Supporting Information

for

A Novel 1,5-Benzoheteroazepine Synthesis *via* a One-Pot Coupling-Isomerization-Cyclocondensation Sequence

Roland U. Braun, Kirsten Zeitler,[§] and Thomas J. J. Müller*

Tables of data collection parameters, bond lengths and angles, positional and thermal parameter, and least-squares planes for **7a**.

Table 1. Crystal data and structure refinement for **7a**.

Identification code	Braun1 Mueller M2199 1/00
Empirical formula	C21 H17 N3 O2
Formula weight	343.38
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	P21/c
Unit cell dimensions	a = 13.337(5) A alpha = 90 deg. b = 13.157(6) A beta = 107.38(5) deg. c = 10.000(7) A gamma = 90 deg.
Volume	1675(2) A^3
Z	4
Density (calculated)	1.362 Mg/m^3
Absorption coefficient	0.090 mm^-1
F(000)	720
Crystal size	.53 x .43 x .30 mm
Theta range for data collection	2.64 to 23.98 deg.
Index ranges	-15<=h<=15, -15<=k<=15, -11<=l<=11
Reflections collected	5296
Independent reflections	1986 [R(int) = 0.0244]
Absorption correction	Semi-empirical from psi-scans

Max. and min. transmission	0.9992 and 0.9323
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1986 / 0 / 236
Goodness-of-fit on F^2	1.095
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0867
R indices (all data)	R1 = 0.0494, wR2 = 0.0964
Extinction coefficient	0.0029(8)
Largest diff. peak and hole	0.164 and -0.205 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7a**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	8247(2)	2704(1)	1135(2)	56(1)
N(2)	6247(1)	1590(1)	-27(2)	45(1)
N(3)	9110(2)	6823(2)	4814(2)	54(1)
O(1)	9302(2)	6648(1)	6057(2)	75(1)
O(2)	9212(2)	7666(1)	4364(2)	94(1)
C(1)	8028(2)	1782(2)	1676(2)	44(1)
C(2)	8830(2)	1291(2)	2691(2)	57(1)
C(3)	8718(2)	318(2)	3126(2)	63(1)
C(4)	7782(2)	-193(2)	2583(2)	59(1)
C(5)	6980(2)	278(2)	1597(2)	49(1)
C(6)	7077(2)	1256(2)	1119(2)	42(1)
C(7)	5976(2)	2528(2)	-164(2)	43(1)
C(8)	6471(2)	3305(2)	939(2)	47(1)
C(9)	7565(2)	3601(2)	906(2)	46(1)
C(10)	5148(2)	2825(2)	-1461(2)	44(1)
C(11)	4579(2)	2081(2)	-2348(2)	54(1)
C(12)	3851(2)	2329(2)	-3600(3)	61(1)
C(13)	3667(2)	3329(2)	-3988(3)	62(1)
C(14)	4205(2)	4079(2)	-3127(3)	64(1)
C(15)	4940(2)	3831(2)	-1874(3)	59(1)
C(16)	8006(2)	4438(2)	1947(2)	40(1)
C(17)	8116(2)	5409(2)	1491(2)	48(1)
C(18)	8479(2)	6195(2)	2417(2)	49(1)
C(19)	8738(2)	5992(2)	3819(2)	41(1)
C(20)	8645(2)	5033(2)	4326(2)	45(1)
C(21)	8283(2)	4259(2)	3384(2)	46(1)

Table 3. Selected bond lengths [A] and angles [deg] for **7a**.

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [A] and angles [deg] for **7a**.

N(1)-C(1)	1.394(3)
N(1)-C(9)	1.465(3)
N(2)-C(7)	1.282(3)
N(2)-C(6)	1.405(3)
N(3)-O(1)	1.214(3)
N(3)-O(2)	1.219(2)
N(3)-C(19)	1.462(3)
C(1)-C(2)	1.394(3)
C(1)-C(6)	1.406(3)
C(2)-C(3)	1.375(3)
C(3)-C(4)	1.377(3)
C(4)-C(5)	1.368(3)
C(5)-C(6)	1.392(3)
C(7)-C(10)	1.483(3)
C(7)-C(8)	1.504(3)
C(8)-C(9)	1.521(3)
C(9)-C(16)	1.509(3)
C(10)-C(11)	1.385(3)
C(10)-C(15)	1.390(3)
C(11)-C(12)	1.375(3)
C(12)-C(13)	1.373(3)
C(13)-C(14)	1.364(3)
C(14)-C(15)	1.380(3)
C(16)-C(17)	1.379(3)
C(16)-C(21)	1.392(3)
C(17)-C(18)	1.377(3)
C(18)-C(19)	1.366(3)
C(19)-C(20)	1.379(3)
C(20)-C(21)	1.373(3)

