-S(1A)-C(15A)	111.84(9)
O(2A)-S(1A)-C(11A)	115.47(8)
O(3A)-S(1A)-C(11A)	111.55(8)
C(15A)-S(1A)-C(11A)	80.51(9)
C(9A)-O(1A)-C(2A)	98.04(12)
C(14A)-N(1A)-C(13A)	106.2(2)
C(14A)-N(1A)-H(1NA)	108.9(14)
C(13A)-N(1A)-H(1NA)	110.0(14)
C(14A)-C(1A)-C(10A)	91.64(13)
C(14A)-C(1A)-C(2A)	120.2(2)
C(10A)-C(1A)-C(2A)	102.29(14)
C(14A)-C(1A)-H(1A)	113.3
C(10A)-C(1A)-H(1A)	113.3
C(2A)-C(1A)-H(1A)	113.3
O(1A)-C(2A)-C(16A)	111.0(2)
O(1A)-C(2A)-C(3A)	99.91(14)
C(16A)-C(2A)-C(3A)	118.1(2)
O(1A)-C(2A)-C(1A)	99.89(14)
C(16A)-C(2A)-C(1A)	117.2(2)
C(3A)-C(2A)-C(1A)	107.9(2)
C(4A)-C(3A)-C(8A)	121.5(2)
C(4A)-C(3A)-C(2A)	132.9(2)
C(8A)-C(3A)-C(2A)	105.4(2)
C(3A)-C(4A)-C(5A)	117.4(2)
C(3A)-C(4A)-H(4A)	121.3
C(5A)-C(4A)-H(4A)	121.3
C(6A)-C(5A)-C(4A)	121.0(2)
C(6A)-C(5A)-H(5A)	119.5
C(4A)-C(5A)-H(5A)	119.5

C(5A)-C(6A)-C(7A)	121.3(2)
C(5A)-C(6A)-H(6A)	119.3
C(7A)-C(6A)-H(6A)	119.3
C(8A)-C(7A)-C(6A)	117.4(2)
C(8A)-C(7A)-H(7A)	121.3
C(6A)-C(7A)-H(7A)	121.3
C(7A)-C(8A)-C(3A)	121.2(2)
C(7A)-C(8A)-C(9A)	133.1(2)
C(3A)-C(8A)-C(9A)	105.7(2)
O(1A)-C(9A)-C(22A)	110.74(14)
O(1A)-C(9A)-C(8A)	100.16(14)
C(22A)-C(9A)-C(8A)	117.9(2)
O(1A)-C(9A)-C(10A)	98.79(13)
C(22A)-C(9A)-C(10A)	117.4(2)
C(8A)-C(9A)-C(10A)	108.79(14)
C(11A)-C(10A)-C(1A)	88.64(13)
C(11A)-C(10A)-C(9A)	124.5(2)
C(1A)-C(10A)-C(9A)	101.99(14)
C(11A)-C(10A)-H(10A)	112.6
C(1A)-C(10A)-H(10A)	112.6
C(9A)-C(10A)-H(10A)	112.6
C(10A)-C(11A)-C(12A)	119.6(2)
C(10A)-C(11A)-C(14A)	91.44(13)
C(12A)-C(11A)-C(14A)	103.25(14)
C(10A)-C(11A)-S(1A)	131.97(13)
C(12A)-C(11A)-S(1A)	89.13(12)
C(14A)-C(11A)-S(1A)	120.39(12)
C(13A)-C(12A)-C(11A)	104.7(2)
C(13A)-C(12A)-C(15A)	116.4(2)
C(11A)-C(12A)-C(15A)	96.18(14)
C(13A)-C(12A)-H(12A)	112.7
C(11A)-C(12A)-H(12A)	112.7
C(15A)-C(12A)-H(12A)	112.7
N(1A)-C(13A)-C(12A)	106.9(2)
N(1A)-C(13A)-H(13A)	110.3
C(12A)-C(13A)-H(13A)	110.3
N(1A)-C(13A)-H(13B)	110.3
C(12A)-C(13A)-H(13B)	110.3
H(13A)-C(13A)-H(13B)	108.6
