Efficient C-B Bond Formation Promoted by *N*-Heterocyclic Carbenes. Synthesis of Tertiary and Quaternary B-Substituted Carbons through Metal-Free Catalytic Boron Conjugate Additions to Cyclic and Acyclic α,β -Unsaturated Carbonyls

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SUPPORTING INFORMATION, PART II

■ Crystal data of bicyclic β -boroketone **16**

Table 1. Crystal Data and Structure Refinement for **16**

Identification code	16
Empirical formula	C ₁₆ H ₂₅ B O ₄
Formula weight	292.17
Temperature	100(2) K
Wavelength	0.71073 $\approx$
Crystal system	Orthorhombic
Space group	P 21 21 21

Unit cell dimensions	$a = 7.4202(8) \text{ \AA}$	$\alpha = 90^\circ$
	$b = 10.7636(11) \text{ \AA}$	$\beta = 90^\circ$
	$c = 19.946(2) \text{ \AA}$	$\gamma = 90^\circ$
Volume	$1593.0(3) \text{ \AA}^3$	
Z	4	
Density (calculated)	1.218 Mg/m^3	
Absorption coefficient	0.084 mm^{-1}	
F(000)	632	
Crystal size	$0.10 \times 0.10 \times 0.05 \text{ mm}^3$	
Theta range for data collection	2.78 to 27.98°	
Index ranges	$-9 \leq h \leq 9$, $-12 \leq k \leq 14$, $-26 \leq l \leq 26$	
Reflections collected	15283	
Independent reflections	3813 [$R(\text{int}) = 0.0342$]	
Completeness to $\theta = 27.98^\circ$	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9958 and 0.9916	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3813 / 25 / 265	
Goodness-of-fit on F^2	1.035	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0377$, $wR2 = 0.0938$	
R indices (all data)	$R1 = 0.0406$, $wR2 = 0.0960$	
Absolute structure parameter	-0.1(7)	
Extinction coefficient	na	
Largest diff. peak and hole	0.374 and $-0.134 \text{ e. \AA}^{-3}$	

Table 2. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\approx 2 \times 10^3$) for **16** (U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.)

	x	y	z	U(eq)
O(1)	-350(2)	643(1)	1608(1)	25(1)
O(2)	4673(2)	3439(1)	3669(1)	28(1)
O(3)	1742(1)	3293(1)	802(1)	18(1)
O(4)	2922(1)	5032(1)	1291(1)	18(1)
C(1)	960(2)	1244(1)	1762(1)	17(1)
C(2)	2874(2)	994(1)	1537(1)	21(1)
C(3)	4021(2)	1983(1)	1885(1)	19(1)
C(4)	2681(2)	3063(1)	2044(1)	14(1)
C(5)	3409(2)	3922(1)	2598(1)	16(1)
C(6)	3411(2)	3347(1)	3288(1)	18(1)
C(7)	1708(2)	2681(1)	3482(1)	19(1)
C(8)	1149(2)	1740(1)	2946(1)	17(1)
C(9)	942(2)	2349(1)	2244(1)	15(1)
C(10)	-800(2)	3090(1)	2205(1)	20(1)
C(11)	1530(2)	4288(1)	306(1)	17(1)
C(12)	2873(2)	5293(1)	568(1)	17(1)
C(13)	1960(2)	3760(1)	-377(1)	26(1)
C(14)	-426(2)	4704(1)	338(1)	22(1)
C(15)	4786(2)	5117(2)	312(1)	28(1)
C(16)	2275(2)	6624(1)	461(1)	22(1)
B(1)	2419(2)	3825(1)	1370(1)	15(1)

Table 3. Bond Lengths [$\approx$] and Angles [∞] for **16**

O(1)-C(1)	1.2072(17)
O(2)-C(6)	1.2098(17)
O(3)-B(1)	1.3657(17)
O(3)-C(11)	1.4669(15)
O(4)-B(1)	1.3612(18)
O(4)-C(12)	1.4701(15)
C(1)-C(2)	1.514(2)
C(1)-C(9)	1.5286(18)
C(2)-C(3)	1.529(2)
C(2)-H(2A)	0.969(14)
C(2)-H(2B)	0.971(14)
C(3)-C(4)	1.5623(18)
C(3)-H(3A)	0.977(14)
C(3)-H(3B)	0.990(13)
C(4)-C(5)	1.5380(17)
C(4)-C(9)	1.5539(17)
C(4)-B(1)	1.5863(19)
C(5)-C(6)	1.5092(18)
C(5)-H(5A)	0.982(14)
C(5)-H(5B)	0.992(13)
C(6)-C(7)	1.5040(19)
C(7)-C(8)	1.5304(18)
C(7)-H(7A)	0.987(14)
C(7)-H(7B)	0.981(13)
C(8)-C(9)	1.5543(17)
C(8)-H(8A)	0.992(13)
C(8)-H(8B)	0.986(13)
C(9)-C(10)	1.5201(19)
C(10)-H(10A)	0.987(14)
C(10)-H(10B)	0.970(14)
C(10)-H(10C)	0.977(14)
C(11)-C(13)	1.5096(19)
C(11)-C(14)	1.5200(19)
C(11)-C(12)	1.5609(18)

C(12)-C(16)	1.5144(19)
C(12)-C(15)	1.521(2)
C(13)-H(13A)	1.000(15)
C(13)-H(13B)	0.967(15)
C(13)-H(13C)	0.992(14)
C(14)-H(14A)	0.989(14)
C(14)-H(14B)	0.958(14)
C(14)-H(14C)	1.008(14)
C(15)-H(15A)	0.963(15)
C(15)-H(15B)	0.996(15)
C(15)-H(15C)	0.957(15)
C(16)-H(16A)	0.963(14)
C(16)-H(16B)	0.966(15)
C(16)-H(16C)	0.965(14)

B(1)-O(3)-C(11)	107.05(10)
B(1)-O(4)-C(12)	106.79(10)
O(1)-C(1)-C(2)	125.76(12)
O(1)-C(1)-C(9)	124.73(12)
C(2)-C(1)-C(9)	109.46(11)
C(1)-C(2)-C(3)	105.28(11)
C(1)-C(2)-H(2A)	107.8(11)
C(3)-C(2)-H(2A)	110.4(10)
C(1)-C(2)-H(2B)	110.7(10)
C(3)-C(2)-H(2B)	115.4(10)
H(2A)-C(2)-H(2B)	107.0(14)
C(2)-C(3)-C(4)	104.85(11)
C(2)-C(3)-H(3A)	111.4(10)
C(4)-C(3)-H(3A)	111.2(10)
C(2)-C(3)-H(3B)	110.1(10)
C(4)-C(3)-H(3B)	109.5(10)
H(3A)-C(3)-H(3B)	109.7(14)
C(5)-C(4)-C(9)	113.90(10)
C(5)-C(4)-C(3)	111.71(11)
C(9)-C(4)-C(3)	102.26(10)
C(5)-C(4)-B(1)	109.93(10)

C(9)-C(4)-B(1)	111.76(10)
C(3)-C(4)-B(1)	106.87(10)
C(6)-C(5)-C(4)	114.12(11)
C(6)-C(5)-H(5A)	106.0(10)
C(4)-C(5)-H(5A)	108.2(10)
C(6)-C(5)-H(5B)	106.4(10)
C(4)-C(5)-H(5B)	110.2(10)
H(5A)-C(5)-H(5B)	111.9(14)
O(2)-C(6)-C(7)	121.82(12)
O(2)-C(6)-C(5)	122.70(13)
C(7)-C(6)-C(5)	115.45(11)
C(6)-C(7)-C(8)	111.28(11)
C(6)-C(7)-H(7A)	105.9(10)
C(8)-C(7)-H(7A)	111.9(10)
C(6)-C(7)-H(7B)	109.6(10)
C(8)-C(7)-H(7B)	110.9(10)
H(7A)-C(7)-H(7B)	107.0(14)
C(7)-C(8)-C(9)	112.18(10)
C(7)-C(8)-H(8A)	109.8(10)
C(9)-C(8)-H(8A)	108.1(10)
C(7)-C(8)-H(8B)	108.0(10)
C(9)-C(8)-H(8B)	110.3(10)
H(8A)-C(8)-H(8B)	108.3(14)
C(10)-C(9)-C(1)	112.53(11)
C(10)-C(9)-C(4)	115.69(11)
C(1)-C(9)-C(4)	102.53(10)
C(10)-C(9)-C(8)	110.57(11)
C(1)-C(9)-C(8)	103.70(10)
C(4)-C(9)-C(8)	110.94(10)
C(9)-C(10)-H(10A)	110.8(11)
C(9)-C(10)-H(10B)	109.2(11)
H(10A)-C(10)-H(10B)	109.5(15)
C(9)-C(10)-H(10C)	109.6(11)
H(10A)-C(10)-H(10C)	107.2(15)
H(10B)-C(10)-H(10C)	110.6(16)
O(3)-C(11)-C(13)	108.10(11)

O(3)-C(11)-C(14)	106.79(11)
C(13)-C(11)-C(14)	110.58(11)
O(3)-C(11)-C(12)	102.19(9)
C(13)-C(11)-C(12)	115.34(12)
C(14)-C(11)-C(12)	113.03(11)
O(4)-C(12)-C(16)	109.03(11)
O(4)-C(12)-C(15)	106.42(11)
C(16)-C(12)-C(15)	110.10(12)
O(4)-C(12)-C(11)	102.28(10)
C(16)-C(12)-C(11)	114.90(11)
C(15)-C(12)-C(11)	113.42(12)
C(11)-C(13)-H(13A)	110.3(12)
C(11)-C(13)-H(13B)	111.4(12)
H(13A)-C(13)-H(13B)	108.6(17)
C(11)-C(13)-H(13C)	112.7(11)
H(13A)-C(13)-H(13C)	107.2(16)
H(13B)-C(13)-H(13C)	106.3(17)
C(11)-C(14)-H(14A)	107.5(12)
C(11)-C(14)-H(14B)	110.0(12)
H(14A)-C(14)-H(14B)	109.4(16)
C(11)-C(14)-H(14C)	113.0(11)
H(14A)-C(14)-H(14C)	108.4(16)
H(14B)-C(14)-H(14C)	108.6(16)
C(12)-C(15)-H(15A)	108.1(12)
C(12)-C(15)-H(15B)	110.7(12)
H(15A)-C(15)-H(15B)	109.6(18)
C(12)-C(15)-H(15C)	109.3(13)
H(15A)-C(15)-H(15C)	108.2(17)
H(15B)-C(15)-H(15C)	110.8(17)
C(12)-C(16)-H(16A)	110.2(11)
C(12)-C(16)-H(16B)	112.8(11)
H(16A)-C(16)-H(16B)	104.8(15)
C(12)-C(16)-H(16C)	109.0(11)
H(16A)-C(16)-H(16C)	112.1(16)
H(16B)-C(16)-H(16C)	107.9(17)
O(4)-B(1)-O(3)	113.90(12)

O(4)-B(1)-C(4)	123.89(12)
O(3)-B(1)-C(4)	122.13(12)

Symmetry transformations used to generate equivalent atoms.

Table 4. Anisotropic Displacement Parameters ($\approx 2 \times 10^3$) for **16** [The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U^{11} + \dots + 2hk a^* b^* U^{12})$.]

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
O(1)	31(1)	21(1)	22(1)	1(1)	-4(1)	-10(1)
O(2)	32(1)	27(1)	24(1)	5(1)	-11(1)	-8(1)
O(3)	23(1)	16(1)	16(1)	2(1)	-2(1)	-2(1)
O(4)	23(1)	18(1)	16(1)	3(1)	-2(1)	-4(1)
C(1)	25(1)	14(1)	13(1)	2(1)	-3(1)	-1(1)
C(2)	27(1)	16(1)	20(1)	-3(1)	-2(1)	4(1)
C(3)	18(1)	19(1)	19(1)	-1(1)	0(1)	4(1)
C(4)	14(1)	13(1)	15(1)	0(1)	-1(1)	-1(1)
C(5)	19(1)	15(1)	15(1)	0(1)	-2(1)	-3(1)
C(6)	25(1)	12(1)	16(1)	-2(1)	-2(1)	-1(1)
C(7)	26(1)	18(1)	14(1)	1(1)	0(1)	-3(1)
C(8)	21(1)	16(1)	15(1)	3(1)	1(1)	-4(1)
C(9)	16(1)	14(1)	15(1)	0(1)	1(1)	-2(1)
C(10)	16(1)	23(1)	22(1)	2(1)	1(1)	0(1)
C(11)	20(1)	16(1)	14(1)	2(1)	-1(1)	-1(1)
C(12)	18(1)	18(1)	15(1)	2(1)	-1(1)	-3(1)
C(13)	37(1)	24(1)	16(1)	0(1)	1(1)	4(1)
C(14)	20(1)	25(1)	23(1)	2(1)	-4(1)	-2(1)
C(15)	18(1)	34(1)	32(1)	10(1)	2(1)	-2(1)
C(16)	28(1)	18(1)	20(1)	4(1)	-2(1)	-2(1)
B(1)	13(1)	17(1)	16(1)	1(1)	1(1)	0(1)

Table 5. Hydrogen Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($\approx^2 \times 10^3$) for **16**

	x	y	z	U(eq)
H(2A)	2920(20)	1100(16)	1055(7)	25
H(2B)	3210(20)	140(14)	1630(8)	25
H(3A)	5000(20)	2267(15)	1596(8)	22
H(3B)	4520(20)	1651(15)	2308(7)	22
H(5A)	4673(19)	4115(15)	2495(8)	20
H(5B)	2660(20)	4684(14)	2629(8)	20
H(7A)	790(20)	3333(15)	3546(8)	23
H(7B)	1880(20)	2273(16)	3918(7)	23
H(8A)	-21(19)	1358(15)	3069(8)	21
H(8B)	2070(20)	1080(14)	2932(8)	21
H(10A)	-1840(20)	2567(16)	2328(9)	30
H(10B)	-960(30)	3398(17)	1751(7)	30
H(10C)	-750(20)	3777(16)	2524(8)	30
H(13A)	1090(20)	3081(16)	-492(10)	38
H(13B)	3170(20)	3429(19)	-393(10)	38
H(13C)	1880(30)	4390(16)	-738(8)	38
H(14A)	-1190(20)	3969(15)	249(9)	34
H(14B)	-650(30)	5324(16)	4(8)	34
H(14C)	-770(30)	5054(17)	789(8)	34
H(15A)	5560(30)	5681(18)	552(10)	42
H(15B)	4860(30)	5295(19)	-178(8)	42
H(15C)	5170(30)	4287(15)	406(10)	42
H(16A)	3160(20)	7189(16)	639(9)	33
H(16B)	1180(20)	6822(17)	699(9)	33
H(16C)	2060(30)	6757(17)	-11(7)	33

