Supporting Information for

Platinum-Catalyzed Diboration Using a Commercially Available Catalyst: Diboration of Aldimines to α-Aminoboronate Esters

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General considerations. All reactions were carried out under a nitrogen atmosphere using dry solvents. Alkenes, alkynes, B_2cat_2, and $Pt(cod)Cl_2$ were purchased from Aldrich Chemical Co. and used without further purification. ^1H, ^{13}C, and ^{11}B NMR spectra were obtained on a Varian 300 MHz spectrometer. ^1H and ^{13}C NMR spectra were referenced to residual protiated solvents, and ^{11}B NMR spectra were referenced to external $BF_3{\cdot}Et_2O$. The yields in this section are representative, and thus may differ from those in Tables 1 and 2.

General procedure for obtaining the ^1H NMR yield for the Pt-catalyzed diboration of vinylarenes, alkenes, alkynes, and aldimines . A 2 mL screw-capped vial equipped with a mini-stir bar was charged with $Pt(cod)Cl_2$ (**1**) (0.004 - 0.007 mmol, 3 - 5 mol % of Pt), B_2cat_2 (0.14 - 0.018 mmol), substrate (0.12 **-** 0.14 mmol), and trimethoxybenzene as an internal standard (ca. 0.10 mmol). Benzene (0.5 mL) was added to the vial and the solution was stirred. At the end of the reaction, the solution was then transferred to a NMR tube. The ^1H NMR yield of the product was obtained with respect to the trimethoxybenzene.

(4-OMe-C_6H_4)CH(Bcat)CH_2Bcat[1] (Table 1, entry 1). Reaction of 18.0 mg (0.13 mmol) of 4-vinylanisole, 38.0 mg (0.16 mmol) of B_2cat_2, 1.8 mg (0.005 mmol) of **1**, and 17.6 mg (0.10 mmol) of trimethoxybenzene in 0.5 mL of C_6D_6 at room temperature for 3 hr gave the product in 97 % yield by ^1H NMR spectroscopy with respect to trimethoxybenzene. ^1H, ^{13}C, $^{11}B\{^1H\}$ NMR spectra were published previously.[2]

(4-Cl-C_6H_4)CH(Bcat)CH_2Bcat[1] (Table 1, entry 2). Reaction of 16.5 mg (0.12 mmol) of 4-chlorostyrene, 38.6 mg (0.16 mmol) of B_2cat_2, 2.5 mg (0.007 mmol) of **1**, and 11.4 mg (0.067 mmol) of trimethoxybenzene in 0.5 mL of C_6D_6 at room temperature for 3 hr gave the product in 97 % yield by ^1H NMR spectroscopy with respect to trimethoxybenzene. ^1H NMR (C_6D_6) δ 1.63 (dd, 16.7 Hz, 6.7 Hz, 1H), 1.95 (dd, 16.7 Hz, 9.4 Hz, 1H), 3.11 (dd, 9.3 Hz, 7.1 Hz, 1H), 6.68-6.72 (m, 4H), 6.69-6.92 (m, 4H), 6.98 (d, 8.5 Hz, 2H), 7.05 (d, 8.3 Hz, 2H); $^{11}B\{^1H\}$ (C_6D_6) δ 34.8 (br, B-C).

$CH_3(CH_2)_5$CH(Bcat)CH_2Bcat (Table 1, entry 3). Reaction of 16.1 mg (0.14 mmol) of 1-octene, 36.7 mg (0.15 mmol) of B_2cat_2, 1.4 mg (0.004 mmol) of **1**, and 13.0 mg (0.077 mmol) of trimethoxybenzene in 0.5 mL of C_6D_6 at room temperature for 3 hr gave the product in 94 % yield by ^1H NMR spectroscopy with respect to trimethoxybenzene. ^1H

NMR (C_6D_6) δ 0.84 (t, 6 Hz, 3H), 1.18-1.20 (m, 6H), 1.36-1.38 (m, 2H), 1.43-1.67 (m, 3H), 1.72-2.03 (m, 2H), 6.71-6.75 (m, 4H), 6.93-6.98 (m, 4H); $^{11}B\{^1H\}$ (C_6D_6) δ 35.7 (br, B-C).