N(1A)-C(14A)-C(1A)	116.2(2)
N(1A)-C(14A)-C(11A)	109.2(2)
C(1A)-C(14A)-C(11A)	87.57(13)
N(1A)-C(14A)-H(14A)	113.7
C(1A)-C(14A)-H(14A)	113.7
C(11A)-C(14A)-H(14A)	113.7
C(12A)-C(15A)-S(1A)	89.29(12)
C(12A)-C(15A)-H(15A)	113.8
S(1A)-C(15A)-H(15A)	113.8
C(12A)-C(15A)-H(15B)	113.8
S(1A)-C(15A)-H(15B)	113.8
H(15A)-C(15A)-H(15B)	111.0
C(21A)-C(16A)-C(17A)	118.8(2)
C(21A)-C(16A)-C(2A)	120.4(2)

C(17A)-C(16A)-C(2A)	120.8(2)
C(18A)-C(17A)-C(16A)	120.5(2)
C(18A)-C(17A)-H(17A)	119.8
C(16A)-C(17A)-H(17A)	119.8
C(19A)-C(18A)-C(17A)	120.3(2)
C(19A)-C(18A)-H(18A)	119.9
C(17A)-C(18A)-H(18A)	119.9
C(20A)-C(19A)-C(18A)	119.6(2)
C(20A)-C(19A)-H(19A)	120.2
C(18A)-C(19A)-H(19A)	120.2
C(19A)-C(20A)-C(21A)	120.4(2)
C(19A)-C(20A)-H(20A)	119.8
C(21A)-C(20A)-H(20A)	119.8
C(16A)-C(21A)-C(20A)	120.6(2)
C(16A)-C(21A)-H(21A)	119.7
C(20A)-C(21A)-H(21A)	119.7
C(27A)-C(22A)-C(23A)	118.8(2)
C(27A)-C(22A)-C(9A)	120.8(2)
C(23A)-C(22A)-C(9A)	120.4(2)
C(22A)-C(23A)-C(24A)	120.5(2)
C(22A)-C(23A)-H(23A)	119.8
C(24A)-C(23A)-H(23A)	119.8
C(25A)-C(24A)-C(23A)	120.1(2)
C(25A)-C(24A)-H(24A)	119.9
C(23A)-C(24A)-H(24A)	119.9
C(24A)-C(25A)-C(26A)	120.3(2)
C(24A)-C(25A)-H(25A)	119.8
C(26A)-C(25A)-H(25A)	119.8
C(25A)-C(26A)-C(27A)	119.5(2)
C(25A)-C(26A)-H(26A)	120.2
C(27A)-C(26A)-H(26A)	120.2
C(22A)-C(27A)-C(26A)	120.7(2)
C(22A)-C(27A)-H(27A)	119.6
C(26A)-C(27A)-H(27A)	119.6
O(3B)-S(1B)-O(2B)	117.53(9)
O(3B)-S(1B)-C(15B)	111.78(9)
O(2B)-S(1B)-C(15B)	114.36(9)
O(3B)-S(1B)-C(11B)	111.32(8)
O(2B)-S(1B)-C(11B)	115.77(8)
C(15B)-S(1B)-C(11B)	80.48(9)
C(9B)-O(1B)-C(2B)	97.95(13)
C(14B)-N(1B)-C(13B)	106.2(2)
C(14B)-N(1B)-H(1NB)	107.0(13)
C(13B)-N(1B)-H(1NB)	109.3(13)
C(14B)-C(1B)-C(2B)	120.2(2)
C(14B)-C(1B)-C(10B)	91.68(13)
C(2B)-C(1B)-C(10B)	102.1(2)
C(14B)-C(1B)-H(1B)	113.3
C(2B)-C(1B)-H(1B)	113.3
C(10B)-C(1B)-H(1B)	113.3
O(1B)-C(2B)-C(16B)	110.9(2)
O(1B)-C(2B)-C(3B)	100.01(14)
C(16B)-C(2B)-C(3B)	117.9(2)