Table 6. Torsion Angles [$^{\circ}$] for **16**

O(1)-C(1)-C(2)-C(3)	-178.27(13)
C(9)-C(1)-C(2)-C(3)	-0.72(15)
C(1)-C(2)-C(3)-C(4)	-23.17(14)
C(2)-C(3)-C(4)-C(5)	160.15(11)
C(2)-C(3)-C(4)-C(9)	37.96(13)
C(2)-C(3)-C(4)-B(1)	-79.58(12)
C(9)-C(4)-C(5)-C(6)	43.93(16)
C(3)-C(4)-C(5)-C(6)	-71.31(14)
B(1)-C(4)-C(5)-C(6)	170.23(11)
C(4)-C(5)-C(6)-O(2)	135.83(14)
C(4)-C(5)-C(6)-C(7)	-46.05(16)
O(2)-C(6)-C(7)-C(8)	-130.22(14)
C(5)-C(6)-C(7)-C(8)	51.64(15)
C(6)-C(7)-C(8)-C(9)	-55.61(15)
O(1)-C(1)-C(9)-C(10)	-33.25(18)
C(2)-C(1)-C(9)-C(10)	149.17(11)
O(1)-C(1)-C(9)-C(4)	-158.21(13)
C(2)-C(1)-C(9)-C(4)	24.21(14)
O(1)-C(1)-C(9)-C(8)	86.27(15)
C(2)-C(1)-C(9)-C(8)	-91.31(12)
C(5)-C(4)-C(9)-C(10)	79.13(14)
C(3)-C(4)-C(9)-C(10)	-160.19(11)
B(1)-C(4)-C(9)-C(10)	-46.21(14)
C(5)-C(4)-C(9)-C(1)	-158.02(11)
C(3)-C(4)-C(9)-C(1)	-37.34(12)
B(1)-C(4)-C(9)-C(1)	76.65(13)
C(5)-C(4)-C(9)-C(8)	-47.86(14)
C(3)-C(4)-C(9)-C(8)	72.83(12)
B(1)-C(4)-C(9)-C(8)	-173.19(11)
C(7)-C(8)-C(9)-C(10)	-75.75(14)
C(7)-C(8)-C(9)-C(1)	163.41(11)
C(7)-C(8)-C(9)-C(4)	54.00(15)
B(1)-O(3)-C(11)-C(13)	144.26(12)
B(1)-O(3)-C(11)-C(14)	-96.74(12)

B(1)-O(3)-C(11)-C(12)	22.16(13)
B(1)-O(4)-C(12)-C(16)	145.35(11)
B(1)-O(4)-C(12)-C(15)	-95.92(13)
B(1)-O(4)-C(12)-C(11)	23.29(13)
O(3)-C(11)-C(12)-O(4)	-27.26(12)
C(13)-C(11)-C(12)-O(4)	-144.26(11)
C(14)-C(11)-C(12)-O(4)	87.13(12)
O(3)-C(11)-C(12)-C(16)	-145.22(11)
C(13)-C(11)-C(12)-C(16)	97.78(14)
C(14)-C(11)-C(12)-C(16)	-30.83(16)
O(3)-C(11)-C(12)-C(15)	86.91(13)
C(13)-C(11)-C(12)-C(15)	-30.09(16)
C(14)-C(11)-C(12)-C(15)	-158.70(12)
C(12)-O(4)-B(1)-O(3)	-10.46(15)
C(12)-O(4)-B(1)-C(4)	166.29(12)
C(11)-O(3)-B(1)-O(4)	-8.46(15)
C(11)-O(3)-B(1)-C(4)	174.72(11)
C(5)-C(4)-B(1)-O(4)	5.23(18)
C(9)-C(4)-B(1)-O(4)	132.73(13)
C(3)-C(4)-B(1)-O(4)	-116.17(13)
C(5)-C(4)-B(1)-O(3)	-178.27(11)
C(9)-C(4)-B(1)-O(3)	-50.78(16)
C(3)-C(4)-B(1)-O(3)	60.32(15)

Symmetry transformations used to generate equivalent atoms.

■ Crystal data of product **22**.

Table 1. Crystal Data and Structure Refinement for **22**

Identification code	22	
Empirical formula	C ₁₉ H ₂₇ B O ₄	
Formula weight	330.22	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /n	
Unit cell dimensions	a = 5.9436(8) Å	α = 90°
	b = 16.888(2) Å	β = 93.841(2)°
	c = 17.475(2) Å	γ = 90°
Volume	1750.2(4) Å ³	
Z	4	
Density (calculated)	1.253 Mg/m ³	
Absorption coefficient	0.085 mm ⁻¹	
F(000)	712	
Crystal size	0.14 x 0.07 x 0.06 mm ³	

Theta range for data collection	2.34 to 28.30°.
Index ranges	-7<=h<=7, -21<=k<=21, -23<=l<=23
Reflections collected	20649
Independent reflections	4265 [R(int) = 0.0222]
Completeness to theta = 28.30°	98.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9949 and 0.9882
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4265 / 27 / 298
Goodness-of-fit on F ²	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0417, wR2 = 0.1060
R indices (all data)	R1 = 0.0468, wR2 = 0.1104
Extinction coefficient	na
Largest diff. peak and hole	0.446 and -0.157 e.Å ⁻³

Table 2. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **22** (U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.)

	x	y	z	U(eq)
O(1)	4424(1)	850(1)	4913(1)	21(1)
O(2)	2258(1)	12(1)	6072(1)	17(1)
O(3)	2929(1)	2618(1)	6314(1)	17(1)
O(4)	832(1)	3471(1)	5543(1)	17(1)
B(1)	1214(2)	2698(1)	5759(1)	14(1)
C(1)	2567(2)	1142(1)	4774(1)	16(1)
C(2)	1855(2)	1470(1)	3992(1)	19(1)
C(3)	702(2)	2276(1)	4043(1)	19(1)
C(4)	-1214(2)	2238(1)	4579(1)	18(1)
C(5)	-287(2)	2005(1)	5392(1)	14(1)
C(6)	812(2)	1172(1)	5371(1)	13(1)
C(7)	1806(2)	845(1)	6140(1)	14(1)
C(8)	234(2)	924(1)	6781(1)	14(1)
C(9)	-1864(2)	551(1)	6733(1)	16(1)
C(10)	-3257(2)	589(1)	7340(1)	18(1)
C(11)	-2586(2)	1018(1)	7995(1)	19(1)
C(12)	-521(2)	1403(1)	8042(1)	19(1)
C(13)	889(2)	1351(1)	7438(1)	16(1)
C(14)	3513(2)	3416(1)	6590(1)	16(1)
C(15)	2714(2)	3935(1)	5889(1)	17(1)
C(16)	6022(2)	3438(1)	6808(1)	22(1)
C(17)	2187(2)	3569(1)	7293(1)	20(1)
C(18)	4458(2)	3982(1)	5292(1)	25(1)
C(19)	1854(2)	4750(1)	6083(1)	24(1)

Table 3. Bond Lengths [Å] and Angles [°] for **22**

O(1)-C(1)	1.2183(13)
O(2)-C(7)	1.4392(12)
O(2)-H(2O)	0.829(12)
O(3)-B(1)	1.3652(14)
O(3)-C(14)	1.4660(12)
O(4)-B(1)	1.3745(13)
O(4)-C(15)	1.4616(13)
B(1)-C(5)	1.5803(15)
C(1)-C(2)	1.5087(14)
C(1)-C(6)	1.5251(14)
C(2)-C(3)	1.5304(15)
C(2)-H(2A)	0.967(12)
C(2)-H(2B)	0.982(12)
C(3)-C(4)	1.5232(15)
C(3)-H(3A)	0.983(12)
C(3)-H(3B)	0.989(12)
C(4)-C(5)	1.5408(14)
C(4)-H(4A)	0.991(12)
C(4)-H(4B)	0.974(12)
C(5)-C(6)	1.5536(14)
C(5)-H(5)	0.987(11)
C(6)-C(7)	1.5342(13)
C(6)-H(6)	0.993(11)
C(7)-C(8)	1.5119(13)
C(7)-H(7)	0.976(11)
C(8)-C(13)	1.3895(14)
C(8)-C(9)	1.3945(14)
C(9)-C(10)	1.3898(14)
C(9)-H(9)	0.951(12)
C(10)-C(11)	1.3892(16)
C(10)-H(10)	0.965(12)
C(11)-C(12)	1.3863(16)
C(11)-H(11)	0.954(12)
C(12)-C(13)	1.3943(15)

C(12)-H(12)	0.970(12)
C(13)-H(13)	0.948(12)
C(14)-C(16)	1.5150(15)
C(14)-C(17)	1.5250(15)
C(14)-C(15)	1.5555(15)
C(15)-C(19)	1.5148(15)
C(15)-C(18)	1.5211(15)
C(16)-H(16A)	0.985(13)
C(16)-H(16B)	0.986(13)
C(16)-H(16C)	0.989(13)
C(17)-H(17A)	0.982(13)
C(17)-H(17B)	0.980(13)
C(17)-H(17C)	0.979(13)
C(18)-H(18A)	0.997(13)
C(18)-H(18B)	1.006(13)
C(18)-H(18C)	0.984(13)
C(19)-H(19A)	0.970(13)
C(19)-H(19B)	0.978(13)
C(19)-H(19C)	0.983(13)
C(7)-O(2)-H(2O)	107.4(10)
B(1)-O(3)-C(14)	106.98(8)
B(1)-O(4)-C(15)	106.73(8)
O(3)-B(1)-O(4)	113.00(9)
O(3)-B(1)-C(5)	126.08(9)
O(4)-B(1)-C(5)	120.90(9)
O(1)-C(1)-C(2)	121.66(9)
O(1)-C(1)-C(6)	121.93(9)
C(2)-C(1)-C(6)	116.38(9)
C(1)-C(2)-C(3)	111.92(9)
C(1)-C(2)-H(2A)	109.2(9)
C(3)-C(2)-H(2A)	112.0(9)
C(1)-C(2)-H(2B)	105.3(8)
C(3)-C(2)-H(2B)	108.6(9)
H(2A)-C(2)-H(2B)	109.6(12)
C(4)-C(3)-C(2)	110.75(9)
C(4)-C(3)-H(3A)	109.0(8)

C(2)-C(3)-H(3A)	109.0(8)
C(4)-C(3)-H(3B)	110.5(9)
C(2)-C(3)-H(3B)	109.7(8)
H(3A)-C(3)-H(3B)	107.7(12)
C(3)-C(4)-C(5)	110.02(9)
C(3)-C(4)-H(4A)	109.1(8)
C(5)-C(4)-H(4A)	109.6(8)
C(3)-C(4)-H(4B)	109.2(8)
C(5)-C(4)-H(4B)	109.3(8)
H(4A)-C(4)-H(4B)	109.6(12)
C(4)-C(5)-C(6)	109.51(8)
C(4)-C(5)-B(1)	110.05(8)
C(6)-C(5)-B(1)	116.96(8)
C(4)-C(5)-H(5)	108.5(8)
C(6)-C(5)-H(5)	107.5(8)
B(1)-C(5)-H(5)	103.9(8)
C(1)-C(6)-C(7)	110.30(8)
C(1)-C(6)-C(5)	110.75(8)
C(7)-C(6)-C(5)	116.26(8)
C(1)-C(6)-H(6)	104.4(8)
C(7)-C(6)-H(6)	108.3(8)
C(5)-C(6)-H(6)	106.0(8)
O(2)-C(7)-C(8)	105.96(8)
O(2)-C(7)-C(6)	110.02(8)
C(8)-C(7)-C(6)	113.39(8)
O(2)-C(7)-H(7)	110.5(8)
C(8)-C(7)-H(7)	108.5(8)
C(6)-C(7)-H(7)	108.5(8)
C(13)-C(8)-C(9)	118.96(9)
C(13)-C(8)-C(7)	120.31(9)
C(9)-C(8)-C(7)	120.70(9)
C(10)-C(9)-C(8)	120.61(10)
C(10)-C(9)-H(9)	118.9(8)
C(8)-C(9)-H(9)	120.4(8)
C(11)-C(10)-C(9)	119.97(10)
C(11)-C(10)-H(10)	120.1(8)

C(9)-C(10)-H(10)	120.0(8)
C(12)-C(11)-C(10)	119.88(10)
C(12)-C(11)-H(11)	119.2(9)
C(10)-C(11)-H(11)	121.0(9)
C(11)-C(12)-C(13)	119.98(10)
C(11)-C(12)-H(12)	121.8(9)
C(13)-C(12)-H(12)	118.2(9)
C(8)-C(13)-C(12)	120.58(10)
C(8)-C(13)-H(13)	118.8(9)
C(12)-C(13)-H(13)	120.6(9)
O(3)-C(14)-C(16)	108.23(8)
O(3)-C(14)-C(17)	107.37(8)
C(16)-C(14)-C(17)	110.27(9)
O(3)-C(14)-C(15)	101.82(8)
C(16)-C(14)-C(15)	115.35(9)
C(17)-C(14)-C(15)	113.08(9)
O(4)-C(15)-C(19)	108.61(9)
O(4)-C(15)-C(18)	106.44(8)
C(19)-C(15)-C(18)	111.19(9)
O(4)-C(15)-C(14)	102.06(8)
C(19)-C(15)-C(14)	115.13(9)
C(18)-C(15)-C(14)	112.57(9)
C(14)-C(16)-H(16A)	111.7(9)
C(14)-C(16)-H(16B)	108.6(10)
H(16A)-C(16)-H(16B)	108.2(13)
C(14)-C(16)-H(16C)	109.1(10)
H(16A)-C(16)-H(16C)	109.7(13)
H(16B)-C(16)-H(16C)	109.3(13)
C(14)-C(17)-H(17A)	108.6(9)
C(14)-C(17)-H(17B)	112.2(9)
H(17A)-C(17)-H(17B)	108.5(13)
C(14)-C(17)-H(17C)	110.6(9)
H(17A)-C(17)-H(17C)	109.9(13)
H(17B)-C(17)-H(17C)	107.1(13)
C(15)-C(18)-H(18A)	110.1(10)
C(15)-C(18)-H(18B)	108.8(10)

H(18A)-C(18)-H(18B)	110.9(14)
C(15)-C(18)-H(18C)	112.0(10)
H(18A)-C(18)-H(18C)	107.3(14)
H(18B)-C(18)-H(18C)	107.7(13)
C(15)-C(19)-H(19A)	111.0(10)
C(15)-C(19)-H(19B)	110.1(10)
H(19A)-C(19)-H(19B)	107.4(13)
C(15)-C(19)-H(19C)	109.4(10)
H(19A)-C(19)-H(19C)	109.5(14)
H(19B)-C(19)-H(19C)	109.4(14)

Symmetry transformations used to generate equivalent atoms.