$CH_3(CH_2)_5$(Bcat)C=CHBcat (Table 1, entry 4). Reaction of 14.9 mg (0.14 mmol) of 1-octyne, 37.6 mg (0.16 mmol) of B_2cat_2, 2.3 mg (0.006 mmol) of **1**, and 13.2 mg (0.079 mmol) of trimethoxybenzene in 0.5 mL of C_6D_6 at 55 °C for 3 hr gave the product in 94 % yield by ^1H NMR spectroscopy with respect to trimethoxybenzene. ^1H, ^{13}C, $^{11}B\{^1H\}$ NMR spectra were published previously.[3]

(4-Me-C_6H_4)(Bcat)C=C(Bcat)(4-Me-C_6H_4) (Table 1, entry 5). Reaction of 26.0 mg (0.13 mmol) of ditolylacetylene, 34.1 mg (0.14 mmol) of B_2cat_2, 2.3 mg (0.006 mmol) of **1**, and 12.4 mg (0.074 mmol) of trimethoxybenzene in 0.5 mL of C_6D_6 at 55 °C for 3 hr gave the product in 98 % yield by ^1H NMR spectroscopy with respect to trimethoxybenzene. ^1H and $^{11}B\{^1H\}$ NMR spectra were published previously. [3]

(2,6-Me_2-C_6H_3)N(Bcat)CH(Bcat)(C_6H_5) (2) (Table 2, entry 1). Reaction of 25.8 mg (0.12 mmol) of N-benzylidene-2,6-dimethylaniline[4,5], 39.4 mg (0.17 mmol) of B_2cat_2, 1.4 mg (0.004 mmol) of **1**, and 9.4 mg (0.056 mmol) of trimethoxybenzene in 0.5 mL of C_6D_6 at room temperature for 15 hr gave the product in 90 % yield by ^1H NMR spectroscopy with respect to trimethoxybenzene. ^1H NMR (C_6D_6) δ 1.62 (s, 3H), 2.66 (s, 3H), 4.17 (s, 1H), 6.55 (br m, 2H), 6.61 (br m, 2H), 6.75 (dd, 5.9 Hz, 3.4 Hz, 2H), 6.84 (d, 6.6 Hz, 1H), 6.94-7.03 (m, 4H), 7.09-7.15 (m, 3H), 7.47-7.49 (m, 2H); ^{13}C NMR (C_6D_6) δ 18.66, 18.81, 54.44 (br, B-C), 111.86, 112.88, 122.18, 123.00, 126.88, 127.69, 128.28, 128.70, 128.87, 129.53, 130.53, 136.38, 137.33, 140.36, 143.01, 148.91; $^{11}B\{^1H\}$ (C_6D_6) δ 26.1 (br, B-N), 33.4 (br, B-C).

(2,6-iPr_2-C_6H_3)N(Bcat)CH(Bcat)(C_6H_5) (Table 2, entry 2). Reaction of 35.3 mg (0.13 mmol) of N-benzylidene-2,6-diisopropylaniline[6,7], 44.0 mg (0.18 mmol) of B_2cat_2, 1.8 mg (0.005 mmol) of **1**, and 11.3 mg (0.067 mmol) of trimethoxybenzene in 0.5 mL of C_6D_6 at room temperature for 15 hr gave the product in 84 % yield by ^1H NMR spectroscopy with respect to trimethoxybenzene. ^1H NMR (C_6D_6) δ 0.42 (d, 6.6 Hz, 3H), 1.07 (d, 6.6 Hz, 3H), 1.40 (d, 6.6 Hz, 3H), 1.48 (d, 6.6 Hz, 3H), 2.94 (septet, 6.8 Hz, 1H), 4.15 (septet, 6.6 Hz, 1H), 4.28 (s, 1H), 6.59 (br d, 19.8 Hz, 2H), 6.72-6.75 (m, 2H), 6.97-7.05 (m, 4H), 7.08-7.26 (m, 6H), 7.48 (d, 7.8 Hz, 2H); ^{13}C NMR (C_6D_6) δ 23.32, 23.98, 24.85, 25.90, 28.22, 29.27, 56.62 (br, B-C), 111.83, 112.91, 122.27, 122.99, 124.41, 124.85, 127.77, 127.94, 128.52, 128.74, 130.67, 139.87, 139.94, 146.84, 147.69, 148.92; $^{11}B\{^1H\}$ (C_6D_6) δ 26.5 (br, B-N), 34.6 (br, B-C).

(4-OMe-C_6H_4)N(Bcat)CH(Bcat)(C_6H_5) (Table 2, entry 3). Reaction of 27.1 mg (0.13 mmol) of N-benzylidene-4-methoxyaniline[8], 40.1 mg (0.17 mmol) of B_2cat_2, 2.5 mg (0.007 mmol) of **1**, and 13.8 mg (0.082 mmol) of trimethoxybenzene in 0.5 mL of C_6D_6 at 55 °C for 3 hr gave the product in 71 % yield by ^1H NMR spectroscopy with respect to trimethoxybenzene. ^1H NMR (C_6D_6) δ 3.21 (s, 3H), 4.90 (s, 1H), 6.57-6.77 (m, 5H),

6.97-7.04 (m, 4H), 7.06-7.11 (m, 4H), 7.24 (d, 7.8 Hz, 2H), 7.43 (d, 7.6 Hz, 2H); $^{11}B\{^1H\}$ (C_6D_6) δ 26.4 (br, B-N), 34.2 (br, B-C).