O(1B)-C(2B)-C(1B)	99.88(13)
C(16B)-C(2B)-C(1B)	117.4(2)
C(3B)-C(2B)-C(1B)	107.9(2)
C(4B)-C(3B)-C(8B)	121.4(2)
C(4B)-C(3B)-C(2B)	133.3(2)
C(8B)-C(3B)-C(2B)	105.2(2)
C(3B)-C(4B)-C(5B)	117.5(2)
C(3B)-C(4B)-H(4B)	121.3
C(5B)-C(4B)-H(4B)	121.3
C(6B)-C(5B)-C(4B)	121.0(2)
C(6B)-C(5B)-H(5B)	119.5
C(4B)-C(5B)-H(5B)	119.5
C(5B)-C(6B)-C(7B)	121.3(2)
C(5B)-C(6B)-H(6B)	119.4
C(7B)-C(6B)-H(6B)	119.4
C(8B)-C(7B)-C(6B)	117.6(2)
C(8B)-C(7B)-H(7B)	121.2
C(6B)-C(7B)-H(7B)	121.2
C(7B)-C(8B)-C(3B)	121.2(2)
C(7B)-C(8B)-C(9B)	133.1(2)
C(3B)-C(8B)-C(9B)	105.7(2)
O(1B)-C(9B)-C(22B)	110.57(14)
O(1B)-C(9B)-C(8B)	100.48(14)
C(22B)-C(9B)-C(8B)	116.8(2)
O(1B)-C(9B)-C(10B)	99.11(14)
C(22B)-C(9B)-C(10B)	118.2(2)
C(8B)-C(9B)-C(10B)	108.7(2)
C(11B)-C(10B)-C(9B)	124.3(2)
C(11B)-C(10B)-C(1B)	88.45(13)
C(9B)-C(10B)-C(1B)	101.75(14)
C(11B)-C(10B)-H(10B)	112.8
C(9B)-C(10B)-H(10B)	112.8
C(1B)-C(10B)-H(10B)	112.8
C(10B)-C(11B)-C(12B)	119.4(2)
C(10B)-C(11B)-C(14B)	91.67(13)
C(12B)-C(11B)-C(14B)	103.2(2)
C(10B)-C(11B)-S(1B)	132.22(14)
C(12B)-C(11B)-S(1B)	89.05(12)
C(14B)-C(11B)-S(1B)	120.11(13)
C(13B)-C(12B)-C(15B)	116.7(2)
C(13B)-C(12B)-C(11B)	104.4(2)
C(15B)-C(12B)-C(11B)	96.2(2)
C(13B)-C(12B)-H(12B)	112.7
C(15B)-C(12B)-H(12B)	112.7
C(11B)-C(12B)-H(12B)	112.7
N(1B)-C(13B)-C(12B)	106.9(2)
N(1B)-C(13B)-H(13C)	110.3
C(12B)-C(13B)-H(13C)	110.3
N(1B)-C(13B)-H(13D)	110.3
C(12B)-C(13B)-H(13D)	110.3
H(13C)-C(13B)-H(13D)	108.6
N(1B)-C(14B)-C(1B)	116.1(2)
N(1B)-C(14B)-C(11B)	109.3(2)

C(1B)-C(14B)-C(11B)	87.51(13)
N(1B)-C(14B)-H(14B)	113.7
C(1B)-C(14B)-H(14B)	113.7
C(11B)-C(14B)-H(14B)	113.7
C(12B)-C(15B)-S(1B)	89.49(12)
C(12B)-C(15B)-H(15C)	113.7
S(1B)-C(15B)-H(15C)	113.7
C(12B)-C(15B)-H(15D)	113.7
S(1B)-C(15B)-H(15D)	113.7
H(15C)-C(15B)-H(15D)	111.0
C(17B)-C(16B)-C(21B)	118.6(2)
C(17B)-C(16B)-C(2B)	120.3(2)
C(21B)-C(16B)-C(2B)	121.1(2)
C(16B)-C(17B)-C(18B)	120.6(2)
C(16B)-C(17B)-H(17B)	119.7