Table 4. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **22** [The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U^{11} + \dots + 2hka^*b^*U^{12})$.]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	21(1)	23(1)	20(1)	1(1)	6(1)	3(1)
O(2)	19(1)	13(1)	18(1)	0(1)	5(1)	2(1)
O(3)	18(1)	14(1)	18(1)	-1(1)	-2(1)	-1(1)
O(4)	20(1)	14(1)	17(1)	-2(1)	-2(1)	0(1)
B(1)	16(1)	16(1)	13(1)	-1(1)	2(1)	1(1)
C(1)	20(1)	13(1)	15(1)	-2(1)	3(1)	-3(1)
C(2)	25(1)	20(1)	13(1)	-1(1)	3(1)	-2(1)
C(3)	25(1)	17(1)	13(1)	1(1)	-1(1)	-3(1)
C(4)	18(1)	18(1)	16(1)	1(1)	-3(1)	-1(1)
C(5)	15(1)	14(1)	14(1)	0(1)	1(1)	-1(1)
C(6)	15(1)	13(1)	12(1)	0(1)	1(1)	-1(1)
C(7)	15(1)	12(1)	13(1)	0(1)	1(1)	0(1)
C(8)	16(1)	13(1)	12(1)	2(1)	1(1)	2(1)
C(9)	18(1)	16(1)	15(1)	-1(1)	0(1)	-1(1)
C(10)	16(1)	17(1)	19(1)	2(1)	2(1)	0(1)
C(11)	22(1)	19(1)	17(1)	2(1)	6(1)	2(1)
C(12)	25(1)	19(1)	14(1)	-2(1)	2(1)	0(1)
C(13)	17(1)	17(1)	16(1)	0(1)	0(1)	-2(1)
C(14)	16(1)	14(1)	18(1)	-3(1)	0(1)	-1(1)
C(15)	19(1)	15(1)	18(1)	-2(1)	1(1)	-2(1)
C(16)	16(1)	24(1)	26(1)	-4(1)	-1(1)	-2(1)
C(17)	18(1)	26(1)	16(1)	-3(1)	0(1)	0(1)
C(18)	30(1)	23(1)	23(1)	1(1)	8(1)	-6(1)
C(19)	32(1)	14(1)	26(1)	-4(1)	-1(1)	1(1)

Table 5. Hydrogen Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **22**

	x	y	z	U(eq)
H(2O)	3310(20)	-37(8)	5785(8)	20
H(2A)	3150(20)	1492(8)	3686(8)	23
H(2B)	760(20)	1088(8)	3764(8)	23
H(3A)	1820(20)	2668(8)	4241(8)	22
H(3B)	130(20)	2450(8)	3525(7)	22
H(4A)	-1950(20)	2764(7)	4593(8)	21
H(4B)	-2310(20)	1844(8)	4388(8)	21
H(5)	-1560(20)	1971(8)	5725(7)	17
H(6)	-400(20)	806(8)	5169(7)	16
H(7)	3190(20)	1133(8)	6285(7)	16
H(9)	-2360(20)	266(8)	6285(7)	19
H(10)	-4680(20)	313(8)	7309(8)	21
H(11)	-3530(20)	1052(9)	8415(7)	23
H(12)	-10(20)	1713(8)	8488(7)	23
H(13)	2320(20)	1603(8)	7470(8)	20
H(16A)	6910(30)	3299(9)	6372(8)	33
H(16B)	6440(30)	3979(8)	6976(9)	33
H(16C)	6370(30)	3065(9)	7236(8)	33
H(17A)	2510(30)	3141(8)	7664(8)	30
H(17B)	560(20)	3586(9)	7165(9)	30
H(17C)	2610(30)	4080(8)	7526(9)	30
H(18A)	5040(30)	3443(8)	5183(9)	38
H(18B)	3740(30)	4231(10)	4812(8)	38
H(18C)	5760(20)	4311(9)	5467(9)	38
H(19A)	530(20)	4713(10)	6379(9)	36
H(19B)	1410(30)	5041(9)	5613(8)	36
H(19C)	3050(20)	5042(9)	6379(9)	36

Table 6. Torsion Angles [°] for **22**

C(14)-O(3)-B(1)-O(4)	10.18(12)
C(14)-O(3)-B(1)-C(5)	-168.31(9)
C(15)-O(4)-B(1)-O(3)	10.58(11)
C(15)-O(4)-B(1)-C(5)	-170.84(9)
O(1)-C(1)-C(2)-C(3)	-134.74(11)
C(6)-C(1)-C(2)-C(3)	47.19(12)
C(1)-C(2)-C(3)-C(4)	-52.46(12)
C(2)-C(3)-C(4)-C(5)	60.84(11)
C(3)-C(4)-C(5)-C(6)	-61.44(11)
C(3)-C(4)-C(5)-B(1)	68.44(11)
O(3)-B(1)-C(5)-C(4)	-153.96(10)
O(4)-B(1)-C(5)-C(4)	27.66(13)
O(3)-B(1)-C(5)-C(6)	-28.19(15)
O(4)-B(1)-C(5)-C(6)	153.43(9)
O(1)-C(1)-C(6)-C(7)	3.86(13)
C(2)-C(1)-C(6)-C(7)	-178.08(8)
O(1)-C(1)-C(6)-C(5)	134.00(10)
C(2)-C(1)-C(6)-C(5)	-47.94(11)
C(4)-C(5)-C(6)-C(1)	53.64(11)
B(1)-C(5)-C(6)-C(1)	-72.40(11)
C(4)-C(5)-C(6)-C(7)	-179.44(8)
B(1)-C(5)-C(6)-C(7)	54.52(12)
C(1)-C(6)-C(7)-O(2)	-66.77(10)
C(5)-C(6)-C(7)-O(2)	166.09(8)
C(1)-C(6)-C(7)-C(8)	174.78(8)
C(5)-C(6)-C(7)-C(8)	47.64(12)
O(2)-C(7)-C(8)-C(13)	118.30(10)
C(6)-C(7)-C(8)-C(13)	-120.92(10)
O(2)-C(7)-C(8)-C(9)	-59.79(11)
C(6)-C(7)-C(8)-C(9)	60.98(12)
C(13)-C(8)-C(9)-C(10)	-1.53(15)
C(7)-C(8)-C(9)-C(10)	176.59(9)
C(8)-C(9)-C(10)-C(11)	1.55(16)
C(9)-C(10)-C(11)-C(12)	-0.34(16)

C(10)-C(11)-C(12)-C(13)	-0.84(16)
C(9)-C(8)-C(13)-C(12)	0.33(15)
C(7)-C(8)-C(13)-C(12)	-177.79(9)
C(11)-C(12)-C(13)-C(8)	0.85(16)
B(1)-O(3)-C(14)-C(16)	-146.82(9)
B(1)-O(3)-C(14)-C(17)	94.16(10)
B(1)-O(3)-C(14)-C(15)	-24.85(10)
B(1)-O(4)-C(15)-C(19)	-147.13(9)
B(1)-O(4)-C(15)-C(18)	93.06(10)
B(1)-O(4)-C(15)-C(14)	-25.12(10)
O(3)-C(14)-C(15)-O(4)	30.00(9)
C(16)-C(14)-C(15)-O(4)	146.93(9)
C(17)-C(14)-C(15)-O(4)	-84.87(10)
O(3)-C(14)-C(15)-C(19)	147.43(9)
C(16)-C(14)-C(15)-C(19)	-95.65(12)
C(17)-C(14)-C(15)-C(19)	32.56(13)
O(3)-C(14)-C(15)-C(18)	-83.71(10)
C(16)-C(14)-C(15)-C(18)	33.21(13)
C(17)-C(14)-C(15)-C(18)	161.42(9)

Symmetry transformations used to generate equivalent atoms.

Table 7. Hydrogen Bonds for **22** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...O(1)	0.829(12)	2.269(13)	2.8489(11)	127.3(12)
O(2)-H(2O)...O(1)#1	0.829(12)	2.327(13)	3.0698(11)	149.5(13)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

■ Crystal data of product (23) of tandem conjugate boron addition/aldol reaction with *p*-chlorobenzaldehyde

Table 1. Crystal Data and Structure Refinement for **23**

Identification code	23	
Empirical formula	C ₁₉ H ₂₆ B Cl O ₄	
Formula weight	364.66	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /c	
Unit cell dimensions	a = 12.399(2) Å	α = 90°
	b = 32.215(5) Å	β = 109.176(2)°
	c = 9.9188(17) Å	γ = 90°
Volume	3742.2(11) Å ³	
Z	8	
Density (calculated)	1.294 Mg/m ³	
Absorption coefficient	0.224 mm ⁻¹	
F(000)	1552	
Crystal size	0.27 x 0.08 x 0.03 mm ³	

Theta range for data collection	2.26 to 25.50°
Index ranges	-15 ≤ h ≤ 15, -39 ≤ k ≤ 39, -12 ≤ l ≤ 12
Reflections collected	46054
Independent reflections	6941 [R(int) = 0.0750]
Completeness to theta = 25.50°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9933 and 0.9419
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6941 / 52 / 607
Goodness-of-fit on F ²	1.046
Final R indices [I > 2σ(I)]	R1 = 0.0481, wR2 = 0.0957
R indices (all data)	R1 = 0.0741, wR2 = 0.1048
Extinction coefficient	na
Largest diff. peak and hole	0.288 and -0.230 e. Å ⁻³

Table 2. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\approx^2 \times 10^3$) for **23** (U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.)

	x	y	z	U(eq)
Cl(1)	8400(1)	-2643(1)	7173(1)	38(1)
O(1)	14807(2)	-3519(1)	13329(2)	30(1)
O(2)	12746(2)	-3107(1)	12859(2)	26(1)
O(3)	14256(1)	-3553(1)	8016(2)	20(1)
O(4)	14558(1)	-3077(1)	9787(2)	19(1)
B(1)	14017(2)	-3436(1)	9201(3)	15(1)
C(1)	14262(2)	-3744(1)	12362(2)	19(1)
C(2)	14629(2)	-4181(1)	12219(3)	26(1)
C(3)	14574(2)	-4287(1)	10694(3)	22(1)
C(4)	13430(2)	-4165(1)	9633(3)	18(1)
C(5)	13192(2)	-3702(1)	9750(2)	15(1)
C(6)	13154(2)	-3607(1)	11261(2)	16(1)
C(7)	12854(2)	-3159(1)	11475(2)	18(1)
C(8)	11745(2)	-3026(1)	10406(2)	18(1)
C(9)	11716(2)	-2755(1)	9315(2)	20(1)
C(10)	10695(2)	-2637(1)	8317(3)	23(1)
C(11)	9698(2)	-2796(1)	8424(3)	25(1)
C(12)	9693(2)	-3069(1)	9488(3)	27(1)
C(13)	10718(2)	-3182(1)	10467(3)	23(1)
C(14)	14856(2)	-3211(1)	7617(2)	22(1)
C(15)	15376(2)	-2982(1)	9047(2)	20(1)
C(16)	15705(3)	-3384(1)	6984(3)	31(1)
C(17)	13947(2)	-2957(1)	6532(3)	30(1)
C(18)	16501(2)	-3165(1)	9966(3)	34(1)
C(19)	15469(3)	-2519(1)	8926(3)	31(1)
Cl(2)	14913(1)	-4700(1)	7103(1)	27(1)
O(5)	8849(2)	-4220(1)	-216(2)	44(1)
O(6)	11156(2)	-4427(1)	701(2)	28(1)
O(7)	8950(2)	-4339(1)	5103(2)	26(1)
O(8)	9551(2)	-3932(1)	3635(2)	27(1)
B(2)	9332(2)	-4322(1)	3972(3)	16(1)

C(20)	8749(2)	-4492(1)	583(2)	24(1)
C(21)	7615(2)	-4690(1)	368(3)	25(1)
C(22)	7390(2)	-4783(1)	1761(3)	21(1)
C(23)	8399(2)	-4995(1)	2822(2)	18(1)
C(24)	9475(2)	-4725(1)	3153(2)	16(1)
C(25)	9768(2)	-4653(1)	1774(2)	17(1)
C(26)	10813(2)	-4381(1)	1940(2)	19(1)
C(27)	11830(2)	-4475(1)	3225(2)	18(1)
C(28)	12337(2)	-4862(1)	3475(3)	21(1)
C(29)	13285(2)	-4938(1)	4657(3)	21(1)
C(30)	13724(2)	-4615(1)	5597(2)	20(1)
C(31)	13239(2)	-4227(1)	5380(3)	21(1)
C(32)	12298(2)	-4160(1)	4191(2)	19(1)
C(33)	9081(2)	-3927(1)	5742(2)	22(1)
C(34)	9158(2)	-3645(1)	4512(3)	27(1)
C(35)	8076(3)	-3844(1)	6234(3)	37(1)
C(36)	10166(3)	-3939(1)	6998(3)	43(1)
C(37)	8015(3)	-3486(1)	3568(3)	54(1)
C(38)	10003(3)	-3295(1)	4946(4)	53(1)

Table 3. Bond Lengths [$\approx$] and Angles [∞] for **23**

Cl(1)-C(11)	1.750(2)
O(1)-C(1)	1.216(3)
O(2)-C(7)	1.432(3)
O(2)-H(2O)	0.844(17)
O(3)-B(1)	1.356(3)
O(3)-C(14)	1.454(3)
O(4)-B(1)	1.367(3)
O(4)-C(15)	1.467(2)
B(1)-C(5)	1.562(3)
C(1)-C(2)	1.501(3)
C(1)-C(6)	1.512(3)
C(2)-C(3)	1.530(3)
C(2)-H(2A)	0.981(16)
C(2)-H(2B)	0.985(16)
C(3)-C(4)	1.514(3)
C(3)-H(3A)	0.995(16)
C(3)-H(3B)	0.964(16)
C(4)-C(5)	1.534(3)
C(4)-H(4A)	0.977(16)
C(4)-H(4B)	0.990(16)
C(5)-C(6)	1.545(3)
C(5)-H(5)	0.980(16)
C(6)-C(7)	1.525(3)
C(6)-H(6)	0.997(15)
C(7)-C(8)	1.496(3)
C(7)-H(7)	0.986(16)
C(8)-C(9)	1.383(3)
C(8)-C(13)	1.388(3)
C(9)-C(10)	1.379(3)
C(9)-H(9)	0.952(16)
C(10)-C(11)	1.373(3)
C(10)-H(10)	0.942(16)
C(11)-C(12)	1.377(4)
C(12)-C(13)	1.371(4)

C(12)-H(12)	0.956(16)
C(13)-H(13)	0.930(16)
C(14)-C(16)	1.500(3)
C(14)-C(17)	1.518(4)
C(14)-C(15)	1.540(3)
C(15)-C(19)	1.505(3)
C(15)-C(18)	1.513(4)
C(16)-H(16A)	0.972(17)
C(16)-H(16B)	1.001(17)
C(16)-H(16C)	0.975(17)
C(17)-H(17A)	1.000(17)
C(17)-H(17B)	0.972(17)
C(17)-H(17C)	0.979(17)
C(18)-H(18A)	0.986(17)
C(18)-H(18B)	0.985(17)
C(18)-H(18C)	0.999(17)
C(19)-H(19A)	1.000(17)
C(19)-H(19B)	1.008(17)
C(19)-H(19C)	0.999(17)
Cl(2)-C(30)	1.741(2)
O(5)-C(20)	1.213(3)
O(6)-C(26)	1.433(3)
O(6)-H(6O)	0.830(17)
O(7)-B(2)	1.354(3)
O(7)-C(33)	1.457(3)
O(8)-B(2)	1.348(3)
O(8)-C(34)	1.459(3)
B(2)-C(24)	1.572(3)
C(20)-C(21)	1.495(3)
C(20)-C(25)	1.511(3)
C(21)-C(22)	1.526(3)
C(21)-H(21A)	0.976(16)
C(21)-H(21B)	0.980(16)
C(22)-C(23)	1.509(3)
C(22)-H(22A)	0.990(16)
C(22)-H(22B)	0.994(16)