Isolated yields: (4-OMe-C_6H_4)CH(Bcat)CH_2Bcat (Table 1, entry 1). Into a 20 mL screw-capped vial equipped with a stir bar was charged **1** (14.4 mg, 0.038 mmol, 3 mol %), B_2cat_2 (135.2 mg, 0.57 mmol), 4-vinylanisole (66.4 mg, 0.50 mmol), and 2.0 mL of benzene. The reaction was stirred at room temperature overnight, after which time the vial was placed in a -5 °C freezer. The benzene solvent was removed by sublimation under vacuum to yield a dark brown powder. The solid was then extracted with hexanes. The clear hexanes solution was decanted, filtered through Celite, and placed in a –35 °C freezer overnight. The product (89.6 mg) crystallized out of solution as a white solid. The dark brown powder that was not extracted with hexanes was dissolved in ca. 2.0 mL of ether and filtered through Celite. To this light brown ether solution was added ca. 10 mL of hexanes and the solution was placed in a –35 °C freezer overnight. A light brown solid (55.3 mg) precipitated out of solution. This product was >97 % pure by ^1H NMR spectroscopy. The product from the reaction was isolated in a combined yield of 79 % (144.9 mg).

(4-Me-C_6H_4)(Bcat)C=C(Bcat)(4-Me-C_6H_4) (Table 1, entry 5). Into a 20 mL screw-capped vial equipped with a stir bar was charged **1** (15.0 mg, 0.04 mmol, 7 mol %), B_2cat_2 (136.3 mg, 0.57 mmol), ditolylacetylene (111.7 mg, 0.54 mmol), and 2.0 mL of benzene. The reaction was stirred at 70 °C overnight, after which time the vial was placed in a –5 °C freezer. The benzene solvent was removed by sublimation under vacuum to yield a dark brown powder. The solid dissolved in ca. 2 mL of ether and the solution was filtered through Celite. To this light brown solution was added ca. 10 mL hexanes and the solution was placed in a –35 °C freezer overnight. The product (109.0 mg) precipitated out of solution as an off-white solid. This procedure was repeated and a second crop of off-white powder was isolated in 26.5 mg. The combined fractions resulted in an isolated yield of 56 % (135.5 mg), and the product was >97 % pure by ^1H NMR spectroscopy.

(2,6-Me_2-C_6H_3)N(Bcat)CH(Bcat)(C_6H_5) (Table 2, entry 1). Into a 20 mL screw-capped vial equipped with a stir bar was charged **1** (14.4 mg, 0.038 mmol, 3 mol %), B_2cat_2 (125.3 mg, 0.53 mmol), N-benzylidene-2,6-dimethylaniline (101.5 mg, 0.49 mmol), and 2.0 mL of benzene. The reaction was stirred for at room temperature overnight, after which time the vial was placed in a –5 °C freezer. The benzene solvent was removed by sublimation under vacuum to yield a dark brown powder. The solid was then dissolved in 2.0 mL of ether, and the solution was placed in a –35 °C freezer overnight, after which time the product precipitated as a white solid in 78 % yield (169 mg).

References

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7) Jordan, A. Y.; Meyer, T. Y. J. Organomet.Chem. **1999**, 591, 104-113.
8) N -benzylidene-4-methoxyaniline is commercially available from Aldrich Chemicals Inc.

Experimental details for crystal structure **2**.

A block-shaped, colorless crystal of **2** was attached to a glass fiber using vacuum grease, and then cooled to 203 K under a liquid nitrogen vapor stream on the goniometer. The data were collected on a Bruker P4/CCD/PC diffractometer, with a sealed MoKα X-ray source. A hemisphere of data was collected using a combination of ϕ and ω scans, with 30 second exposures and 0.3 ° frame widths. Data collection, indexing, and initial cell refinement were handled using SMART software.[1] Frame integration and final cell refinement were carried out using SAINT software.[2] The SADABS program was used to perform the absorption correction.[3] The structure was solved using Patterson and difference Fourier techniques. The hydrogen atom positions were fixed in ideal positions, and refined using a riding model, with isotropic temperature factors fixed to 1.2 (methine and methylene) or 1.5 (methyl) times the equivalent isotropic U of the carbon atom they were bonded to. The C-H distances were fixed at 0.98 Å (methine), 0.97 Å (methylene), or 0.96 Å (methyl). The final refinement included anisotropic temperature factors on all non-hydrogen atoms. Structure solution, refinement, graphics, and creation of publication materials were performed using SHELXTL 5.1 software.[4]

Crystals of **2** were shown to adopt the space group $P2_1/c$. Refinement revealed that there were two molecules in the asymmetric unit with one molecule each possessing *R* and *S* chirality about the carbon atom bound to boron.