C(18B)-C(17B)-H(17B)	119.7
C(19B)-C(18B)-C(17B)	120.3(2)
C(19B)-C(18B)-H(18B)	119.9
C(17B)-C(18B)-H(18B)	119.9
C(18B)-C(19B)-C(20B)	119.8(2)
C(18B)-C(19B)-H(19B)	120.1
C(20B)-C(19B)-H(19B)	120.1
C(19B)-C(20B)-C(21B)	120.0(2)
C(19B)-C(20B)-H(20B)	120.0
C(21B)-C(20B)-H(20B)	120.0
C(20B)-C(21B)-C(16B)	120.8(2)
C(20B)-C(21B)-H(21B)	119.6
C(16B)-C(21B)-H(21B)	119.6
C(23B)-C(22B)-C(27B)	119.0(2)
C(23B)-C(22B)-C(9B)	120.9(2)
C(27B)-C(22B)-C(9B)	120.0(2)
C(22B)-C(23B)-C(24B)	120.6(2)
C(22B)-C(23B)-H(23B)	119.7
C(24B)-C(23B)-H(23B)	119.7
C(25B)-C(24B)-C(23B)	120.0(2)
C(25B)-C(24B)-H(24B)	120.0
C(23B)-C(24B)-H(24B)	120.0
C(24B)-C(25B)-C(26B)	120.0(2)
C(24B)-C(25B)-H(25B)	120.0
C(26B)-C(25B)-H(25B)	120.0
C(25B)-C(26B)-C(27B)	120.2(2)
C(25B)-C(26B)-H(26B)	119.9
C(27B)-C(26B)-H(26B)	119.9
C(22B)-C(27B)-C(26B)	120.2(2)
C(22B)-C(27B)-H(27B)	119.9
C(26B)-C(27B)-H(27B)	119.9

Anisotropic displacement parameters ($Å^2$ x 10^3) for **23**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
S(1A)	28(1)	29(1)	33(1)	-6(1)	1(1)	-2(1)
O(1A)	29(1)	29(1)	31(1)	-6(1)	1(1)	-1(1)
O(2A)	39(1)	39(1)	32(1)	-3(1)	-5(1)	-2(1)
O(3A)	33(1)	37(1)	41(1)	-6(1)	5(1)	-8(1)
N(1A)	41(1)	26(1)	36(1)	-8(1)	-4(1)	-6(1)
C(1A)	29(1)	30(1)	26(1)	-9(1)	-1(1)	-6(1)
C(2A)	32(1)	28(1)	28(1)	-5(1)	0(1)	-2(1)
C(3A)	32(1)	29(1)	30(1)	-12(1)	-1(1)	0(1)
C(4A)	40(1)	35(1)	32(1)	-13(1)	3(1)	-1(1)
C(5A)	54(1)	40(1)	30(1)	-14(1)	-6(1)	1(1)
C(6A)	47(1)	39(1)	43(1)	-19(1)	-16(1)	0(1)
C(7A)	39(1)	29(1)	43(1)	-14(1)	-5(1)	-5(1)
C(8A)	35(1)	26(1)	33(1)	-13(1)	-2(1)	-1(1)
C(9A)	26(1)	29(1)	31(1)	-8(1)	1(1)	-2(1)
C(10A)	30(1)	28(1)	24(1)	-6(1)	-1(1)	-4(1)
C(11A)	30(1)	28(1)	26(1)	-8(1)	1(1)	-4(1)
C(12A)	45(1)	31(1)	29(1)	-11(1)	3(1)	-1(1)
C(13A)	52(1)	33(1)	39(1)	-17(1)	-3(1)	-5(1)
C(14A)	31(1)	29(1)	27(1)	-8(1)	-2(1)	-5(1)
C(15A)	39(1)	30(1)	43(1)	-12(1)	8(1)	0(1)
C(16A)	30(1)	38(1)	26(1)	-6(1)	-2(1)	-3(1)