C(23)-C(24)	1.537(3)
C(23)-H(23A)	1.006(16)
C(23)-H(23B)	0.988(16)
C(24)-C(25)	1.544(3)
C(24)-H(24)	0.987(16)
C(25)-C(26)	1.528(3)
C(25)-H(25)	0.978(16)
C(26)-C(27)	1.500(3)
C(26)-H(26)	0.988(16)
C(27)-C(28)	1.381(3)
C(27)-C(32)	1.385(3)
C(28)-C(29)	1.383(3)
C(28)-H(28)	0.952(16)
C(29)-C(30)	1.383(3)
C(29)-H(29)	0.945(16)
C(30)-C(31)	1.374(3)
C(31)-C(32)	1.376(3)
C(31)-H(31)	0.945(16)
C(32)-H(32)	0.940(16)
C(33)-C(36)	1.504(4)
C(33)-C(35)	1.504(4)
C(33)-C(34)	1.548(3)
C(34)-C(38)	1.503(4)
C(34)-C(37)	1.509(4)
C(35)-H(35A)	0.987(17)
C(35)-H(35B)	1.009(17)
C(35)-H(35C)	0.980(17)
C(36)-H(36A)	0.987(18)
C(36)-H(36B)	0.979(18)
C(36)-H(36C)	0.989(18)
C(37)-H(37A)	0.996(18)
C(37)-H(37B)	0.986(18)
C(37)-H(37C)	1.003(18)
C(38)-H(38A)	0.973(18)
C(38)-H(38B)	1.016(18)
C(38)-H(38C)	0.978(18)

C(7)-O(2)-H(2O)	104.3(19)
B(1)-O(3)-C(14)	107.63(17)
B(1)-O(4)-C(15)	106.70(16)
O(3)-B(1)-O(4)	112.75(19)
O(3)-B(1)-C(5)	120.4(2)
O(4)-B(1)-C(5)	126.89(19)
O(1)-C(1)-C(2)	121.8(2)
O(1)-C(1)-C(6)	122.2(2)
C(2)-C(1)-C(6)	115.9(2)
C(1)-C(2)-C(3)	112.67(19)
C(1)-C(2)-H(2A)	105.2(15)
C(3)-C(2)-H(2A)	110.3(15)
C(1)-C(2)-H(2B)	110.3(15)
C(3)-C(2)-H(2B)	110.1(15)
H(2A)-C(2)-H(2B)	108(2)
C(4)-C(3)-C(2)	110.9(2)
C(4)-C(3)-H(3A)	108.6(14)
C(2)-C(3)-H(3A)	110.2(14)
C(4)-C(3)-H(3B)	110.8(15)
C(2)-C(3)-H(3B)	109.4(14)
H(3A)-C(3)-H(3B)	107(2)
C(3)-C(4)-C(5)	110.99(19)
C(3)-C(4)-H(4A)	108.8(14)
C(5)-C(4)-H(4A)	110.1(14)
C(3)-C(4)-H(4B)	112.2(13)
C(5)-C(4)-H(4B)	107.0(13)
H(4A)-C(4)-H(4B)	107.7(19)
C(4)-C(5)-C(6)	109.47(18)
C(4)-C(5)-B(1)	110.03(18)
C(6)-C(5)-B(1)	117.54(18)
C(4)-C(5)-H(5)	108.0(13)
C(6)-C(5)-H(5)	107.9(13)
B(1)-C(5)-H(5)	103.4(13)
C(1)-C(6)-C(7)	112.44(19)
C(1)-C(6)-C(5)	109.44(18)

C(7)-C(6)-C(5)	114.13(18)
C(1)-C(6)-H(6)	104.4(13)
C(7)-C(6)-H(6)	107.8(13)
C(5)-C(6)-H(6)	108.1(13)
O(2)-C(7)-C(8)	107.01(18)
O(2)-C(7)-C(6)	110.37(18)
C(8)-C(7)-C(6)	112.43(19)
O(2)-C(7)-H(7)	108.3(13)
C(8)-C(7)-H(7)	109.7(14)
C(6)-C(7)-H(7)	109.0(13)
C(9)-C(8)-C(13)	118.3(2)
C(9)-C(8)-C(7)	121.1(2)
C(13)-C(8)-C(7)	120.6(2)
C(10)-C(9)-C(8)	121.1(2)
C(10)-C(9)-H(9)	117.6(15)
C(8)-C(9)-H(9)	121.2(15)
C(11)-C(10)-C(9)	118.7(2)
C(11)-C(10)-H(10)	120.8(15)
C(9)-C(10)-H(10)	120.4(15)
C(10)-C(11)-C(12)	121.9(2)
C(10)-C(11)-Cl(1)	118.9(2)
C(12)-C(11)-Cl(1)	119.3(2)
C(13)-C(12)-C(11)	118.4(2)
C(13)-C(12)-H(12)	121.7(16)
C(11)-C(12)-H(12)	119.9(16)
C(12)-C(13)-C(8)	121.6(2)
C(12)-C(13)-H(13)	119.6(15)
C(8)-C(13)-H(13)	118.8(15)
O(3)-C(14)-C(16)	108.96(19)
O(3)-C(14)-C(17)	105.93(19)
C(16)-C(14)-C(17)	111.3(2)
O(3)-C(14)-C(15)	102.08(17)
C(16)-C(14)-C(15)	115.1(2)
C(17)-C(14)-C(15)	112.6(2)
O(4)-C(15)-C(19)	109.36(19)
O(4)-C(15)-C(18)	105.67(18)

C(19)-C(15)-C(18)	110.7(2)
O(4)-C(15)-C(14)	102.18(17)
C(19)-C(15)-C(14)	114.9(2)
C(18)-C(15)-C(14)	113.1(2)
C(14)-C(16)-H(16A)	109.2(17)
C(14)-C(16)-H(16B)	110.1(16)
H(16A)-C(16)-H(16B)	109(2)
C(14)-C(16)-H(16C)	109.9(17)
H(16A)-C(16)-H(16C)	109(2)
H(16B)-C(16)-H(16C)	110(2)
C(14)-C(17)-H(17A)	107.0(16)
C(14)-C(17)-H(17B)	110.0(17)
H(17A)-C(17)-H(17B)	108(2)
C(14)-C(17)-H(17C)	111.9(16)
H(17A)-C(17)-H(17C)	111(2)
H(17B)-C(17)-H(17C)	109(2)
C(15)-C(18)-H(18A)	106.5(17)
C(15)-C(18)-H(18B)	107.9(17)
H(18A)-C(18)-H(18B)	109(2)
C(15)-C(18)-H(18C)	111.9(17)
H(18A)-C(18)-H(18C)	112(2)
H(18B)-C(18)-H(18C)	109(2)
C(15)-C(19)-H(19A)	108.1(16)
C(15)-C(19)-H(19B)	109.3(16)
H(19A)-C(19)-H(19B)	108(2)
C(15)-C(19)-H(19C)	108.8(16)
H(19A)-C(19)-H(19C)	110(2)
H(19B)-C(19)-H(19C)	113(2)
C(26)-O(6)-H(6O)	100(2)
B(2)-O(7)-C(33)	107.70(17)
B(2)-O(8)-C(34)	107.96(17)
O(8)-B(2)-O(7)	113.4(2)
O(8)-B(2)-C(24)	125.0(2)
O(7)-B(2)-C(24)	121.6(2)
O(5)-C(20)-C(21)	120.5(2)
O(5)-C(20)-C(25)	121.4(2)

C(21)-C(20)-C(25)	118.0(2)
C(20)-C(21)-C(22)	113.5(2)
C(20)-C(21)-H(21A)	104.9(15)
C(22)-C(21)-H(21A)	108.6(15)
C(20)-C(21)-H(21B)	107.7(15)
C(22)-C(21)-H(21B)	113.4(15)
H(21A)-C(21)-H(21B)	108(2)
C(23)-C(22)-C(21)	111.3(2)
C(23)-C(22)-H(22A)	109.8(14)
C(21)-C(22)-H(22A)	108.5(14)
C(23)-C(22)-H(22B)	112.3(14)
C(21)-C(22)-H(22B)	109.8(14)
H(22A)-C(22)-H(22B)	104.9(19)
C(22)-C(23)-C(24)	110.77(19)
C(22)-C(23)-H(23A)	108.8(13)
C(24)-C(23)-H(23A)	109.2(13)
C(22)-C(23)-H(23B)	109.4(14)
C(24)-C(23)-H(23B)	109.2(13)
H(23A)-C(23)-H(23B)	109.4(18)
C(23)-C(24)-C(25)	109.62(18)
C(23)-C(24)-B(2)	110.00(18)
C(25)-C(24)-B(2)	115.70(18)
C(23)-C(24)-H(24)	107.7(13)
C(25)-C(24)-H(24)	105.8(13)
B(2)-C(24)-H(24)	107.6(13)
C(20)-C(25)-C(26)	110.38(19)
C(20)-C(25)-C(24)	111.39(18)
C(26)-C(25)-C(24)	115.39(18)
C(20)-C(25)-H(25)	103.9(14)
C(26)-C(25)-H(25)	107.7(14)
C(24)-C(25)-H(25)	107.3(13)
O(6)-C(26)-C(27)	107.72(18)
O(6)-C(26)-C(25)	109.17(18)
C(27)-C(26)-C(25)	114.96(18)
O(6)-C(26)-H(26)	107.9(13)
C(27)-C(26)-H(26)	109.7(14)

C(25)-C(26)-H(26)	107.2(14)
C(28)-C(27)-C(32)	118.3(2)
C(28)-C(27)-C(26)	122.7(2)
C(32)-C(27)-C(26)	119.0(2)
C(27)-C(28)-C(29)	121.5(2)
C(27)-C(28)-H(28)	120.6(15)
C(29)-C(28)-H(28)	117.9(15)
C(28)-C(29)-C(30)	118.4(2)
C(28)-C(29)-H(29)	122.3(15)
C(30)-C(29)-H(29)	119.4(15)
C(31)-C(30)-C(29)	121.6(2)
C(31)-C(30)-Cl(2)	118.81(18)
C(29)-C(30)-Cl(2)	119.62(18)
C(30)-C(31)-C(32)	118.7(2)
C(30)-C(31)-H(31)	120.2(15)
C(32)-C(31)-H(31)	121.0(15)
C(31)-C(32)-C(27)	121.6(2)
C(31)-C(32)-H(32)	120.1(15)
C(27)-C(32)-H(32)	118.3(15)
O(7)-C(33)-C(36)	106.1(2)
O(7)-C(33)-C(35)	108.5(2)
C(36)-C(33)-C(35)	110.3(2)
O(7)-C(33)-C(34)	102.58(17)
C(36)-C(33)-C(34)	113.5(2)
C(35)-C(33)-C(34)	115.1(2)
O(8)-C(34)-C(38)	108.0(2)
O(8)-C(34)-C(37)	105.9(2)
C(38)-C(34)-C(37)	110.3(3)
O(8)-C(34)-C(33)	102.56(17)
C(38)-C(34)-C(33)	115.6(2)
C(37)-C(34)-C(33)	113.6(2)
C(33)-C(35)-H(35A)	107.1(18)
C(33)-C(35)-H(35B)	110.1(17)
H(35A)-C(35)-H(35B)	112(2)
C(33)-C(35)-H(35C)	109.7(18)
H(35A)-C(35)-H(35C)	106(2)

H(35B)-C(35)-H(35C)	113(3)
C(33)-C(36)-H(36A)	106(2)
C(33)-C(36)-H(36B)	111.0(19)
H(36A)-C(36)-H(36B)	113(3)
C(33)-C(36)-H(36C)	112.7(19)
H(36A)-C(36)-H(36C)	109(3)
H(36B)-C(36)-H(36C)	105(3)
C(34)-C(37)-H(37A)	108(2)
C(34)-C(37)-H(37B)	110(2)
H(37A)-C(37)-H(37B)	111(3)
C(34)-C(37)-H(37C)	107(2)
H(37A)-C(37)-H(37C)	115(3)
H(37B)-C(37)-H(37C)	105(3)
C(34)-C(38)-H(38A)	108(2)
C(34)-C(38)-H(38B)	110(2)
H(38A)-C(38)-H(38B)	110(3)
C(34)-C(38)-H(38C)	110(2)
H(38A)-C(38)-H(38C)	107(3)
H(38B)-C(38)-H(38C)	111(3)

Symmetry transformations used to generate equivalent atoms.

Table 4. Anisotropic Displacement Parameters ($\approx 2 \times 10^3$) for **23** [The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12})$.]

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	25(1)	29(1)	51(1)	-2(1)	-1(1)	8(1)
O(1)	34(1)	31(1)	18(1)	-1(1)	0(1)	-1(1)
O(2)	36(1)	31(1)	16(1)	-5(1)	14(1)	0(1)
O(3)	30(1)	18(1)	17(1)	-3(1)	14(1)	-7(1)
O(4)	21(1)	22(1)	16(1)	-3(1)	10(1)	-5(1)
B(1)	19(1)	15(1)	10(1)	3(1)	4(1)	5(1)
C(1)	26(1)	23(1)	12(1)	4(1)	10(1)	-3(1)
C(2)	28(2)	24(1)	26(1)	8(1)	10(1)	6(1)
C(3)	28(1)	17(1)	26(1)	4(1)	14(1)	5(1)
C(4)	24(1)	14(1)	21(1)	-1(1)	13(1)	-3(1)
C(5)	16(1)	16(1)	12(1)	-1(1)	4(1)	1(1)
C(6)	19(1)	16(1)	14(1)	1(1)	8(1)	-2(1)
C(7)	28(1)	17(1)	15(1)	-3(1)	13(1)	-3(1)
C(8)	24(1)	14(1)	20(1)	-6(1)	12(1)	0(1)
C(9)	23(1)	16(1)	24(1)	-2(1)	11(1)	-2(1)
C(10)	28(1)	17(1)	25(1)	0(1)	9(1)	2(1)
C(11)	20(1)	18(1)	32(2)	-6(1)	2(1)	7(1)
C(12)	22(1)	24(1)	38(2)	-7(1)	14(1)	-2(1)
C(13)	27(1)	20(1)	27(1)	-1(1)	16(1)	0(1)
C(14)	28(1)	20(1)	21(1)	0(1)	14(1)	-7(1)
C(15)	22(1)	24(1)	18(1)	1(1)	11(1)	-4(1)
C(16)	44(2)	27(2)	33(2)	-4(1)	27(1)	-4(1)
C(17)	38(2)	33(2)	20(1)	7(1)	12(1)	-1(1)
C(18)	23(2)	44(2)	34(2)	0(1)	6(1)	-6(1)
C(19)	42(2)	25(1)	33(2)	-6(1)	23(1)	-9(1)
Cl(2)	22(1)	36(1)	21(1)	4(1)	7(1)	5(1)
O(5)	38(1)	64(1)	24(1)	23(1)	2(1)	-13(1)
O(6)	29(1)	44(1)	16(1)	-3(1)	13(1)	-10(1)
O(7)	46(1)	17(1)	22(1)	-2(1)	22(1)	-2(1)
O(8)	46(1)	16(1)	26(1)	2(1)	22(1)	2(1)
B(2)	14(1)	20(1)	13(1)	3(1)	2(1)	0(1)