1. SMART Version 4.210, **1996**, Bruker Analytical X-Ray Systems, 6300 Enterprise Lane, Madison, WI 53719.
2. SAINT Version 4.05, **1996**, Bruker Analytical X-Ray Systems, 6300 Enterprise Lane, Madison, WI 53719.
3. SADABS, **1996**, George Sheldrick, University of Göttingen, Germany.
4. SHELXTL Version 5.1, **1997**, Bruker Analytical X-Ray Systems, 6300 Enterprise Lane, Madison, WI 53719.

Table 1. Crystal data and structure refinement for **2**.

Identification code	**2**	
Empirical formula	C54 H46 B4 N2 O8	
Formula weight	894.17	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 8.4702(5) Å	α= 90°.
	b = 16.3243(11) Å	β= 90.4990(10)°.
	c = 32.945(2) Å	γ = 90°.
Volume	4555.1(5) $Å^3$	
Z	4	
Density (calculated)	1.304 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	1872	
Crystal size	0.08 x 0.10 x 0.13mm^3	
Theta range for data collection	1.24 to 23.30°.	
Index ranges	-9<=h<=9, -18<=k<=18, -34<=l<=36	
Reflections collected	14042	
Independent reflections	6217 [R(int) = 0.0493]	
Completeness to theta = 23.30°	94.4 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6217 / 0 / 613	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2σ(I)]	R1 = 0.0663, wR2 = 0.1241	
R indices (all data)	R1 = 0.1085, wR2 = 0.1407	
Largest diff. peak and hole	0.328 and -0.254 ex$Å^{-3}$	

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

	x	y	z	U(eq)
N(1)	6357(4)	7639(2)	285(1)	27(1)
N(2)	4078(4)	4881(2)	2646(1)	33(1)
B(1)	4304(6)	8073(3)	-233(1)	33(1)
B(2)	6532(5)	6889(3)	92(1)	28(1)
B(3)	6136(6)	5425(3)	2151(1)	38(1)
B(4)	3722(6)	4209(3)	2405(1)	32(1)
O(1)	2985(3)	7622(2)	-123(1)	34(1)
O(2)	4266(3)	8272(2)	-640(1)	36(1)
O(3)	7268(3)	6206(2)	263(1)	35(1)
O(4)	5948(3)	6724(2)	-299(1)	35(1)
O(5)	7431(3)	4926(2)	2213(1)	42(1)
O(6)	6171(3)	5801(2)	1775(1)	44(1)
O(7)	2830(3)	3534(2)	2527(1)	38(1)
O(8)	4237(3)	4114(2)	2002(1)	36(1)
C(1)	5623(4)	8358(2)	75(1)	28(1)
C(2)	6822(4)	8925(2)	-119(1)	28(1)
C(3)	7775(5)	8648(2)	-434(1)	34(1)
C(4)	8805(5)	9166(3)	-630(1)	41(1)
C(5)	8915(5)	9976(2)	-512(1)	41(1)
C(6)	7996(5)	10262(2)	-197(1)	41(1)
C(7)	6969(5)	9735(2)	-2(1)	32(1)
C(8)	6891(5)	7754(2)	700(1)	27(1)
C(9)	8502(5)	7821(2)	786(1)	33(1)
C(10)	8974(5)	7920(3)	1190(1)	42(1)
C(11)	7883(6)	7930(3)	1498(1)	46(1)
C(12)	6304(6)	7847(2)	1409(1)	40(1)
C(13)	5771(5)	7767(2)	1012(1)	31(1)
C(14)	9740(5)	7763(3)	464(1)	42(1)
C(15)	4017(5)	7703(3)	930(1)	43(1)
C(16)	2159(5)	7498(2)	-484(1)	34(1)
C(17)	2929(5)	7891(2)	-793(1)	37(1)
C(18)	2378(6)	7877(3)	-1188(1)	52(1)
C(19)	999(7)	7433(3)	-1254(2)	65(2)
C(20)	223(6)	7046(3)	-941(2)	61(2)
C(21)	789(5)	7065(3)	-546(1)	48(1)
C(22)	7060(5)	5591(2)	-27(1)	33(1)
C(23)	6270(5)	5893(2)	-359(1)	32(1)
C(24)	5865(5)	5414(2)	-684(1)	43(1)
C(25)	6312(6)	4595(3)	-661(1)	47(1)
C(26)	7118(5)	4295(3)	-330(1)	48(1)
C(27)	7528(5)	4786(2)	1(1)	45(1)