C(17A)	37(1)	38(1)	43(1)	-7(1)	3(1)	-4(1)
C(18A)	38(1)	51(1)	56(1)	-11(1)	5(1)	-16(1)
C(19A)	28(1)	66(2)	52(1)	-18(1)	2(1)	-2(1)
C(20A)	34(1)	54(2)	51(1)	-18(1)	0(1)	6(1)
C(21A)	35(1)	41(1)	45(1)	-17(1)	1(1)	-2(1)
C(22A)	33(1)	28(1)	32(1)	-6(1)	-4(1)	-3(1)
C(23A)	48(1)	33(1)	39(1)	-14(1)	2(1)	-3(1)
C(24A)	69(2)	27(1)	44(1)	-11(1)	-8(1)	-3(1)
C(25A)	57(2)	32(1)	52(1)	0(1)	-5(1)	-14(1)
C(26A)	44(1)	44(1)	64(2)	4(1)	13(1)	-5(1)
C(27A)	42(1)	31(1)	59(1)	1(1)	12(1)	2(1)
S(1B)	30(1)	30(1)	33(1)	-5(1)	-3(1)	-3(1)
O(1B)	31(1)	32(1)	29(1)	-4(1)	-1(1)	-5(1)
O(2B)	40(1)	38(1)	32(1)	-1(1)	3(1)	-5(1)
O(3B)	34(1)	38(1)	41(1)	-4(1)	-7(1)	2(1)
N(1B)	39(1)	29(1)	34(1)	-7(1)	0(1)	1(1)
C(1B)	30(1)	34(1)	25(1)	-9(1)	2(1)	0(1)
C(2B)	33(1)	33(1)	26(1)	-5(1)	0(1)	-3(1)
C(3B)	36(1)	31(1)	28(1)	-11(1)	1(1)	-5(1)
C(4B)	48(1)	35(1)	29(1)	-11(1)	-3(1)	-5(1)
C(5B)	60(1)	40(1)	28(1)	-13(1)	7(1)	-9(1)
C(6B)	51(1)	39(1)	40(1)	-18(1)	17(1)	-7(1)
C(7B)	39(1)	31(1)	40(1)	-14(1)	5(1)	-2(1)

C(8B)	38(1)	26(1)	30(1)	-10(1)	1(1)	-5(1)
C(9B)	28(1)	31(1)	29(1)	-7(1)	0(1)	-4(1)
C(10B)	30(1)	32(1)	23(1)	-6(1)	2(1)	-1(1)
C(11B)	31(1)	30(1)	24(1)	-7(1)	-2(1)	0(1)
C(12B)	45(1)	34(1)	28(1)	-10(1)	-6(1)	-2(1)
C(13B)	50(1)	37(1)	39(1)	-16(1)	-1(1)	2(1)
C(14B)	31(1)	31(1)	25(1)	-7(1)	0(1)	1(1)
C(15B)	42(1)	33(1)	46(1)	-13(1)	-12(1)	-4(1)
C(16B)	33(1)	41(1)	26(1)	-6(1)	1(1)	-4(1)
C(17B)	38(1)	46(1)	47(1)	-20(1)	-2(1)	-4(1)
C(18B)	41(1)	56(2)	54(1)	-21(1)	-5(1)	-11(1)
C(19B)	31(1)	69(2)	50(1)	-15(1)	-6(1)	-6(1)
C(20B)	41(1)	51(2)	61(2)	-6(1)	-13(1)	6(1)
C(21B)	43(1)	41(1)	47(1)	-4(1)	-10(1)	-5(1)
C(22B)	33(1)	30(1)	26(1)	-5(1)	4(1)	-2(1)
C(23B)	44(1)	32(1)	47(1)	-2(1)	-8(1)	-8(1)
C(24B)	40(1)	42(1)	48(1)	0(1)	-11(1)	-4(1)
C(25B)	41(1)	34(1)	36(1)	0(1)	4(1)	4(1)
C(26B)	53(1)	30(1)	35(1)	-10(1)	6(1)	-3(1)
C(27B)	40(1)	35(1)	30(1)	-10(1)	4(1)	-4(1)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **23**.