C(20)	30(1)	32(1)	11(1)	-2(1)	8(1)	-6(1)
C(21)	23(1)	31(1)	18(1)	-1(1)	4(1)	-3(1)
C(22)	19(1)	23(1)	22(1)	-3(1)	7(1)	-2(1)
C(23)	20(1)	18(1)	19(1)	-1(1)	10(1)	-3(1)
C(24)	16(1)	18(1)	13(1)	0(1)	6(1)	-1(1)
C(25)	20(1)	19(1)	12(1)	-2(1)	7(1)	-5(1)
C(26)	24(1)	25(1)	12(1)	0(1)	10(1)	-5(1)
C(27)	18(1)	22(1)	17(1)	-2(1)	12(1)	-5(1)
C(28)	27(1)	22(1)	19(1)	-7(1)	14(1)	-9(1)
C(29)	25(1)	20(1)	25(1)	0(1)	17(1)	1(1)
C(30)	18(1)	28(1)	17(1)	1(1)	8(1)	-1(1)
C(31)	24(1)	21(1)	20(1)	-3(1)	11(1)	-6(1)
C(32)	21(1)	19(1)	20(1)	0(1)	11(1)	0(1)
C(33)	33(1)	14(1)	18(1)	-2(1)	9(1)	3(1)
C(34)	43(2)	18(1)	25(1)	0(1)	18(1)	7(1)
C(35)	50(2)	32(2)	38(2)	-7(1)	28(2)	1(1)
C(36)	51(2)	44(2)	25(2)	-10(1)	1(2)	21(2)
C(37)	76(3)	48(2)	35(2)	12(2)	14(2)	37(2)
C(38)	84(3)	22(2)	72(3)	-14(2)	50(2)	-15(2)

Table 5. Hydrogen Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($\approx 2 \times 10^{-3}$) for **23**

	x	y	z	U(eq)
H(2O)	13397(17)	-3167(9)	13430(30)	39
H(2A)	14099(19)	-4358(7)	12510(30)	31
H(2B)	15405(16)	-4230(8)	12890(20)	31
H(3A)	15185(17)	-4136(7)	10450(20)	27
H(3B)	14710(20)	-4579(5)	10630(30)	27
H(4A)	12834(17)	-4331(6)	9820(20)	22
H(4B)	13391(19)	-4217(7)	8634(18)	22
H(5)	12438(15)	-3640(7)	9060(20)	18
H(6)	12563(17)	-3789(6)	11440(20)	19
H(7)	13473(17)	-2976(6)	11410(20)	22
H(9)	12396(16)	-2630(7)	9260(20)	24
H(10)	10680(20)	-2449(7)	7580(20)	28
H(12)	8985(17)	-3178(7)	9520(30)	32
H(13)	10730(20)	-3361(7)	11210(20)	27
H(16A)	15300(20)	-3508(8)	6060(20)	47
H(16B)	16180(20)	-3602(7)	7630(30)	47
H(16C)	16200(20)	-3162(7)	6850(30)	47
H(17A)	13540(20)	-3148(7)	5730(20)	45
H(17B)	14300(20)	-2739(7)	6150(30)	45
H(17C)	13410(20)	-2830(8)	6950(30)	45
H(18A)	16670(20)	-3044(8)	10930(20)	51
H(18B)	17090(20)	-3076(9)	9570(30)	51
H(18C)	16480(20)	-3474(6)	9990(30)	51
H(19A)	15820(20)	-2403(8)	9910(20)	47
H(19B)	14681(17)	-2397(8)	8500(30)	47
H(19C)	15970(20)	-2457(8)	8350(30)	47
H(6O)	10592(19)	-4324(9)	90(30)	42
H(21A)	7640(20)	-4952(6)	-110(20)	30
H(21B)	7029(18)	-4514(7)	-290(20)	30
H(22A)	7230(20)	-4518(6)	2160(20)	25

H(22B)	6675(16)	-4947(7)	1560(20)	25
H(23A)	8536(19)	-5267(6)	2400(20)	22
H(23B)	8231(19)	-5048(7)	3710(20)	22
H(24)	10120(16)	-4884(6)	3790(20)	19
H(25)	9914(19)	-4925(5)	1430(20)	21
H(26)	10580(20)	-4090(5)	1980(20)	23
H(28)	12038(19)	-5085(6)	2830(20)	25
H(29)	13633(19)	-5202(6)	4850(30)	26
H(31)	13558(19)	-4010(6)	6030(20)	25
H(32)	11944(19)	-3899(6)	4030(20)	23
H(35A)	8130(30)	-4038(8)	7020(30)	55
H(35B)	7341(19)	-3883(9)	5420(30)	55
H(35C)	8140(30)	-3566(6)	6650(30)	55
H(36A)	10070(30)	-4166(8)	7620(30)	65
H(36B)	10320(30)	-3670(7)	7480(30)	65
H(36C)	10850(20)	-3997(10)	6720(30)	65
H(37A)	8130(30)	-3353(10)	2720(30)	81
H(37B)	7700(30)	-3286(9)	4100(30)	81
H(37C)	7470(30)	-3727(9)	3360(40)	81
H(38A)	10000(30)	-3150(10)	4080(30)	80
H(38B)	10790(20)	-3409(11)	5470(30)	80
H(38C)	9760(30)	-3096(9)	5530(30)	80

Table 6. Torsion Angles [$^{\circ}$] for **23**

C(14)-O(3)-B(1)-O(4)	-10.2(3)
C(14)-O(3)-B(1)-C(5)	169.3(2)
C(15)-O(4)-B(1)-O(3)	-9.7(2)
C(15)-O(4)-B(1)-C(5)	170.9(2)
O(1)-C(1)-C(2)-C(3)	-133.7(2)
C(6)-C(1)-C(2)-C(3)	48.3(3)
C(1)-C(2)-C(3)-C(4)	-49.6(3)
C(2)-C(3)-C(4)-C(5)	57.3(3)
C(3)-C(4)-C(5)-C(6)	-61.3(2)
C(3)-C(4)-C(5)-B(1)	69.3(2)
O(3)-B(1)-C(5)-C(4)	41.2(3)
O(4)-B(1)-C(5)-C(4)	-139.5(2)
O(3)-B(1)-C(5)-C(6)	167.4(2)
O(4)-B(1)-C(5)-C(6)	-13.3(3)
O(1)-C(1)-C(6)-C(7)	2.7(3)
C(2)-C(1)-C(6)-C(7)	-179.34(19)
O(1)-C(1)-C(6)-C(5)	130.6(2)
C(2)-C(1)-C(6)-C(5)	-51.4(2)
C(4)-C(5)-C(6)-C(1)	56.4(2)
B(1)-C(5)-C(6)-C(1)	-70.0(2)
C(4)-C(5)-C(6)-C(7)	-176.59(19)
B(1)-C(5)-C(6)-C(7)	57.0(3)
C(1)-C(6)-C(7)-O(2)	-59.3(2)
C(5)-C(6)-C(7)-O(2)	175.27(18)
C(1)-C(6)-C(7)-C(8)	-178.70(17)
C(5)-C(6)-C(7)-C(8)	55.9(2)
O(2)-C(7)-C(8)-C(9)	131.2(2)
C(6)-C(7)-C(8)-C(9)	-107.5(2)
O(2)-C(7)-C(8)-C(13)	-50.4(3)
C(6)-C(7)-C(8)-C(13)	70.9(3)
C(13)-C(8)-C(9)-C(10)	0.6(3)
C(7)-C(8)-C(9)-C(10)	179.0(2)
C(8)-C(9)-C(10)-C(11)	0.0(3)
C(9)-C(10)-C(11)-C(12)	-0.6(4)

C(9)-C(10)-C(11)-Cl(1)	179.25(18)
C(10)-C(11)-C(12)-C(13)	0.5(4)
Cl(1)-C(11)-C(12)-C(13)	-179.31(18)
C(11)-C(12)-C(13)-C(8)	0.1(4)
C(9)-C(8)-C(13)-C(12)	-0.7(3)
C(7)-C(8)-C(13)-C(12)	-179.1(2)
B(1)-O(3)-C(14)-C(16)	146.4(2)
B(1)-O(3)-C(14)-C(17)	-93.7(2)
B(1)-O(3)-C(14)-C(15)	24.3(2)
B(1)-O(4)-C(15)-C(19)	146.1(2)
B(1)-O(4)-C(15)-C(18)	-94.7(2)
B(1)-O(4)-C(15)-C(14)	23.9(2)
O(3)-C(14)-C(15)-O(4)	-28.7(2)
C(16)-C(14)-C(15)-O(4)	-146.60(19)
C(17)-C(14)-C(15)-O(4)	84.4(2)
O(3)-C(14)-C(15)-C(19)	-147.0(2)
C(16)-C(14)-C(15)-C(19)	95.1(3)
C(17)-C(14)-C(15)-C(19)	-33.9(3)
O(3)-C(14)-C(15)-C(18)	84.4(2)
C(16)-C(14)-C(15)-C(18)	-33.5(3)
C(17)-C(14)-C(15)-C(18)	-162.5(2)
C(34)-O(8)-B(2)-O(7)	-7.2(3)
C(34)-O(8)-B(2)-C(24)	172.0(2)
C(33)-O(7)-B(2)-O(8)	-9.3(3)
C(33)-O(7)-B(2)-C(24)	171.5(2)
O(5)-C(20)-C(21)-C(22)	-141.5(2)
C(25)-C(20)-C(21)-C(22)	41.3(3)
C(20)-C(21)-C(22)-C(23)	-47.6(3)
C(21)-C(22)-C(23)-C(24)	58.8(3)
C(22)-C(23)-C(24)-C(25)	-61.4(2)
C(22)-C(23)-C(24)-B(2)	66.9(2)
O(8)-B(2)-C(24)-C(23)	-131.5(2)
O(7)-B(2)-C(24)-C(23)	47.6(3)
O(8)-B(2)-C(24)-C(25)	-6.6(3)
O(7)-B(2)-C(24)-C(25)	172.4(2)
O(5)-C(20)-C(25)-C(26)	9.6(3)

C(21)-C(20)-C(25)-C(26)	-173.3(2)
O(5)-C(20)-C(25)-C(24)	139.1(2)
C(21)-C(20)-C(25)-C(24)	-43.8(3)
C(23)-C(24)-C(25)-C(20)	52.1(2)
B(2)-C(24)-C(25)-C(20)	-73.0(2)
C(23)-C(24)-C(25)-C(26)	178.97(19)
B(2)-C(24)-C(25)-C(26)	53.9(3)
C(20)-C(25)-C(26)-O(6)	-67.3(2)
C(24)-C(25)-C(26)-O(6)	165.37(19)
C(20)-C(25)-C(26)-C(27)	171.59(19)
C(24)-C(25)-C(26)-C(27)	44.2(3)
O(6)-C(26)-C(27)-C(28)	-64.2(3)
C(25)-C(26)-C(27)-C(28)	57.7(3)
O(6)-C(26)-C(27)-C(32)	114.6(2)
C(25)-C(26)-C(27)-C(32)	-123.5(2)
C(32)-C(27)-C(28)-C(29)	0.2(3)
C(26)-C(27)-C(28)-C(29)	179.0(2)
C(27)-C(28)-C(29)-C(30)	-0.1(3)
C(28)-C(29)-C(30)-C(31)	0.3(3)
C(28)-C(29)-C(30)-Cl(2)	179.62(17)
C(29)-C(30)-C(31)-C(32)	-0.5(3)
Cl(2)-C(30)-C(31)-C(32)	-179.81(17)
C(30)-C(31)-C(32)-C(27)	0.5(3)
C(28)-C(27)-C(32)-C(31)	-0.4(3)
C(26)-C(27)-C(32)-C(31)	-179.2(2)
B(2)-O(7)-C(33)-C(36)	-98.9(2)
B(2)-O(7)-C(33)-C(35)	142.6(2)
B(2)-O(7)-C(33)-C(34)	20.4(2)
B(2)-O(8)-C(34)-C(38)	141.7(2)
B(2)-O(8)-C(34)-C(37)	-100.1(3)
B(2)-O(8)-C(34)-C(33)	19.2(2)
O(7)-C(33)-C(34)-O(8)	-23.6(2)
C(36)-C(33)-C(34)-O(8)	90.5(2)
C(35)-C(33)-C(34)-O(8)	-141.1(2)
O(7)-C(33)-C(34)-C(38)	-140.8(2)
C(36)-C(33)-C(34)-C(38)	-26.7(3)

C(35)-C(33)-C(34)-C(38)	101.7(3)
O(7)-C(33)-C(34)-C(37)	90.3(2)
C(36)-C(33)-C(34)-C(37)	-155.7(2)
C(35)-C(33)-C(34)-C(37)	-27.3(3)

Symmetry transformations used to generate equivalent atoms.

Table 7. Hydrogen Bonds for **23** [$\approx$ and ∞]

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle$ (DHA)
O(2)-H(2O)...O(1)	0.844(17)	2.11(2)	2.781(2)	136(3)
O(6)-H(6O)...O(5)	0.830(17)	2.11(2)	2.782(3)	138(3)

Symmetry transformations used to generate equivalent atoms.

■ **Crystal data of product (24) of tandem conjugate boron addition/aldol reaction with *p*-bromobenzaldehyde**

Table 1. Crystal data and structure refinement for **24**

Identification code	24	
Empirical formula	C ₁₉ H ₂₆ B Br O ₄	
Formula weight	409.12	
Temperature	100(2) K	
Wavelength	0.71073 $\approx$	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	$a = 12.509(3) \approx$	$\alpha = 90^\circ$
	$b = 32.442(7) \approx$	$\beta = 108.603(3)^\circ$
	$c = 9.963(2) \approx$	$\gamma = 90^\circ$
Volume	$3832.0(15) \approx^3$	
Z	8	
Density (calculated)	1.418 Mg/m ³	
Absorption coefficient	2.165 mm ⁻¹	
F(000)	1696	
Crystal size	0.12 x 0.04 x 0.02 mm ³	
Theta range for data collection	1.72 to 28.31 $^\circ$.	
Index ranges	-16 $\leq h \leq$ 16, -43 $\leq k \leq$ 42, -13 $\leq l \leq$ 13	

Reflections collected	46848
Independent reflections	9443 [R(int) = 0.0370]
Completeness to theta = 28.31°	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9580 and 0.7811
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9443 / 52 / 607
Goodness-of-fit on F ²	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0323, wR2 = 0.0730
R indices (all data)	R1 = 0.0432, wR2 = 0.0777
Extinction coefficient	na
Largest diff. peak and hole	0.581 and -0.252 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\approx^2 \times 10^3$) for **24** (U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.)

	x	y	z	U(eq)
Br(1)	3328(1)	2628(1)	7135(1)	30(1)
B(1)	8980(2)	3436(1)	9199(2)	14(1)
O(1)	9787(1)	3510(1)	13309(1)	26(1)
O(2)	7738(1)	3103(1)	12874(1)	23(1)
O(3)	9183(1)	3548(1)	7980(1)	17(1)
O(4)	9539(1)	3086(1)	9790(1)	16(1)
C(1)	9246(2)	3737(1)	12361(2)	18(1)
C(2)	9621(2)	4172(1)	12222(2)	23(1)
C(3)	9562(2)	4278(1)	10702(2)	21(1)
C(4)	8420(2)	4164(1)	9659(2)	17(1)
C(5)	8165(1)	3703(1)	9764(2)	13(1)
C(6)	8144(1)	3605(1)	11277(2)	14(1)
C(7)	7848(2)	3157(1)	11494(2)	15(1)
C(8)	6747(2)	3028(1)	10430(2)	16(1)
C(9)	6723(2)	2758(1)	9338(2)	17(1)
C(10)	5712(2)	2642(1)	8347(2)	21(1)
C(11)	4719(2)	2798(1)	8466(2)	21(1)
C(12)	4709(2)	3067(1)	9533(2)	23(1)
C(13)	5729(2)	3182(1)	10515(2)	20(1)
C(14)	9789(2)	3209(1)	7584(2)	16(1)
C(15)	10342(1)	2993(1)	9027(2)	16(1)
C(16)	10617(2)	3386(1)	6915(2)	25(1)
C(17)	8904(2)	2946(1)	6539(2)	24(1)
C(18)	11452(2)	3182(1)	9891(2)	26(1)
C(19)	10453(2)	2529(1)	8942(2)	24(1)
Br(2)	9982(1)	334(1)	12176(1)	22(1)
B(2)	4315(2)	670(1)	8970(2)	15(1)
O(5)	3866(1)	771(1)	4787(2)	41(1)
O(6)	6151(1)	575(1)	5707(1)	26(1)
O(7)	3952(1)	652(1)	10122(1)	23(1)
O(8)	4506(1)	1060(1)	8612(1)	21(1)