C(28)	4884(5)	5626(2)	2487(1)	34(1)
C(29)	3721(5)	6301(2)	2372(1)	34(1)
C(30)	2740(5)	6236(3)	2033(1)	43(1)
C(31)	1684(5)	6845(3)	1939(1)	50(1)
C(32)	1585(5)	7540(3)	2174(2)	54(1)
C(33)	2545(6)	7613(3)	2514(2)	56(1)
C(34)	3593(5)	6993(2)	2613(1)	43(1)
C(35)	3572(5)	4921(2)	3065(1)	33(1)
C(36)	4693(5)	4834(2)	3370(1)	38(1)
C(37)	4202(6)	4918(3)	3773(1)	45(1)
C(38)	2649(6)	5040(3)	3862(1)	48(1)
C(39)	1542(6)	5095(3)	3554(1)	47(1)
C(40)	1971(5)	5058(2)	3151(1)	36(1)
C(41)	6383(5)	4610(3)	3283(1)	49(1)
C(42)	718(5)	5124(3)	2828(1)	51(1)
C(43)	7553(5)	5514(2)	1598(1)	39(1)
C(44)	8317(5)	4986(2)	1859(1)	35(1)
C(45)	9712(5)	4623(3)	1768(1)	48(1)
C(46)	10354(6)	4828(3)	1391(1)	51(1)
C(47)	9587(6)	5350(3)	1130(1)	54(1)
C(48)	8147(6)	5708(3)	1226(1)	54(1)
C(49)	2829(5)	3005(2)	2196(1)	32(1)
C(50)	3676(5)	3348(2)	1885(1)	31(1)
C(51)	3935(5)	2940(3)	1528(1)	40(1)
C(52)	3260(6)	2165(3)	1496(1)	50(1)
C(53)	2375(5)	1836(3)	1802(1)	50(1)
C(54)	2134(5)	2255(3)	2162(1)	44(1)

Table 3. Bond lengths [Å] and angles [°] for **2**.

Bond lengths [Å]	
N(1)-B(2)	1.389(5)
N(1)-C(8)	1.448(4)
N(1)-C(1)	1.495(4)
N(2)-B(4)	1.386(5)
N(2)-C(35)	1.450(4)
N(2)-C(28)	1.492(5)
B(1)-O(2)	1.382(5)
B(1)-O(1)	1.389(5)
B(1)-C(1)	1.571(6)
B(2)-O(3)	1.395(5)
B(2)-O(4)	1.400(5)
B(3)-O(5)	1.380(5)
B(3)-O(6)	1.384(5)
B(3)-C(28)	1.572(6)
B(4)-O(7)	1.397(5)
B(4)-O(8)	1.412(5)
O(1)-C(16)	1.391(4)
O(2)-C(17)	1.383(5)
O(3)-C(22)	1.395(4)
O(4)-C(23)	1.398(4)
O(5)-C(44)	1.397(4)
O(6)-C(43)	1.394(5)
O(7)-C(49)	1.391(4)
O(8)-C(50)	1.390(4)
C(1)-C(2)	1.520(5)
C(2)-C(7)	1.384(5)
C(2)-C(3)	1.394(5)
C(3)-C(4)	1.381(5)
C(4)-C(5)	1.381(6)
C(5)-C(6)	1.382(5)
C(6)-C(7)	1.385(5)
C(8)-C(9)	1.395(5)
C(8)-C(13)	1.404(5)
C(9)-C(10)	1.396(5)
C(9)-C(14)	1.501(5)
C(10)-C(11)	1.380(6)
C(11)-C(12)	1.375(6)
C(12)-C(13)	1.386(5)
C(13)-C(15)	1.512(6)
C(16)-C(17)	1.374(5)
C(16)-C(21)	1.372(6)
C(17)-C(18)	1.378(6)
C(18)-C(19)	1.390(7)

C(19)-C(20)	1.379(7)
C(20)-C(21)	1.383(6)
C(22)-C(23)	1.368(5)
C(22)-C(27)	1.375(5)
C(23)-C(24)	1.367(5)
C(24)-C(25)	1.391(6)
C(25)-C(26)	1.373(6)
C(26)-C(27)	1.395(6)
C(28)-C(29)	1.524(5)
C(29)-C(34)	1.387(5)
C(29)-C(30)	1.390(5)
C(30)-C(31)	1.371(6)
C(31)-C(32)	1.378(6)
C(32)-C(33)	1.383(6)
C(33)-C(34)	1.384(6)
C(35)-C(36)	1.386(5)
C(35)-C(40)	1.406(5)
C(36)-C(37)	1.400(5)
C(36)-C(41)	1.507(6)
C(37)-C(38)	1.365(6)
C(38)-C(39)	1.379(6)
C(39)-C(40)	1.380(5)
C(40)-C(42)	1.501(6)
C(43)-C(48)	1.366(5)
C(43)-C(44)	1.375(5)
C(44)-C(45)	1.358(6)
C(45)-C(46)	1.401(6)
C(46)-C(47)	1.370(6)
C(47)-C(48)	1.392(6)
C(49)-C(54)	1.362(5)
C(49)-C(50)	1.374(5)
C(50)-C(51)	1.373(5)
C(51)-C(52)	1.391(6)
C(52)-C(53)	1.371(6)
C(53)-C(54)	1.385(6)

