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The synthesis of Benzo[C]carbazoles

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APPENDIX

TABLE 1. CRYSTAL DATA AND STRUCTURE REFINEMENT FOR 2M_JN1_S.

Identification code	2m_jn1_s	
Empirical formula	C18 H15 N	
Formula weight	245.31	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 11.4419(14) Å	α= 90°.
	b = 14.1679(17) Å	β= 90°.
	c = 16.1234(19) Å	γ = 90°.
Volume	2613.7(5) $Å^3$	
Z	8	
Density (calculated)	1.247 Mg/m^3	
Absorption coefficient	0.072 mm^{-1}	
F(000)	1040	
Crystal size	0.40 x 0.36 x 0.20 mm^3	
Theta range for data collection	2.53 to 26.00°.	
Index ranges	-10<=h<=14, -15<=k<=17, -19<=l<=19	
Reflections collected	14591	
Independent reflections	2566 [R(int) = 0.0481]	
Completeness to theta = 26.00°	100.0 %	
Absorption correction	None	
Max. and min. transmission	0.9857 and 0.9717	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2566 / 0 / 174	
Goodness-of-fit on F^2	1.073	
Final R indices [I>2sigma(I)]	R1 = 0.0758, wR2 = 0.2184	
R indices (all data)	R1 = 0.1143, wR2 = 0.2517	
Largest diff. peak and hole	0.741 and -0.286 $e.Å^{-3}$	

TABLE 2: ATOMIC COORDINATES (X104) AND EQUIVALENT ISOTROPIC DISPLACEMENT PARAMETERS (Å2X 103) FOR 2M_JN1_S. U(EQ) IS DEFINED AS ONE THIRD OF THE TRACE OF THE ORTHOGONALIZED UIJ TENSOR.

	x	y	z	U(eq)
C(1)	-2212(4)	10328(3)	3428(2)	76(1)
C(2)	-3297(4)	9936(3)	3451(2)	86(1)
C(3)	-3451(4)	9026(3)	3768(2)	83(1)
C(4)	-2523(4)	8534(3)	4062(2)	72(1)
C(5)	-399(3)	8415(3)	4339(2)	66(1)
C(6)	734(4)	8759(3)	4336(2)	89(1)
C(8)	2459(3)	11731(3)	3410(2)	71(1)
C(9)	2009(4)	12518(3)	3024(2)	77(1)
C(10)	832(4)	12584(3)	2844(2)	78(1)
C(11)	70(3)	11872(2)	3051(2)	68(1)
C(12)	-500(4)	7427(3)	4683(3)	93(1)
C(13)	3160(4)	9844(3)	4175(3)	98(1)
C(4A)	-1382(3)	8912(2)	4049(2)	61(1)
C(6A)	893(4)	9635(3)	4031(2)	79(1)
C(7A)	1709(3)	10992(2)	3610(2)	58(1)
C(11A)	488(3)	11049(2)	3440(2)	57(1)
C(11B)	-58(3)	10192(2)	3713(2)	55(1)
C(11C)	-1219(3)	9846(2)	3719(2)	60(1)
N(7)	1989(3)	10141(2)	3963(2)	69(1)

TABLE 3: BOND LENGTHS [Å] AND ANGLES [°] FOR 2M_JN1_S.

C(1)-C(2)	1.361(5)	C(4)-H(4)	0.9300
C(1)-C(11C)	1.406(5)	C(5)-C(6)	1.386(6)
C(1)-H(1)	0.9300	C(5)-C(4A)	1.407(5)
C(2)-C(3)	1.398(6)	C(5)-C(12)	1.510(5)
C(2)-H(2)	0.9300	C(6)-C(6A)	1.347(5)
C(3)-C(4)	1.356(6)	C(6)-H(6)	0.9300
C(3)-H(3)	0.9300	C(8)-C(9)	1.377(5)
C(4)-C(4A)	1.411(5)	C(8)-C(7A)	1.392(5)