C(20)	3758(2)	504(1)	5589(2)	22(1)
C(21)	2632(2)	305(1)	5393(2)	23(1)
C(22)	2404(2)	214(1)	6781(2)	20(1)
C(23)	3405(2)	-1(1)	7827(2)	18(1)
C(24)	4468(1)	270(1)	8154(2)	14(1)
C(25)	4766(2)	343(1)	6782(2)	16(1)
C(26)	5791(2)	620(1)	6936(2)	17(1)
C(27)	6798(1)	536(1)	8222(2)	16(1)
C(28)	7242(2)	855(1)	9169(2)	17(1)
C(29)	8184(2)	796(1)	10347(2)	19(1)
C(30)	8682(1)	412(1)	10567(2)	18(1)
C(31)	8253(2)	86(1)	9661(2)	20(1)
C(32)	7313(2)	151(1)	8484(2)	20(1)
C(33)	4065(2)	1064(1)	10746(2)	20(1)
C(34)	4106(2)	1343(1)	9489(2)	20(1)
C(35)	4919(2)	1703(1)	9885(3)	37(1)
C(36)	2954(2)	1491(1)	8575(2)	35(1)
C(37)	5153(2)	1062(1)	11979(2)	36(1)
C(38)	3073(2)	1140(1)	11270(2)	31(1)

Table 3. Bond lengths [$\approx$] and angles [∞] for **24**

Br(1)-C(11)	1.9008(19)
B(1)-O(4)	1.364(2)
B(1)-O(3)	1.367(2)
B(1)-C(5)	1.573(2)
O(1)-C(1)	1.218(2)
O(2)-C(7)	1.435(2)
O(2)-H(2O)	0.814(16)
O(3)-C(14)	1.460(2)
O(4)-C(15)	1.4712(19)
C(1)-C(2)	1.507(3)
C(1)-C(6)	1.517(2)
C(2)-C(3)	1.532(3)
C(2)-H(2A)	0.977(16)
C(2)-H(2B)	0.989(15)
C(3)-C(4)	1.519(3)
C(3)-H(3A)	0.984(15)
C(3)-H(3B)	0.992(15)
C(4)-C(5)	1.540(2)
C(4)-H(4A)	0.957(15)
C(4)-H(4B)	0.995(15)
C(5)-C(6)	1.549(2)
C(5)-H(5)	0.977(15)
C(6)-C(7)	1.533(2)
C(6)-H(6)	0.985(14)
C(7)-C(8)	1.505(2)
C(7)-H(7)	0.978(15)
C(8)-C(9)	1.390(2)
C(8)-C(13)	1.394(2)
C(9)-C(10)	1.386(3)
C(9)-H(9)	0.934(15)
C(10)-C(11)	1.380(3)
C(10)-H(10)	0.941(15)
C(11)-C(12)	1.380(3)
C(12)-C(13)	1.388(3)

C(12)-H(12)	0.948(15)
C(13)-H(13)	0.943(15)
C(14)-C(16)	1.513(3)
C(14)-C(17)	1.519(3)
C(14)-C(15)	1.550(2)
C(15)-C(18)	1.512(3)
C(15)-C(19)	1.516(3)
C(16)-H(16A)	0.956(16)
C(16)-H(16B)	0.968(16)
C(16)-H(16C)	0.989(16)
C(17)-H(17A)	0.976(16)
C(17)-H(17B)	0.969(16)
C(17)-H(17C)	0.970(16)
C(18)-H(18A)	0.975(16)
C(18)-H(18B)	0.964(16)
C(18)-H(18C)	0.968(16)
C(19)-H(19A)	0.959(16)
C(19)-H(19B)	0.964(16)
C(19)-H(19C)	0.974(16)
Br(2)-C(30)	1.9008(18)
B(2)-O(8)	1.357(2)
B(2)-O(7)	1.363(2)
B(2)-C(24)	1.575(3)
O(5)-C(20)	1.214(2)
O(6)-C(26)	1.441(2)
O(6)-H(6O)	0.816(16)
O(7)-C(33)	1.462(2)
O(8)-C(34)	1.462(2)
C(20)-C(21)	1.505(3)
C(20)-C(25)	1.523(3)
C(21)-C(22)	1.528(3)
C(21)-H(21A)	0.976(15)
C(21)-H(21B)	0.966(16)
C(22)-C(23)	1.518(3)
C(22)-H(22A)	0.971(15)
C(22)-H(22B)	0.975(15)

C(23)-C(24)	1.541(2)
C(23)-H(23A)	0.976(15)
C(23)-H(23B)	0.983(15)
C(24)-C(25)	1.545(2)
C(24)-H(24)	0.968(15)
C(25)-C(26)	1.533(2)
C(25)-H(25)	0.981(15)
C(26)-C(27)	1.509(2)
C(26)-H(26)	0.977(15)
C(27)-C(32)	1.391(3)
C(27)-C(28)	1.393(2)
C(28)-C(29)	1.386(3)
C(28)-H(28)	0.957(15)
C(29)-C(30)	1.381(3)
C(29)-H(29)	0.950(15)
C(30)-C(31)	1.381(3)
C(31)-C(32)	1.386(3)
C(31)-H(31)	0.950(15)
C(32)-H(32)	0.955(15)
C(33)-C(38)	1.513(3)
C(33)-C(37)	1.514(3)
C(33)-C(34)	1.561(2)
C(34)-C(35)	1.514(3)
C(34)-C(36)	1.516(3)
C(35)-H(35A)	0.991(17)
C(35)-H(35B)	0.978(17)
C(35)-H(35C)	0.982(17)
C(36)-H(36A)	0.979(17)
C(36)-H(36B)	0.969(17)
C(36)-H(36C)	0.981(17)
C(37)-H(37A)	0.986(17)
C(37)-H(37B)	0.974(17)
C(37)-H(37C)	0.956(17)
C(38)-H(38A)	0.975(16)
C(38)-H(38B)	0.984(17)
C(38)-H(38C)	0.978(16)

O(4)-B(1)-O(3)	113.03(15)
O(4)-B(1)-C(5)	127.25(15)
O(3)-B(1)-C(5)	119.72(15)
C(7)-O(2)-H(2O)	105.2(18)
B(1)-O(3)-C(14)	107.33(13)
B(1)-O(4)-C(15)	106.74(13)
O(1)-C(1)-C(2)	121.64(17)
O(1)-C(1)-C(6)	122.43(16)
C(2)-C(1)-C(6)	115.91(15)
C(1)-C(2)-C(3)	112.51(15)
C(1)-C(2)-H(2A)	110.1(13)
C(3)-C(2)-H(2A)	112.9(13)
C(1)-C(2)-H(2B)	105.9(13)
C(3)-C(2)-H(2B)	109.1(13)
H(2A)-C(2)-H(2B)	105.9(18)
C(4)-C(3)-C(2)	111.15(15)
C(4)-C(3)-H(3A)	112.0(13)
C(2)-C(3)-H(3A)	109.7(13)
C(4)-C(3)-H(3B)	108.5(13)
C(2)-C(3)-H(3B)	111.3(13)
H(3A)-C(3)-H(3B)	104.0(17)
C(3)-C(4)-C(5)	110.98(14)
C(3)-C(4)-H(4A)	110.5(13)
C(5)-C(4)-H(4A)	107.6(13)
C(3)-C(4)-H(4B)	109.3(12)
C(5)-C(4)-H(4B)	107.6(12)
H(4A)-C(4)-H(4B)	110.8(17)
C(4)-C(5)-C(6)	109.50(13)
C(4)-C(5)-B(1)	109.82(14)
C(6)-C(5)-B(1)	116.73(14)
C(4)-C(5)-H(5)	108.0(12)
C(6)-C(5)-H(5)	108.0(12)
B(1)-C(5)-H(5)	104.3(12)
C(1)-C(6)-C(7)	111.85(14)
C(1)-C(6)-C(5)	109.93(14)

C(7)-C(6)-C(5)	114.29(13)
C(1)-C(6)-H(6)	106.3(12)
C(7)-C(6)-H(6)	108.0(12)
C(5)-C(6)-H(6)	106.0(11)
O(2)-C(7)-C(8)	107.17(14)
O(2)-C(7)-C(6)	110.54(14)
C(8)-C(7)-C(6)	111.83(14)
O(2)-C(7)-H(7)	110.1(12)
C(8)-C(7)-H(7)	108.8(12)
C(6)-C(7)-H(7)	108.4(12)
C(9)-C(8)-C(13)	118.74(17)
C(9)-C(8)-C(7)	120.82(16)
C(13)-C(8)-C(7)	120.44(16)
C(10)-C(9)-C(8)	121.03(17)
C(10)-C(9)-H(9)	118.6(13)
C(8)-C(9)-H(9)	120.4(13)
C(11)-C(10)-C(9)	118.77(17)
C(11)-C(10)-H(10)	121.9(14)
C(9)-C(10)-H(10)	119.3(14)
C(12)-C(11)-C(10)	121.82(17)
C(12)-C(11)-Br(1)	119.31(14)
C(10)-C(11)-Br(1)	118.87(15)
C(11)-C(12)-C(13)	118.74(17)
C(11)-C(12)-H(12)	121.6(14)
C(13)-C(12)-H(12)	119.6(14)
C(12)-C(13)-C(8)	120.89(17)
C(12)-C(13)-H(13)	118.7(13)
C(8)-C(13)-H(13)	120.4(13)
O(3)-C(14)-C(16)	108.67(14)
O(3)-C(14)-C(17)	106.35(14)
C(16)-C(14)-C(17)	111.32(15)
O(3)-C(14)-C(15)	101.95(12)
C(16)-C(14)-C(15)	114.55(15)
C(17)-C(14)-C(15)	113.15(15)
O(4)-C(15)-C(18)	106.11(14)
O(4)-C(15)-C(19)	108.87(14)

C(18)-C(15)-C(19)	110.52(16)
O(4)-C(15)-C(14)	102.13(13)
C(18)-C(15)-C(14)	113.64(15)
C(19)-C(15)-C(14)	114.78(15)
C(14)-C(16)-H(16A)	111.0(15)
C(14)-C(16)-H(16B)	109.9(15)
H(16A)-C(16)-H(16B)	109(2)
C(14)-C(16)-H(16C)	111.7(14)
H(16A)-C(16)-H(16C)	107(2)
H(16B)-C(16)-H(16C)	108(2)
C(14)-C(17)-H(17A)	108.0(15)
C(14)-C(17)-H(17B)	111.8(14)
H(17A)-C(17)-H(17B)	108(2)
C(14)-C(17)-H(17C)	111.0(15)
H(17A)-C(17)-H(17C)	109(2)
H(17B)-C(17)-H(17C)	109(2)
C(15)-C(18)-H(18A)	108.2(15)
C(15)-C(18)-H(18B)	112.1(15)
H(18A)-C(18)-H(18B)	109(2)
C(15)-C(18)-H(18C)	110.2(15)
H(18A)-C(18)-H(18C)	109(2)
H(18B)-C(18)-H(18C)	109(2)
C(15)-C(19)-H(19A)	108.6(15)
C(15)-C(19)-H(19B)	107.4(15)
H(19A)-C(19)-H(19B)	108(2)
C(15)-C(19)-H(19C)	110.1(14)
H(19A)-C(19)-H(19C)	112(2)
H(19B)-C(19)-H(19C)	111(2)
O(8)-B(2)-O(7)	113.35(16)
O(8)-B(2)-C(24)	124.85(16)
O(7)-B(2)-C(24)	121.79(16)
C(26)-O(6)-H(6O)	103.2(18)
B(2)-O(7)-C(33)	107.76(14)
B(2)-O(8)-C(34)	107.83(13)
O(5)-C(20)-C(21)	121.06(18)
O(5)-C(20)-C(25)	121.37(17)

C(21)-C(20)-C(25)	117.50(16)
C(20)-C(21)-C(22)	113.76(15)
C(20)-C(21)-H(21A)	105.4(13)
C(22)-C(21)-H(21A)	109.5(13)
C(20)-C(21)-H(21B)	105.7(13)
C(22)-C(21)-H(21B)	115.6(13)
H(21A)-C(21)-H(21B)	106.1(18)
C(23)-C(22)-C(21)	111.05(15)
C(23)-C(22)-H(22A)	110.7(13)
C(21)-C(22)-H(22A)	108.8(13)
C(23)-C(22)-H(22B)	112.1(13)
C(21)-C(22)-H(22B)	109.0(13)
H(22A)-C(22)-H(22B)	105.0(18)
C(22)-C(23)-C(24)	110.53(14)
C(22)-C(23)-H(23A)	109.4(13)
C(24)-C(23)-H(23A)	110.7(12)
C(22)-C(23)-H(23B)	109.5(12)
C(24)-C(23)-H(23B)	109.3(12)
H(23A)-C(23)-H(23B)	107.4(17)
C(23)-C(24)-C(25)	109.61(14)
C(23)-C(24)-B(2)	109.84(14)
C(25)-C(24)-B(2)	115.84(14)
C(23)-C(24)-H(24)	108.2(12)
C(25)-C(24)-H(24)	106.2(12)
B(2)-C(24)-H(24)	106.8(12)
C(20)-C(25)-C(26)	109.49(15)
C(20)-C(25)-C(24)	111.68(14)
C(26)-C(25)-C(24)	115.48(14)
C(20)-C(25)-H(25)	103.4(12)
C(26)-C(25)-H(25)	106.8(12)
C(24)-C(25)-H(25)	109.2(12)
O(6)-C(26)-C(27)	107.47(14)
O(6)-C(26)-C(25)	109.47(14)
C(27)-C(26)-C(25)	115.05(14)
O(6)-C(26)-H(26)	107.3(12)
C(27)-C(26)-H(26)	109.0(12)

C(25)-C(26)-H(26)	108.3(12)
C(32)-C(27)-C(28)	118.74(17)
C(32)-C(27)-C(26)	122.25(16)
C(28)-C(27)-C(26)	118.99(16)
C(29)-C(28)-C(27)	121.21(17)
C(29)-C(28)-H(28)	119.5(13)
C(27)-C(28)-H(28)	119.2(13)
C(30)-C(29)-C(28)	118.56(17)
C(30)-C(29)-H(29)	121.9(13)
C(28)-C(29)-H(29)	119.6(13)
C(29)-C(30)-C(31)	121.69(17)
C(29)-C(30)-Br(2)	118.39(14)
C(31)-C(30)-Br(2)	119.92(14)
C(30)-C(31)-C(32)	119.05(17)
C(30)-C(31)-H(31)	121.1(13)
C(32)-C(31)-H(31)	119.8(13)
C(31)-C(32)-C(27)	120.74(17)
C(31)-C(32)-H(32)	120.0(13)
C(27)-C(32)-H(32)	119.3(13)
O(7)-C(33)-C(38)	108.57(16)
O(7)-C(33)-C(37)	106.37(15)
C(38)-C(33)-C(37)	110.14(17)
O(7)-C(33)-C(34)	102.33(13)
C(38)-C(33)-C(34)	114.97(16)
C(37)-C(33)-C(34)	113.70(18)
O(8)-C(34)-C(35)	108.05(16)
O(8)-C(34)-C(36)	106.32(16)
C(35)-C(34)-C(36)	110.13(18)
O(8)-C(34)-C(33)	102.68(13)
C(35)-C(34)-C(33)	115.44(17)
C(36)-C(34)-C(33)	113.41(17)
C(34)-C(35)-H(35A)	109.5(17)
C(34)-C(35)-H(35B)	111.6(17)
H(35A)-C(35)-H(35B)	107(2)
C(34)-C(35)-H(35C)	111.5(17)
H(35A)-C(35)-H(35C)	110(2)

H(35B)-C(35)-H(35C)	107(2)
C(34)-C(36)-H(36A)	106.9(17)
C(34)-C(36)-H(36B)	112.1(17)
H(36A)-C(36)-H(36B)	108(2)
C(34)-C(36)-H(36C)	109.9(17)
H(36A)-C(36)-H(36C)	111(2)
H(36B)-C(36)-H(36C)	109(2)
C(33)-C(37)-H(37A)	109.3(17)
C(33)-C(37)-H(37B)	110.0(17)
H(37A)-C(37)-H(37B)	109(2)
C(33)-C(37)-H(37C)	113.8(17)
H(37A)-C(37)-H(37C)	109(2)
H(37B)-C(37)-H(37C)	106(2)
C(33)-C(38)-H(38A)	110.0(15)
C(33)-C(38)-H(38B)	112.5(15)
H(38A)-C(38)-H(38B)	108(2)
C(33)-C(38)-H(38C)	109.5(15)
H(38A)-C(38)-H(38C)	106(2)
H(38B)-C(38)-H(38C)	110(2)

Symmetry transformations used to generate equivalent atoms.