Bond Angles [°]

B(2)-N(1)-C(8)	121.0(3)
B(2)-N(1)-C(1)	121.6(3)
C(8)-N(1)-C(1)	117.5(3)
B(4)-N(2)-C(35)	121.1(3)
B(4)-N(2)-C(28)	122.8(3)
C(35)-N(2)-C(28)	116.0(3)
O(2)-B(1)-O(1)	111.5(4)
O(2)-B(1)-C(1)	124.6(4)

O(1)-B(1)-C(1)	123.9(3)
N(1)-B(2)-O(3)	124.6(4)
N(1)-B(2)-O(4)	123.6(3)
O(3)-B(2)-O(4)	111.7(3)
O(5)-B(3)-O(6)	111.8(4)
O(5)-B(3)-C(28)	124.0(4)
O(6)-B(3)-C(28)	123.8(4)
N(2)-B(4)-O(7)	125.1(3)
N(2)-B(4)-O(8)	124.0(4)
O(7)-B(4)-O(8)	110.9(3)
B(1)-O(1)-C(16)	104.7(3)
B(1)-O(2)-C(17)	105.1(3)
C(22)-O(3)-B(2)	104.2(3)
C(23)-O(4)-B(2)	104.4(3)
B(3)-O(5)-C(44)	105.5(3)
B(3)-O(6)-C(43)	104.5(3)
C(49)-O(7)-B(4)	105.1(3)
C(50)-O(8)-B(4)	104.5(3)
N(1)-C(1)-C(2)	113.3(3)
N(1)-C(1)-B(1)	111.0(3)
C(2)-C(1)-B(1)	112.5(3)
C(7)-C(2)-C(3)	117.8(4)
C(7)-C(2)-C(1)	121.6(3)
C(3)-C(2)-C(1)	120.6(3)
C(4)-C(3)-C(2)	121.5(4)
C(5)-C(4)-C(3)	119.7(4)
C(4)-C(5)-C(6)	119.9(4)
C(5)-C(6)-C(7)	119.8(4)
C(2)-C(7)-C(6)	121.4(4)
C(9)-C(8)-C(13)	121.1(3)
C(9)-C(8)-N(1)	119.9(3)
C(13)-C(8)-N(1)	119.0(3)
C(10)-C(9)-C(8)	118.3(4)
C(10)-C(9)-C(14)	119.0(4)
C(8)-C(9)-C(14)	122.7(3)
C(11)-C(10)-C(9)	121.1(4)
C(12)-C(11)-C(10)	119.8(4)
C(11)-C(12)-C(13)	121.4(4)
C(12)-C(13)-C(8)	118.4(4)
C(12)-C(13)-C(15)	119.1(3)
C(8)-C(13)-C(15)	122.5(3)
C(17)-C(16)-C(21)	122.5(4)
C(17)-C(16)-O(1)	109.1(3)
C(21)-C(16)-O(1)	128.4(4)
C(16)-C(17)-C(18)	122.2(4)
C(16)-C(17)-O(2)	109.5(3)

C(18)-C(17)-O(2)	128.4(4)
C(17)-C(18)-C(19)	115.7(5)
C(20)-C(19)-C(18)	121.8(5)
C(19)-C(20)-C(21)	121.9(5)
C(16)-C(21)-C(20)	115.9(5)
C(23)-C(22)-C(27)	122.4(4)
C(23)-C(22)-O(3)	110.2(3)
C(27)-C(22)-O(3)	127.3(4)
C(22)-C(23)-C(24)	122.5(4)
C(22)-C(23)-O(4)	109.4(3)
C(24)-C(23)-O(4)	128.1(4)
C(23)-C(24)-C(25)	116.2(4)
C(26)-C(25)-C(24)	121.3(4)
C(25)-C(26)-C(27)	122.3(4)
C(22)-C(27)-C(26)	115.3(4)
N(2)-C(28)-C(29)	112.3(3)
N(2)-C(28)-B(3)	113.0(3)
C(29)-C(28)-B(3)	114.5(3)
C(34)-C(29)-C(30)	118.3(4)
C(34)-C(29)-C(28)	120.0(4)
C(30)-C(29)-C(28)	121.7(4)
C(31)-C(30)-C(29)	120.7(4)
C(30)-C(31)-C(32)	120.8(4)
C(31)-C(32)-C(33)	119.3(4)
C(32)-C(33)-C(34)	119.9(4)
C(33)-C(34)-C(29)	121.0(4)
C(36)-C(35)-C(40)	121.7(3)
C(36)-C(35)-N(2)	118.7(4)
C(40)-C(35)-N(2)	119.6(3)
C(35)-C(36)-C(37)	118.1(4)
C(35)-C(36)-C(41)	122.2(4)
C(37)-C(36)-C(41)	119.6(4)
C(38)-C(37)-C(36)	120.8(4)
C(37)-C(38)-C(39)	120.1(4)
C(38)-C(39)-C(40)	121.4(4)
C(39)-C(40)-C(35)	117.7(4)
C(39)-C(40)-C(42)	119.3(4)
C(35)-C(40)-C(42)	123.0(3)
C(48)-C(43)-C(44)	122.1(4)
C(48)-C(43)-O(6)	128.0(4)
C(44)-C(43)-O(6)	109.9(3)
C(45)-C(44)-C(43)	122.7(4)
C(45)-C(44)-O(5)	129.0(4)
C(43)-C(44)-O(5)	108.3(3)
C(44)-C(45)-C(46)	115.9(4)
C(47)-C(46)-C(45)	121.3(4)