C(8)-H(8)	0.9300	C(6A)-C(6)-H(6)	121.6
C(9)-C(10)	1.381(5)	C(5)-C(6)-H(6)	121.6
C(9)-H(9)	0.9300	C(9)-C(8)-C(7A)	118.8(4)
C(10)-C(11)	1.375(5)	C(9)-C(8)-H(8)	120.6
C(10)-H(10)	0.9300	C(7A)-C(8)-H(8)	120.6
C(11)-C(11A)	1.407(4)	C(8)-C(9)-C(10)	121.0(4)
C(11)-H(11)	0.9300	C(8)-C(9)-H(9)	119.5
C(12)-H(12A)	0.9600	C(10)-C(9)-H(9)	119.5
C(12)-H(12B)	0.9600	C(11)-C(10)-C(9)	121.2(4)
C(12)-H(12C)	0.9600	C(11)-C(10)-H(10)	119.4
C(13)-N(7)	1.446(5)	C(9)-C(10)-H(10)	119.4
C(13)-H(13A)	0.9600	C(10)-C(11)-C(11A)	120.0(4)
C(13)-H(13B)	0.9600	C(10)-C(11)-H(11)	120.0
C(13)-H(13C)	0.9600	C(11A)-C(11)-H(11)	120.0
C(4A)-C(11C)	1.437(4)	C(5)-C(12)-H(12A)	109.5
C(6A)-C(11B)	1.439(5)	C(5)-C(12)-H(12B)	109.5
C(6A)-N(7)	1.449(5)	H(12A)-C(12)-H(12B)	109.5
C(7A)-N(7)	1.371(4)	C(5)-C(12)-H(12C)	109.5
C(7A)-C(11A)	1.426(5)	H(12A)-C(12)-H(12C)	109.5
C(11A)-C(11B)	1.435(4)	H(12B)-C(12)-H(12C)	109.5
C(11B)-C(11C)	1.415(5)	N(7)-C(13)-H(13A)	109.5
C(2)-C(1)-C(11C)	122.0(4)	N(7)-C(13)-H(13B)	109.5
C(2)-C(1)-H(1)	119.0	H(13A)-C(13)-H(13B)	109.5
C(11C)-C(1)-H(1)	119.0	N(7)-C(13)-H(13C)	109.5
C(1)-C(2)-C(3)	120.1(4)	H(13A)-C(13)-H(13C)	109.5
C(1)-C(2)-H(2)	120.0	H(13B)-C(13)-H(13C)	109.5
C(3)-C(2)-H(2)	120.0	C(5)-C(4A)-C(4)	122.9(3)
C(4)-C(3)-C(2)	120.2(4)	C(5)-C(4A)-C(11C)	118.6(3)
C(4)-C(3)-H(3)	119.9	C(4)-C(4A)-C(11C)	118.4(3)
C(2)-C(3)-H(3)	119.9	C(6)-C(6A)-C(11B)	122.2(4)
C(3)-C(4)-C(4A)	121.6(3)	C(6)-C(6A)-N(7)	126.9(4)
C(3)-C(4)-H(4)	119.2	C(11B)-C(6A)-N(7)	110.8(3)
C(4A)-C(4)-H(4)	119.2	N(7)-C(7A)-C(8)	127.8(3)
C(6)-C(5)-C(4A)	124.8(3)	N(7)-C(7A)-C(11A)	111.0(3)
C(6)-C(5)-C(12)	113.5(4)	C(8)-C(7A)-C(11A)	121.2(3)
C(4A)-C(5)-C(12)	121.7(3)	C(11)-C(11A)-C(7A)	117.7(3)
C(6A)-C(6)-C(5)	116.8(4)	C(11)-C(11A)-C(11B)	133.6(3)

C(7A)-C(11A)-C(11B)	108.7(3)	C(1)-C(11C)-C(4A)	117.7(3)
C(11C)-C(11B)-C(11A)	134.7(3)	C(11B)-C(11C)-C(4A)	116.3(3)
C(11C)-C(11B)-C(6A)	121.2(3)	C(7A)-N(7)-C(13)	124.9(3)
C(11A)-C(11B)-C(6A)	104.1(3)	C(7A)-N(7)-C(6A)	105.3(3)
C(1)-C(11C)-C(11B)	126.0(3)	C(13)-N(7)-C(6A)	129.7(3)

Symmetry transformations used to generate equivalent atoms:

TABLE 4: ANISOTROPIC DISPLACEMENT PARAMETERS (Å2X 103) FOR 2M_JN1_S. THE ANISOTROPIC DISPLACEMENT FACTOR EXPONENT TAKES THE FORM: -2□2[H2 A*2U11 + ... + 2 H K A* B* U12]