Table 4. Anisotropic displacement parameters ($\approx 2 \times 10^3$) for **24** [The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^*U^{12})$]

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Br(1)	19(1)	23(1)	41(1)	2(1)	0(1)	-5(1)
B(1)	13(1)	14(1)	12(1)	-2(1)	2(1)	-2(1)
O(1)	28(1)	28(1)	18(1)	1(1)	-1(1)	1(1)
O(2)	30(1)	26(1)	14(1)	4(1)	10(1)	-2(1)
O(3)	23(1)	15(1)	15(1)	2(1)	10(1)	6(1)
O(4)	17(1)	18(1)	13(1)	3(1)	8(1)	5(1)
C(1)	20(1)	20(1)	14(1)	-4(1)	8(1)	0(1)
C(2)	25(1)	22(1)	21(1)	-6(1)	7(1)	-4(1)
C(3)	24(1)	16(1)	25(1)	-3(1)	12(1)	-3(1)
C(4)	20(1)	14(1)	22(1)	2(1)	12(1)	2(1)
C(5)	13(1)	14(1)	12(1)	2(1)	4(1)	0(1)
C(6)	16(1)	14(1)	12(1)	0(1)	6(1)	2(1)
C(7)	19(1)	16(1)	13(1)	2(1)	8(1)	1(1)
C(8)	19(1)	14(1)	18(1)	5(1)	8(1)	-1(1)
C(9)	18(1)	16(1)	20(1)	2(1)	8(1)	1(1)
C(10)	23(1)	16(1)	24(1)	0(1)	7(1)	-1(1)
C(11)	17(1)	17(1)	26(1)	4(1)	3(1)	-5(1)
C(12)	18(1)	19(1)	36(1)	3(1)	12(1)	1(1)
C(13)	23(1)	17(1)	25(1)	-1(1)	13(1)	0(1)
C(14)	20(1)	17(1)	13(1)	0(1)	8(1)	4(1)
C(15)	16(1)	18(1)	14(1)	0(1)	8(1)	3(1)
C(16)	32(1)	24(1)	26(1)	3(1)	19(1)	3(1)
C(17)	27(1)	30(1)	15(1)	-7(1)	6(1)	0(1)
C(18)	16(1)	32(1)	28(1)	-2(1)	4(1)	2(1)
C(19)	31(1)	18(1)	26(1)	3(1)	15(1)	7(1)
Br(2)	18(1)	29(1)	20(1)	2(1)	6(1)	4(1)
B(2)	15(1)	17(1)	13(1)	1(1)	3(1)	0(1)
O(5)	32(1)	61(1)	24(1)	20(1)	1(1)	-14(1)
O(6)	25(1)	42(1)	15(1)	-4(1)	11(1)	-11(1)
O(7)	41(1)	14(1)	20(1)	-1(1)	18(1)	0(1)
O(8)	31(1)	15(1)	20(1)	2(1)	14(1)	1(1)

C(20)	23(1)	29(1)	13(1)	-1(1)	5(1)	-5(1)
C(21)	18(1)	27(1)	20(1)	0(1)	1(1)	-5(1)
C(22)	16(1)	22(1)	24(1)	-2(1)	7(1)	-3(1)
C(23)	18(1)	16(1)	20(1)	-1(1)	10(1)	-3(1)
C(24)	16(1)	14(1)	12(1)	1(1)	5(1)	-1(1)
C(25)	17(1)	19(1)	13(1)	-3(1)	7(1)	-4(1)
C(26)	19(1)	21(1)	12(1)	-2(1)	8(1)	-6(1)
C(27)	16(1)	20(1)	15(1)	-2(1)	9(1)	-5(1)
C(28)	18(1)	16(1)	19(1)	-2(1)	8(1)	-2(1)
C(29)	19(1)	20(1)	18(1)	-5(1)	7(1)	-4(1)
C(30)	14(1)	24(1)	17(1)	1(1)	7(1)	-1(1)
C(31)	23(1)	18(1)	23(1)	-2(1)	14(1)	1(1)
C(32)	24(1)	19(1)	20(1)	-6(1)	12(1)	-5(1)
C(33)	30(1)	15(1)	16(1)	0(1)	8(1)	4(1)
C(34)	26(1)	15(1)	20(1)	1(1)	10(1)	4(1)
C(35)	48(1)	19(1)	52(2)	-8(1)	27(1)	-7(1)
C(36)	41(1)	33(1)	28(1)	7(1)	5(1)	16(1)
C(37)	44(1)	38(1)	18(1)	-8(1)	-1(1)	18(1)
C(38)	44(1)	25(1)	31(1)	-4(1)	24(1)	2(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\approx 2 \times 10^{-3}$) for **24**

	x	y	z	U(eq)
H(2O)	8355(15)	3159(8)	13430(20)	34
H(2A)	10367(14)	4220(7)	12910(20)	27
H(2B)	9097(17)	4352(6)	12510(20)	27
H(3A)	9741(18)	4571(5)	10640(20)	25
H(3B)	10154(16)	4131(6)	10420(20)	25
H(4A)	8407(17)	4217(6)	8708(17)	20
H(4B)	7821(15)	4324(6)	9890(20)	20
H(5)	7415(13)	3647(6)	9101(18)	16
H(6)	7555(15)	3783(6)	11430(20)	16
H(7)	8448(15)	2979(6)	11390(20)	18
H(9)	7391(15)	2644(6)	9280(20)	21
H(10)	5719(19)	2459(6)	7620(20)	25
H(12)	4025(15)	3169(7)	9620(20)	28
H(13)	5724(18)	3372(6)	11230(20)	25
H(16A)	10232(19)	3507(7)	6014(19)	37
H(16B)	11111(18)	3171(6)	6790(30)	37
H(16C)	11089(19)	3605(6)	7510(20)	37
H(17A)	8481(19)	3122(7)	5760(20)	36
H(17B)	8378(18)	2827(7)	6970(20)	36
H(17C)	9250(20)	2726(6)	6170(20)	36
H(18A)	11640(20)	3081(7)	10860(19)	39
H(18B)	11420(20)	3479(5)	9910(30)	39
H(18C)	12044(18)	3101(7)	9510(30)	39
H(19A)	10817(19)	2425(7)	9878(19)	36
H(19B)	10943(18)	2475(7)	8390(20)	36
H(19C)	9714(15)	2405(7)	8510(20)	36
H(6O)	5618(17)	664(8)	5070(20)	39
H(21A)	2645(18)	47(5)	4890(20)	27
H(21B)	2083(16)	479(6)	4730(20)	27
H(22A)	2239(18)	471(5)	7170(20)	24
H(22B)	1714(14)	52(6)	6580(20)	24

H(23A)	3527(18)	-266(5)	7440(20)	21
H(23B)	3238(17)	-55(6)	8710(18)	21
H(24)	5095(14)	119(6)	8786(19)	17
H(25)	4928(17)	77(5)	6420(20)	19
H(26)	5557(17)	907(5)	6960(20)	20
H(28)	6899(17)	1122(5)	8990(20)	21
H(29)	8456(17)	1017(6)	10990(20)	23
H(31)	8584(17)	-180(5)	9840(20)	24
H(32)	7013(17)	-71(6)	7840(20)	23
H(35A)	4920(20)	1850(8)	9010(20)	55
H(35B)	5691(16)	1610(9)	10370(30)	55
H(35C)	4720(20)	1895(8)	10530(30)	55
H(36A)	3060(20)	1621(8)	7740(20)	53
H(36B)	2640(20)	1697(7)	9050(30)	53
H(36C)	2430(20)	1256(7)	8310(30)	53
H(37A)	5120(20)	845(7)	12650(30)	54
H(37B)	5260(20)	1327(6)	12460(30)	54
H(37C)	5811(18)	1019(9)	11710(30)	54
H(38A)	3120(20)	962(7)	12080(20)	46
H(38B)	2344(16)	1087(8)	10540(20)	46
H(38C)	3100(20)	1424(6)	11610(30)	46

Table 6. Torsion angles [$^{\circ}$] for **24**

O(4)-B(1)-O(3)-C(14)	9.83(19)
C(5)-B(1)-O(3)-C(14)	-169.84(15)
O(3)-B(1)-O(4)-C(15)	10.24(19)
C(5)-B(1)-O(4)-C(15)	-170.12(16)
O(1)-C(1)-C(2)-C(3)	133.53(18)
C(6)-C(1)-C(2)-C(3)	-48.2(2)
C(1)-C(2)-C(3)-C(4)	50.0(2)
C(2)-C(3)-C(4)-C(5)	-57.42(19)
C(3)-C(4)-C(5)-C(6)	60.65(18)
C(3)-C(4)-C(5)-B(1)	-68.75(18)
O(4)-B(1)-C(5)-C(4)	136.55(18)
O(3)-B(1)-C(5)-C(4)	-43.8(2)
O(4)-B(1)-C(5)-C(6)	11.2(3)
O(3)-B(1)-C(5)-C(6)	-169.20(15)
O(1)-C(1)-C(6)-C(7)	-2.7(2)
C(2)-C(1)-C(6)-C(7)	179.02(14)
O(1)-C(1)-C(6)-C(5)	-130.77(17)
C(2)-C(1)-C(6)-C(5)	50.93(19)
C(4)-C(5)-C(6)-C(1)	-55.69(18)
B(1)-C(5)-C(6)-C(1)	69.84(18)
C(4)-C(5)-C(6)-C(7)	177.59(14)
B(1)-C(5)-C(6)-C(7)	-56.9(2)
C(1)-C(6)-C(7)-O(2)	59.97(18)
C(5)-C(6)-C(7)-O(2)	-174.31(13)
C(1)-C(6)-C(7)-C(8)	179.29(14)
C(5)-C(6)-C(7)-C(8)	-54.99(19)
O(2)-C(7)-C(8)-C(9)	-130.92(16)
C(6)-C(7)-C(8)-C(9)	107.79(18)
O(2)-C(7)-C(8)-C(13)	49.7(2)
C(6)-C(7)-C(8)-C(13)	-71.6(2)
C(13)-C(8)-C(9)-C(10)	0.1(3)
C(7)-C(8)-C(9)-C(10)	-179.36(16)
C(8)-C(9)-C(10)-C(11)	-0.4(3)
C(9)-C(10)-C(11)-C(12)	0.5(3)

C(9)-C(10)-C(11)-Br(1)	-178.51(14)
C(10)-C(11)-C(12)-C(13)	-0.4(3)
Br(1)-C(11)-C(12)-C(13)	178.66(14)
C(11)-C(12)-C(13)-C(8)	0.1(3)
C(9)-C(8)-C(13)-C(12)	0.1(3)
C(7)-C(8)-C(13)-C(12)	179.53(17)
B(1)-O(3)-C(14)-C(16)	-145.46(15)
B(1)-O(3)-C(14)-C(17)	94.60(16)
B(1)-O(3)-C(14)-C(15)	-24.14(17)
B(1)-O(4)-C(15)-C(18)	94.94(16)
B(1)-O(4)-C(15)-C(19)	-146.10(15)
B(1)-O(4)-C(15)-C(14)	-24.33(16)
O(3)-C(14)-C(15)-O(4)	28.99(16)
C(16)-C(14)-C(15)-O(4)	146.15(15)
C(17)-C(14)-C(15)-O(4)	-84.80(16)
O(3)-C(14)-C(15)-C(18)	-84.83(17)
C(16)-C(14)-C(15)-C(18)	32.3(2)
C(17)-C(14)-C(15)-C(18)	161.38(16)
O(3)-C(14)-C(15)-C(19)	146.60(15)
C(16)-C(14)-C(15)-C(19)	-96.24(19)
C(17)-C(14)-C(15)-C(19)	32.8(2)
O(8)-B(2)-O(7)-C(33)	-9.2(2)
C(24)-B(2)-O(7)-C(33)	171.63(16)
O(7)-B(2)-O(8)-C(34)	-7.6(2)
C(24)-B(2)-O(8)-C(34)	171.49(16)
O(5)-C(20)-C(21)-C(22)	-142.0(2)
C(25)-C(20)-C(21)-C(22)	41.1(2)
C(20)-C(21)-C(22)-C(23)	-48.1(2)
C(21)-C(22)-C(23)-C(24)	59.5(2)
C(22)-C(23)-C(24)-C(25)	-61.86(18)
C(22)-C(23)-C(24)-B(2)	66.49(18)
O(8)-B(2)-C(24)-C(23)	-129.95(18)
O(7)-B(2)-C(24)-C(23)	49.1(2)
O(8)-B(2)-C(24)-C(25)	-5.1(3)
O(7)-B(2)-C(24)-C(25)	173.93(16)
O(5)-C(20)-C(25)-C(26)	10.7(3)

C(21)-C(20)-C(25)-C(26)	-172.40(16)
O(5)-C(20)-C(25)-C(24)	139.86(19)
C(21)-C(20)-C(25)-C(24)	-43.2(2)
C(23)-C(24)-C(25)-C(20)	52.18(19)
B(2)-C(24)-C(25)-C(20)	-72.77(19)
C(23)-C(24)-C(25)-C(26)	178.14(15)
B(2)-C(24)-C(25)-C(26)	53.2(2)
C(20)-C(25)-C(26)-O(6)	-67.98(19)
C(24)-C(25)-C(26)-O(6)	164.96(15)
C(20)-C(25)-C(26)-C(27)	170.91(15)
C(24)-C(25)-C(26)-C(27)	43.8(2)
O(6)-C(26)-C(27)-C(32)	-64.7(2)
C(25)-C(26)-C(27)-C(32)	57.5(2)
O(6)-C(26)-C(27)-C(28)	114.06(17)
C(25)-C(26)-C(27)-C(28)	-123.75(17)
C(32)-C(27)-C(28)-C(29)	0.4(3)
C(26)-C(27)-C(28)-C(29)	-178.35(15)
C(27)-C(28)-C(29)-C(30)	0.2(3)
C(28)-C(29)-C(30)-C(31)	-1.2(3)
C(28)-C(29)-C(30)-Br(2)	179.44(13)
C(29)-C(30)-C(31)-C(32)	1.5(3)
Br(2)-C(30)-C(31)-C(32)	-179.17(13)
C(30)-C(31)-C(32)-C(27)	-0.8(3)
C(28)-C(27)-C(32)-C(31)	-0.2(3)
C(26)-C(27)-C(32)-C(31)	178.58(16)
B(2)-O(7)-C(33)-C(38)	142.51(17)
B(2)-O(7)-C(33)-C(37)	-98.98(18)
B(2)-O(7)-C(33)-C(34)	20.56(18)
B(2)-O(8)-C(34)-C(35)	142.16(17)
B(2)-O(8)-C(34)-C(36)	-99.63(18)
B(2)-O(8)-C(34)-C(33)	19.72(18)
O(7)-C(33)-C(34)-O(8)	-24.02(17)
C(38)-C(33)-C(34)-O(8)	-141.50(16)
C(37)-C(33)-C(34)-O(8)	90.25(18)
O(7)-C(33)-C(34)-C(35)	-141.32(17)
C(38)-C(33)-C(34)-C(35)	101.2(2)

C(37)-C(33)-C(34)-C(35)	-27.1(2)
O(7)-C(33)-C(34)-C(36)	90.27(18)
C(38)-C(33)-C(34)-C(36)	-27.2(2)
C(37)-C(33)-C(34)-C(36)	-155.46(17)

Symmetry transformations used to generate equivalent atoms.