	x	y	z	U(eq)
H(1NA)	6699(18)	5493(20)	5780(13)	36(6)*
H(1A)	8279(2)	2860(2)	6814(1)	34
H(4A)	8089(2)	2841(2)	4175(1)	43
H(5A)	6513(2)	2617(2)	3430(1)	49
H(6A)	4949(2)	1607(2)	4121(1)	50
H(7A)	4898(2)	755(2)	5581(1)	44
H(10A)	6784(2)	1727(2)	7554(1)	33
H(12A)	5413(2)	3442(2)	7693(1)	42
H(13A)	6283(2)	5532(2)	7021(1)	48
H(13B)	7140(2)	4364(2)	7415(1)	48
H(14A)	6810(2)	3895(2)	5392(1)	35
H(15A)	4557(2)	5311(2)	6195(1)	46
H(15B)	3786(2)	4529(2)	6985(1)	46
H(17A)	9612(2)	3676(2)	5657(1)	49
H(18A)	11565(2)	3772(2)	5342(1)	59
H(19A)	12642(2)	2061(2)	5272(1)	59
H(20A)	11749(2)	271(2)	5487(1)	56
H(21A)	9791(2)	175(2)	5785(1)	48
H(23A)	7418(2)	-1483(2)	6944(1)	47
H(24A)	6611(2)	-3238(2)	7813(1)	56
H(25A)	4950(2)	-3104(2)	8570(1)	60
H(26A)	4108(2)	-1222(2)	8498(2)	68
H(27A)	4928(2)	543(2)	7638(1)	59
H(1NB)	-1852(17)	10553(18)	803(12)	29(5)*

H(1B)	-3248(2)	8001(2)	1848(1)	36
H(4B)	-2737(2)	7819(2)	-767(1)	45
H(5B)	-1031(2)	7559(2)	-1483(1)	51
H(6B)	597(2)	6602(2)	-761(1)	51
H(7B)	568(2)	5811(2)	697(1)	43
H(10B)	-1695(2)	6862(2)	2616(1)	35
H(12B)	-559(2)	8583(2)	2728(1)	43
H(13C)	-2377(2)	9510(2)	2423(1)	49
H(13D)	-1628(2)	10670(2)	2024(1)	49
H(14B)	-1732(2)	8968(2)	430(1)	36
H(15C)	1016(2)	9627(2)	2017(1)	48
H(15D)	242(2)	10401(2)	1218(1)	48
H(17B)	-4274(2)	5250(2)	882(1)	51
H(18B)	-6210(2)	5344(2)	575(1)	58
H(19B)	-7306(2)	7153(2)	295(1)	61
H(20B)	-6477(2)	8875(2)	345(2)	65
H(21B)	-4552(2)	8781(2)	669(1)	55
H(23B)	309(2)	5618(2)	2733(1)	52
H(24B)	1295(2)	3847(2)	3555(1)	56
H(25B)	695(2)	1971(2)	3628(1)	49
H(26B)	-867(2)	1853(2)	2863(1)	48
H(27B)	-1848(2)	3618(2)	2031(1)	42

*Refined isotropically