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	90(3)	73(2)	64(2)	16(2)	0(2)	-1(2)
C(2)	83(3)	100(3)	74(2)	16(2)	-10(2)	5(2)
C(3)	81(3)	91(3)	76(2)	-1(2)	-3(2)	-15(2)
C(4)	91(3)	62(2)	62(2)	-3(2)	6(2)	-14(2)
C(5)	72(2)	76(2)	51(2)	-10(2)	10(2)	-14(2)
C(6)	129(4)	75(3)	62(2)	-7(2)	-1(2)	29(3)
C(8)	76(2)	76(2)	60(2)	-12(2)	15(2)	-10(2)
C(9)	101(3)	69(2)	60(2)	-5(2)	22(2)	-15(2)
C(10)	105(3)	68(2)	60(2)	8(2)	13(2)	0(2)
C(11)	78(2)	71(2)	55(2)	3(2)	1(2)	8(2)
C(12)	118(3)	82(3)	79(3)	3(2)	8(2)	20(2)
C(13)	100(3)	95(3)	98(3)	-17(2)	-23(2)	26(2)
C(4A)	88(2)	54(2)	42(2)	-4(1)	8(2)	-9(2)
C(6A)	118(3)	71(2)	50(2)	-13(2)	6(2)	13(2)
C(7A)	64(2)	62(2)	47(2)	-7(1)	7(1)	1(2)
C(11A)	66(2)	63(2)	44(2)	-5(1)	4(1)	3(2)
C(11B)	73(2)	53(2)	41(1)	-1(1)	-1(1)	10(2)
C(11C)	83(2)	56(2)	41(2)	1(1)	4(2)	-3(2)
N(7)	72(2)	72(2)	64(2)	-6(1)	2(1)	-8(2)

TABLE 5: HYDROGEN COORDINATES (X 10^4) AND ISOTROPIC DISPLACEMENT PARAMETERS (Å2X 10^3) FOR 2M_JN1_S.

	x	y	z	U(eq)
H(1)	-2124	10933	3214	91
H(2)	-3937	10273	3255	103
H(3)	-4192	8757	3776	99
H(4)	-2641	7932	4278	86
H(6)	1356	8402	4536	106
H(8)	3251	11694	3536	85
H(9)	2505	13012	2882	92
H(10)	550	13119	2577	93
H(11)	-723	11934	2935	82
H(12A)	250	7223	4880	140
H(12B)	-765	7008	4254	140
H(12C)	-1050	7423	5133	140
H(13A)	3540	9596	3691	147
H(13B)	3123	9364	4595	147
H(13C)	3594	10374	4381	147

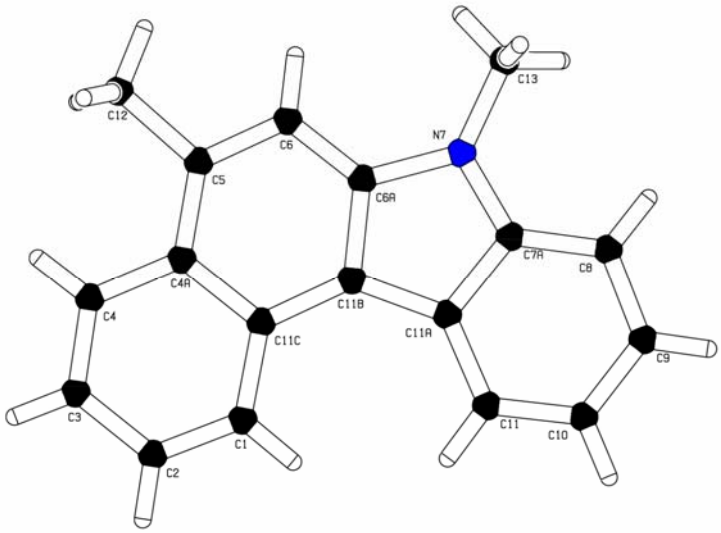
TABLE 6. TORSION ANGLES [°] FOR 2M_JN1_S.