Table 7. Hydrogen bonds for **24** [$\approx$ and ∞].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...O(1)	0.814(16)	2.16(2)	2.791(2)	135(2)
O(6)-H(6O)...O(5)	0.816(16)	2.15(2)	2.783(2)	135(2)

Symmetry transformations used to generate equivalent atoms.

■ DFT calculation.

B₂(pin)₂

Coordinates:

C	-3.01073700	-0.54365300	0.57131400
C	-3.01052300	0.54369600	-0.57142200
B	-0.85163400	-0.00043600	-0.00010100
O	-1.61740200	0.52944700	-1.01334700
O	-1.61762400	-0.53007800	1.01317000
C	-3.29346800	1.96454800	-0.06666400
H	-3.08677500	2.67335100	-0.87297600
H	-4.33827900	2.08319600	0.23626300
H	-2.65318400	2.22253400	0.78129200
C	-3.89981100	0.22580900	-1.77119100
H	-4.95139600	0.16829400	-1.47038000
H	-3.80418900	1.01975300	-2.51715000
H	-3.61958300	-0.71679100	-2.24402800
C	-3.89977600	-0.22534300	1.77116400
H	-4.95141200	-0.16777600	1.47051700
H	-3.80411600	-1.01912800	2.51728700
H	-3.61936700	0.71732200	2.24373500
C	-3.29440000	-1.96436700	0.06659200
H	-3.08798600	-2.67325800	0.87290300
H	-4.33930300	-2.08253000	-0.23624300
H	-2.65431700	-2.22266100	-0.78141300
C	3.01084400	-0.57803600	-0.53596100
C	3.01055100	0.57814600	0.53617300
B	0.85184700	-0.00039100	0.00002500
O	1.61774000	1.02108200	0.51413000
O	1.61826300	-1.02154600	-0.51403000
C	3.90153700	1.77279800	0.20436700
H	3.80767800	2.52788400	0.98987100
H	4.95261000	1.46965300	0.14967700
H	3.62133100	2.23550100	-0.74327000
C	3.29097500	0.09072200	1.96355000
H	4.33614900	-0.20869000	2.08832500
H	3.08081500	0.90478900	2.66239100
H	2.65188300	-0.75563300	2.22973900
C	3.29147200	-0.09063000	-1.96337000
H	4.33503800	0.21489900	-2.08630200

H	3.08781600	-0.90662700	-2.66190700
H	2.64785700	0.75160500	-2.23173700
C	3.90245900	-1.77227800	-0.20432500
H	3.80160400	-2.53097600	-0.98545600
H	4.95429000	-1.47010100	-0.15910800
H	3.62923200	-2.23018700	0.74760800

Item	Value	Threshold	Converged?
Maximum Force	0.000084	0.000450	YES
RMS Force	0.000016	0.000300	YES
Maximum Displacement	0.000121	0.001800	YES
RMS Displacement	0.000027	0.001200	YES

Predicted change in Energy=-1.921522D-05

Optimization completed.

-- Stationary point found.

Charges:

APT atomic charges:

1
 1 C 0.457016
 2 C 0.457035
 3 B 0.944738
 4 O -0.882293
 5 O -0.882291
 6 C -0.017826
 7 H -0.001514
 8 H -0.014193
 9 H -0.001290
 10 C 0.007771
 11 H -0.015234
 12 H -0.004848
 13 H 0.000153
 14 C 0.007773
 15 H -0.015243
 16 H -0.004838
 17 H 0.000149
 18 C -0.017822
 19 H -0.001514
 20 H -0.014204
 21 H -0.001291
 22 C 0.456826
 23 C 0.456876
 24 B 0.944017
 25 O -0.882153
 26 O -0.882177
 27 C 0.007929
 28 H -0.004917
 29 H -0.015246

30 H 0.000192
31 C -0.017813
32 H -0.014238
33 H -0.001493
34 H -0.001229
35 C -0.017809
36 H -0.014170
37 H -0.001634
38 H -0.001200
39 C 0.007871
40 H -0.004717
41 H -0.015266
42 H 0.000117

Sum of APT charges= 0.00000

Thermochemistry:

Zero-point correction= 0.363847 (Hartree/Particle)

Thermal correction to Energy= 0.383655

Thermal correction to Enthalpy= 0.384600

Thermal correction to Gibbs Free Energy= 0.316925

Sum of electronic and zero-point Energies= -822.220336

Sum of electronic and thermal Energies= -822.200528

Sum of electronic and thermal Enthalpies= -822.199583

Sum of electronic and thermal Free Energies= -822.267258

NMR Calculation for B₂(pin)₂

(GIAO at B3LYP/6-311+G(2d,p), gas phase, B₂H₆ (0 ppm) as reference)

δ (ppm) 71.6 ppm

3 B Isotropic = 71.6268 Anisotropy = 22.4592

XX= 72.8443 YX= -0.0008 ZX= 0.0007

XY= -0.0011 YY= 57.7366 ZY= 8.8990

XZ= 0.0001 YZ= 7.3966 ZZ= 84.2995

Eigenvalues: 55.4365 72.8443 86.5996

24 B Isotropic = 71.6268 Anisotropy = 22.4568

XX= 72.8454 YX= 0.0002 ZX= 0.0002

XY= 0.0002 YY= 57.7673 ZY= 8.9395

XZ= -0.0003 YZ= 7.4538 ZZ= 84.2676

Eigenvalues: 55.4370 72.8454 86.5979

NHC-B₂(pin)₂ complex (NHC·1 in Scheme 2)

Coordinates:

C	0.00965700	-1.06114100	-0.66457600
C	0.67757700	-1.94137100	-2.63239700
C	-0.67829500	-1.94230200	-2.62352800
N	-1.07559600	-1.40012400	-1.40946100
H	1.37337600	-2.28300700	-3.38071000
H	-1.38286100	-2.28095400	-3.36488700
N	1.08807500	-1.39831600	-1.42334700
C	-2.48872300	-1.17153100	-1.03165500
C	-3.14274700	-0.13939400	-1.96458000
C	-3.27668600	-2.49108300	-0.99690200
H	-2.44847100	-0.77133800	-0.01785000
C	-4.60149000	0.10921600	-1.54846200
H	-3.11948300	-0.50574700	-3.00129600
H	-2.56192700	0.78777800	-1.93123500
C	-4.73547400	-2.23327700	-0.58458800
H	-3.25956600	-2.96821700	-1.98740700
H	-2.79588200	-3.18387500	-0.29726800
C	-5.40783800	-1.19753400	-1.49873800
H	-5.06844800	0.82083700	-2.23943000
H	-4.61509300	0.58142400	-0.55675300
H	-5.29573000	-3.17540900	-0.59539500
H	-4.75395200	-1.86991300	0.45175100
H	-6.43074400	-0.99979800	-1.15725900
H	-5.49232500	-1.61087200	-2.51430000
C	2.50271500	-1.16252300	-1.05884600
C	3.30622700	-2.47271300	-1.06103100
C	3.14104300	-0.11018100	-1.98102100
H	2.47254400	-0.78444200	-0.03511400
C	4.76427800	-2.20760000	-0.65076700
H	3.28890700	-2.92389600	-2.06350100
H	2.83658200	-3.18826000	-0.37761700
C	4.59867700	0.15253700	-1.56912000
H	3.11484500	-0.46277000	-3.02207200

H	2.55369300	0.81393500	-1.94239800
C	5.42076900	-1.14520600	-1.54578100
H	5.33457600	-3.14301300	-0.68585900
H	4.78502600	-1.86682700	0.39305500
H	5.05162900	0.88025400	-2.25236600
H	4.61226800	0.60966800	-0.57056100
H	6.44118800	-0.93998100	-1.20172500
H	5.50920700	-1.53726800	-2.56928200
B	0.04920300	-0.21150700	0.78593000
O	1.18654800	-0.64264900	1.62815400
O	-1.16376600	-0.56072800	1.58197100
C	0.69499200	-1.45067100	2.70174000
C	-0.75502900	-0.87816700	2.91788800
C	0.68573400	-2.92771100	2.26252900
H	1.69591900	-3.20853300	1.94679700
H	0.38848700	-3.60094900	3.07375600
H	0.00749200	-3.08557700	1.41893100
C	1.63357100	-1.28355200	3.89963700
H	1.24536100	-1.80073200	4.78491900
H	2.61432600	-1.70983900	3.66432900
H	1.77601400	-0.22842000	4.14053100
C	-1.75885200	-1.87162200	3.51063500
H	-1.44352300	-2.20849300	4.50493500
H	-2.73571400	-1.38864700	3.61610600
H	-1.88385200	-2.74822400	2.87081800
C	-0.75797100	0.41123100	3.75991200
H	-1.75151300	0.86638600	3.69543300
H	-0.54482000	0.21296900	4.81605800
H	-0.02721500	1.13044100	3.38327800
B	0.09664000	1.48821500	0.37722800
O	0.66850800	2.48429200	1.15265600
O	-0.52081900	2.04488800	-0.74352400
C	-0.57313500	3.49104300	-0.58318600
C	0.58980400	3.75157400	0.44630200
C	-0.38964900	4.14289700	-1.95277100
H	-1.22799900	3.87338800	-2.60219400
H	-0.36775500	5.23477100	-1.86685800
H	0.53060200	3.81387300	-2.43891800
C	-1.96465800	3.82779100	-0.02795100
H	-2.10902900	4.90772100	0.07766800
H	-2.72333100	3.44784300	-0.71832100
H	-2.12813100	3.35668500	0.94501800
C	0.32271500	4.86003100	1.46391000
H	1.17121200	4.93566000	2.15008700
H	0.20147700	5.82893300	0.96668200
H	-0.57063500	4.65698300	2.05681700

C	1.95565500	3.97819300	-0.21795500
H	2.00714800	4.94864100	-0.72211900
H	2.73080100	3.94856400	0.55266100
H	2.17778700	3.19575900	-0.94932800

Item	Value	Threshold	Converged?
Maximum Force	0.000363	0.000450	YES
RMS Force	0.000063	0.000300	YES
Maximum Displacement	0.001600	0.001800	YES
RMS Displacement	0.000376	0.001200	YES

Predicted change in Energy=-1.306674D-05

Optimization completed.

-- Stationary point found.

Charges:

APT atomic charges:

1

1 C 0.239477
 2 C -0.022846
 3 C -0.025271
 4 N -0.405251
 5 H 0.085011
 6 H 0.085882
 7 N -0.415910
 8 C 0.338745
 9 C 0.042908
 10 C 0.061738
 11 H 0.077023
 12 C 0.118353
 13 H -0.048187
 14 H -0.000368
 15 C 0.119326
 16 H -0.043747
 17 H -0.029915
 18 C 0.116066
 19 H -0.061653
 20 H -0.034698
 21 H -0.064978
 22 H -0.033356
 23 H -0.060536
 24 H -0.050505
 25 C 0.332907
 26 C 0.061129
 27 C 0.063614
 28 H 0.075813
 29 C 0.119304
 30 H -0.043024
 31 H -0.025674

32 C 0.114764
33 H -0.046517
34 H -0.035845
35 C 0.115960
36 H -0.063610
37 H -0.031418
38 H -0.060052
39 H -0.030965
40 H -0.058424
41 H -0.049701
42 B 0.897901
43 O -0.918245
44 O -0.942598
45 C 0.459686
46 C 0.492291
47 C -0.003397
48 H -0.029147
49 H -0.038558
50 H -0.015409
51 C 0.021325
52 H -0.031186
53 H -0.026326
54 H -0.001427
55 C 0.013938
56 H -0.030903
57 H -0.019731
58 H -0.014935
59 C -0.023365
60 H -0.018656
61 H -0.042969
62 H 0.023368
63 B 0.776802
64 O -0.848771
65 O -0.846532
66 C 0.433846
67 C 0.436470
68 C 0.016845
69 H -0.010442
70 H -0.022220
71 H -0.005071
72 C -0.010202
73 H -0.023918
74 H -0.011098
75 H 0.003480
76 C 0.013842
77 H -0.006597

78 H -0.024456

79 H -0.001207

80 C -0.002330

81 H -0.026650

82 H -0.002096

83 H -0.016924

Sum of APT charges= 0.00000

Thermochemistry:

Zero-point correction= 0.738560 (Hartree/Particle)

Thermal correction to Energy= 0.775055

Thermal correction to Enthalpy= 0.776000

Thermal correction to Gibbs Free Energy= 0.670890

Sum of electronic and zero-point Energies= -1517.423498

Sum of electronic and thermal Energies= -1517.387003

Sum of electronic and thermal Enthalpies= -1517.386059

Sum of electronic and thermal Free Energies= -1517.491169

NMR Calculation for NHC-B₂(pin)₂ complex (NHC·1 in Scheme 2)

(GIAO at B3LYP/6-311+G(2d,p), gas phase, B₂H₆ (0 ppm) as reference)

δ (ppm) B⁴² = -158.5 ppm

B⁶³ = -125.8 ppm

42 B Isotropic = 242.0704 Anisotropy = 33.8128

XX= 262.5067 YX= 4.6246 ZX= 10.8595

XY= -14.8824 YY= 229.3467 ZY= 6.3972

XZ= 2.6682 YZ= -1.3156 ZZ= 234.3579

Eigenvalues: 226.6864 234.9126 264.6123

63 B Isotropic = 209.4113 Anisotropy = 38.7484

XX= 193.7259 YX= 8.2950 ZX= 44.6936

XY= -0.0955 YY= 220.1217 ZY= -8.2220

XZ= 14.0640 YZ= 0.4166 ZZ= 214.3864

Eigenvalues: 172.2584 220.7319 235.2436