C(1)-N(1)-C(9)	124.7(2)
C(7)-N(2)-C(6)	121.1(2)
O(1)-N(3)-O(2)	122.6(2)
O(1)-N(3)-C(19)	118.6(2)
O(2)-N(3)-C(19)	118.8(2)
N(1)-C(1)-C(2)	118.8(2)
N(1)-C(1)-C(6)	122.9(2)
C(2)-C(1)-C(6)	117.7(2)
C(3)-C(2)-C(1)	122.0(2)
C(2)-C(3)-C(4)	120.1(2)
C(5)-C(4)-C(3)	119.0(2)
C(4)-C(5)-C(6)	122.2(2)
C(5)-C(6)-C(1)	119.0(2)
C(5)-C(6)-N(2)	115.9(2)
C(1)-C(6)-N(2)	124.6(2)
N(2)-C(7)-C(10)	117.4(2)
N(2)-C(7)-C(8)	121.8(2)
C(10)-C(7)-C(8)	120.8(2)
C(7)-C(8)-C(9)	111.9(2)
N(1)-C(9)-C(16)	112.6(2)

N(1)-C(9)-C(8)	110.1(2)
C(16)-C(9)-C(8)	110.5(2)
C(11)-C(10)-C(15)	117.4(2)
C(11)-C(10)-C(7)	119.7(2)
C(15)-C(10)-C(7)	122.8(2)
C(12)-C(11)-C(10)	121.2(2)
C(13)-C(12)-C(11)	120.2(2)
C(14)-C(13)-C(12)	119.9(2)
C(13)-C(14)-C(15)	120.0(2)
C(14)-C(15)-C(10)	121.3(2)
C(17)-C(16)-C(21)	118.5(2)
C(17)-C(16)-C(9)	120.4(2)
C(21)-C(16)-C(9)	121.2(2)
C(16)-C(17)-C(18)	121.6(2)
C(19)-C(18)-C(17)	118.2(2)
C(18)-C(19)-C(20)	122.3(2)
C(18)-C(19)-N(3)	118.8(2)
C(20)-C(19)-N(3)	118.9(2)
C(21)-C(20)-C(19)	118.5(2)
C(20)-C(21)-C(16)	120.9(2)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for **7a**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	53(1)	36(1)	88(2)	-16(1)	34(1)	-6(1)
N(2)	47(1)	39(1)	47(1)	-2(1)	11(1)	-2(1)
N(3)	60(1)	46(1)	55(1)	-12(1)	15(1)	-6(1)
O(1)	104(2)	70(1)	51(1)	-19(1)	24(1)	-16(1)
O(2)	142(2)	44(1)	80(1)	-7(1)	10(1)	-26(1)
C(1)	47(1)	44(1)	43(1)	-12(1)	14(1)	0(1)
C(2)	50(1)	68(2)	49(1)	-22(1)	10(1)	0(1)
C(3)	70(2)	75(2)	36(1)	-2(1)	6(1)	17(2)
C(4)	78(2)	56(2)	45(1)	6(1)	21(1)	7(1)
C(5)	59(1)	47(1)	43(1)	0(1)	17(1)	-2(1)
C(6)	47(1)	40(1)	38(1)	-6(1)	13(1)	1(1)
C(7)	42(1)	42(1)	47(1)	-4(1)	18(1)	-4(1)
C(8)	51(1)	43(1)	47(1)	-6(1)	14(1)	2(1)
C(9)	56(1)	41(1)	43(1)	-7(1)	18(1)	-7(1)
C(10)	40(1)	46(1)	48(1)	0(1)	14(1)	1(1)
C(11)	52(1)	48(1)	58(2)	2(1)	9(1)	-6(1)
C(12)	50(1)	66(2)	59(2)	-1(1)	5(1)	-10(1)
C(13)	49(1)	76(2)	59(2)	15(2)	12(1)	2(1)
C(14)	62(2)	55(2)	70(2)	14(1)	12(1)	8(1)
C(15)	60(2)	48(2)	65(2)	1(1)	13(1)	3(1)
C(16)	46(1)	34(1)	42(1)	-3(1)	18(1)	-2(1)
C(17)	66(2)	43(1)	37(1)	1(1)	15(1)	-6(1)
C(18)	63(2)	34(1)	49(1)	3(1)	18(1)	-5(1)
C(19)	43(1)	37(1)	43(1)	-7(1)	14(1)	-3(1)
C(20)	53(1)	43(1)	37(1)	1(1)	13(1)	1(1)
C(21)	60(1)	33(1)	45(1)	1(1)	16(1)	-2(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7a**.

	x	y	z	U(eq)
H(1)	9038(2)	2999(1)	1329(2)	67
H(2)	9460(2)	1632(2)	3086(2)	68
H(3)	9274(2)	4(2)	3787(2)	75
H(4)	7698(2)	-847(2)	2883(2)	71
H(5)	6348(2)	-67(2)	1233(2)	59
H(8A)	6514(2)	3031(2)	1855(2)	56
H(8B)	6030(2)	3906(2)	792(2)	56
H(9)	7504(2)	3865(2)	-31(2)	55
H(11)	4691(2)	1401(2)	-2091(2)	65
H(12)	3482(2)	1818(2)	-4185(3)	73
H(13)	3177(2)	3495(2)	-4838(3)	75
H(14)	4077(2)	4757(2)	-3384(3)	77
H(15)	5304(2)	4348(2)	-1295(3)	71
H(17)	7940(2)	5535(2)	534(2)	58
H(18)	8546(2)	6848(2)	2097(2)	58
H(20)	8824(2)	4913(2)	5285(2)	53
H(21)	8221(2)	3607(2)	3709(2)	55