C(46)-C(47)-C(48)	122.0(4)
C(43)-C(48)-C(47)	115.9(4)
C(54)-C(49)-C(50)	122.1(4)
C(54)-C(49)-O(7)	128.3(4)
C(50)-C(49)-O(7)	109.6(3)
C(51)-C(50)-C(49)	122.0(4)
C(51)-C(50)-O(8)	128.0(4)
C(49)-C(50)-O(8)	109.9(3)
C(50)-C(51)-C(52)	115.9(4)
C(53)-C(52)-C(51)	121.8(4)
C(52)-C(53)-C(54)	121.5(4)
C(49)-C(54)-C(53)	116.6(4)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	33(2)	27(2)	21(2)	3(1)	1(1)	3(2)
N(2)	37(2)	34(2)	29(2)	1(2)	9(2)	-1(2)
B(1)	38(3)	30(3)	31(3)	0(2)	2(2)	10(2)
B(2)	31(3)	29(3)	25(2)	6(2)	8(2)	2(2)
B(3)	43(3)	34(3)	36(3)	4(2)	1(2)	-3(2)
B(4)	36(3)	36(3)	24(2)	4(2)	4(2)	5(2)
O(1)	33(2)	35(2)	34(2)	-2(1)	1(1)	1(1)
O(2)	40(2)	42(2)	26(1)	2(1)	-2(1)	4(1)
O(3)	45(2)	28(2)	31(2)	2(1)	-1(1)	8(1)
O(4)	48(2)	26(2)	30(2)	-1(1)	2(1)	4(1)
O(5)	40(2)	51(2)	34(2)	8(1)	5(1)	4(2)
O(6)	51(2)	47(2)	34(2)	13(1)	10(1)	5(2)
O(7)	47(2)	35(2)	33(2)	0(1)	11(1)	-5(1)
O(8)	46(2)	37(2)	26(1)	1(1)	9(1)	-4(1)
C(1)	28(2)	29(2)	25(2)	-3(2)	4(2)	9(2)
C(2)	30(2)	31(2)	24(2)	2(2)	-3(2)	5(2)
C(3)	44(3)	27(2)	29(2)	-1(2)	3(2)	4(2)
C(4)	43(3)	42(3)	40(2)	3(2)	15(2)	5(2)
C(5)	39(3)	35(2)	49(3)	6(2)	11(2)	-1(2)
C(6)	40(3)	27(2)	55(3)	-4(2)	5(2)	-3(2)
C(7)	28(2)	33(2)	36(2)	-7(2)	3(2)	5(2)
C(8)	33(3)	23(2)	24(2)	-1(2)	-2(2)	1(2)
C(9)	36(3)	30(2)	32(2)	2(2)	-2(2)	2(2)
C(10)	40(3)	46(3)	41(3)	-1(2)	-10(2)	5(2)
C(11)	60(4)	51(3)	26(2)	-8(2)	-8(2)	11(2)
C(12)	53(3)	43(3)	24(2)	-2(2)	6(2)	13(2)
C(13)	35(3)	28(2)	29(2)	2(2)	7(2)	5(2)
C(14)	36(3)	46(3)	43(2)	0(2)	4(2)	-3(2)
C(15)	48(3)	44(3)	38(2)	-1(2)	11(2)	-1(2)
C(16)	30(3)	31(2)	42(2)	-9(2)	-4(2)	8(2)
C(17)	31(3)	39(2)	42(3)	-9(2)	-11(2)	14(2)
C(18)	57(4)	60(3)	39(3)	-9(2)	-9(2)	18(3)
C(19)	65(4)	77(4)	53(3)	-34(3)	-26(3)	29(3)
C(20)	47(3)	60(3)	75(4)	-35(3)	-22(3)	12(3)
C(21)	39(3)	44(3)	61(3)	-16(2)	-4(2)	6(2)
C(22)	41(3)	27(2)	33(2)	-3(2)	11(2)	-2(2)
C(23)	45(3)	22(2)	31(2)	-4(2)	10(2)	3(2)
C(24)	57(3)	37(3)	36(2)	0(2)	6(2)	-1(2)
C(25)	65(3)	35(3)	42(3)	-10(2)	13(2)	-7(2)
C(26)	56(3)	30(2)	58(3)	-3(2)	19(3)	5(2)
C(27)	54(3)	31(2)	49(3)	1(2)	10(2)	9(2)

C(28)	39(3)	34(2)	30(2)	1(2)	3(2)	-7(2)
C(29)	37(3)	33(2)	31(2)	4(2)	10(2)	-8(2)
C(30)	46(3)	41(3)	41(3)	3(2)	-4(2)	-3(2)
C(31)	44(3)	55(3)	50(3)	19(2)	-9(2)	-1(3)
C(32)	42(3)	50(3)	72(3)	13(3)	4(3)	6(2)
C(33)	53(3)	41(3)	75(4)	-8(3)	5(3)	4(3)
C(34)	42(3)	38(3)	49(3)	-3(2)	0(2)	-2(2)
C(35)	39(3)	32(2)	26(2)	-4(2)	4(2)	-4(2)
C(36)	43(3)	32(2)	40(2)	3(2)	5(2)	-1(2)
C(37)	62(3)	45(3)	27(2)	-1(2)	2(2)	-1(2)
C(38)	62(4)	52(3)	30(2)	-1(2)	7(2)	4(3)
C(39)	46(3)	49(3)	45(3)	-6(2)	14(2)	7(2)
C(40)	42(3)	33(2)	32(2)	-4(2)	6(2)	-1(2)
C(41)	48(3)	50(3)	50(3)	7(2)	4(2)	3(2)
C(42)	45(3)	65(3)	42(3)	-6(2)	4(2)	5(2)
C(43)	39(3)	41(3)	36(2)	-1(2)	11(2)	-5(2)
C(44)	41(3)	36(2)	29(2)	0(2)	7(2)	-5(2)
C(45)	44(3)	51(3)	49(3)	-9(2)	2(2)	2(2)
C(46)	44(3)	56(3)	52(3)	-17(3)	18(2)	-5(2)
C(47)	63(4)	57(3)	44(3)	-3(2)	25(3)	-7(3)
C(48)	62(4)	55(3)	44(3)	6(2)	9(2)	-5(3)
C(49)	35(3)	30(2)	32(2)	-3(2)	5(2)	3(2)
C(50)	32(2)	28(2)	33(2)	0(2)	-2(2)	5(2)
C(51)	47(3)	45(3)	28(2)	4(2)	4(2)	7(2)
C(52)	64(3)	44(3)	40(3)	-7(2)	-10(2)	7(3)
C(53)	53(3)	37(3)	60(3)	-7(2)	-8(3)	2(2)
C(54)	44(3)	37(3)	50(3)	-2(2)	5(2)	0(2)

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

	x	y	z	U(eq)
H(1A)	5091	8678	285	33
H(3A)	7716	8102	-513	40
H(4A)	9422	8971	-841	50
H(5A)	9606	10328	-643	49
H(6A)	8067	10807	-117	49
H(7A)	6366	9931	211	39
H(10A)	10041	7982	1252	51
H(11A)	8216	7992	1766	55
H(12A)	5577	7845	1619	48
H(14A)	10767	7824	586	63
H(14B)	9575	8189	267	63
H(14C)	9671	7239	333	63
H(15A)	3459	7723	1182	65
H(15B)	3792	7193	795	65
H(15C)	3685	8150	760	65
H(18A)	2896	8146	-1397	62
H(19A)	587	7396	-1516	78
H(20A)	-707	6764	-998	73
H(21A)	271	6801	-336	58
H(24A)	5321	5624	-907	52
H(25A)	6061	4245	-875	56
H(26A)	7399	3744	-326	58
H(27A)	8079	4584	225	54
H(28A)	5494	5844	2716	41
H(30A)	2801	5775	1868	51
H(31A)	1026	6788	1713	60
H(32A)	880	7956	2106	65
H(33A)	2486	8079	2676	67
H(34A)	4221	7041	2845	52
H(37A)	4944	4890	3982	54
H(38A)	2337	5086	4131	58
H(39A)	483	5159	3619	56
H(41A)	6529	4576	2995	74
H(41B)	6623	4090	3405	74
H(41C)	7072	5021	3394	74
H(42A)	-287	5217	2952	76
H(42B)	681	4625	2674	76
H(42C)	960	5573	2651	76
H(45A)	10210	4259	1944	58
H(46A)	11319	4606	1316	61
H(47A)	10043	5469	881	65
H(48A)	7622	6059	1048	64

H(51A)	4527	3167	1320	48
H(52A)	3413	1862	1260	60
H(53A)	1927	1321	1767	60
H(54A)	1529	2036	2369	53