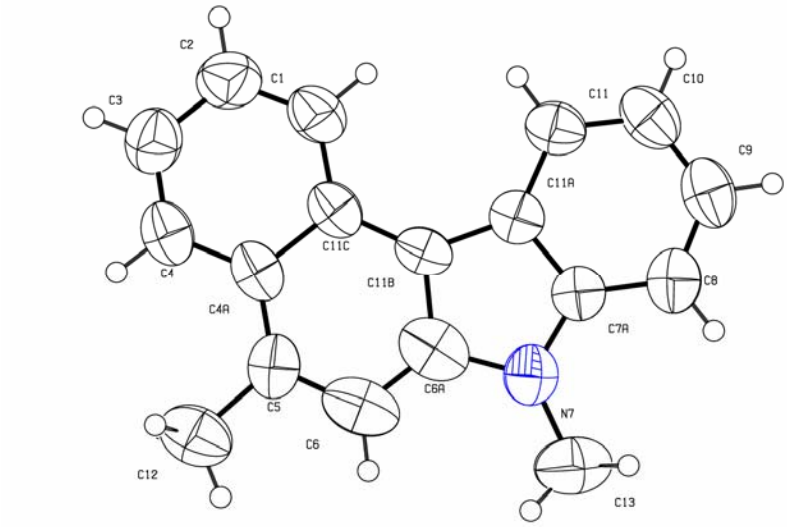
C(11C)-C(1)-C(2)-C(3)	-0.2(6)	C(3)-C(4)-C(4A)-C(5)	-179.1(3)
C(1)-C(2)-C(3)-C(4)	0.7(6)	C(3)-C(4)-C(4A)-C(11C)	0.5(5)
C(2)-C(3)-C(4)-C(4A)	-0.9(6)	C(5)-C(6)-C(6A)-C(11B)	-0.7(5)
C(4A)-C(5)-C(6)-C(6A)	0.0(5)	C(5)-C(6)-C(6A)-N(7)	-179.8(3)
C(12)-C(5)-C(6)-C(6A)	179.5(3)	C(9)-C(8)-C(7A)-N(7)	177.3(3)
C(7A)-C(8)-C(9)-C(10)	0.8(5)	C(9)-C(8)-C(7A)-C(11A)	-1.6(5)
C(8)-C(9)-C(10)-C(11)	0.7(5)	C(10)-C(11)-C(11A)-C(7A)	0.4(4)
C(9)-C(10)-C(11)-C(11A)	-1.3(5)	C(10)-C(11)-C(11A)-C(11B)	-178.4(3)
C(6)-C(5)-C(4A)-C(4)	179.9(3)	N(7)-C(7A)-C(11A)-C(11)	-178.0(3)
C(12)-C(5)-C(4A)-C(4)	0.5(5)	C(8)-C(7A)-C(11A)-C(11)	1.0(4)
C(6)-C(5)-C(4A)-C(11C)	0.3(5)	N(7)-C(7A)-C(11A)-C(11B)	1.1(3)
C(12)-C(5)-C(4A)-C(11C)	-179.2(3)	C(8)-C(7A)-C(11A)-C(11B)	-179.9(3)

C(11)-C(11A)-C(11B)-C(11C)	-1.8(6)	C(6A)-C(11B)-C(11C)-C(4A)	-0.7(4)
C(7A)-C(11A)-C(11B)-C(11C)	179.3(3)	C(5)-C(4A)-C(11C)-C(1)	179.7(3)
C(11)-C(11A)-C(11B)-C(6A)	178.0(3)	C(4)-C(4A)-C(11C)-C(1)	0.0(4)
C(7A)-C(11A)-C(11B)-C(6A)	-1.0(3)	C(5)-C(4A)-C(11C)-C(11B)	0.1(4)
C(6)-C(6A)-C(11B)-C(11C)	1.1(5)	C(4)-C(4A)-C(11C)-C(11B)	-179.6(3)
N(7)-C(6A)-C(11B)-C(11C)	-179.6(3)	C(8)-C(7A)-N(7)-C(13)	-1.9(5)
C(6)-C(6A)-C(11B)-C(11A)	-178.7(3)	C(11A)-C(7A)-N(7)-C(13)	177.1(3)
N(7)-C(6A)-C(11B)-C(11A)	0.6(3)	C(8)-C(7A)-N(7)-C(6A)	-179.7(3)
C(2)-C(1)-C(11C)-C(11B)	179.3(3)	C(11A)-C(7A)-N(7)-C(6A)	-0.7(3)
C(2)-C(1)-C(11C)-C(4A)	-0.2(5)	C(6)-C(6A)-N(7)-C(7A)	179.3(3)
C(11A)-C(11B)-C(11C)-C(1)	-0.5(6)	C(11B)-C(6A)-N(7)-C(7A)	0.1(4)
C(6A)-C(11B)-C(11C)-C(1)	179.7(3)	C(6)-C(6A)-N(7)-C(13)	1.7(6)
C(11A)-C(11B)-C(11C)-C(4A)	179.0(3)	C(11B)-C(6A)-N(7)-C(13)	-177.6(3)

Symmetry transformations used to generate equivalent atoms:

DIAGRAMS:


C13
C12
C6
N7
C5
C6A
C7A
C8
C4A
C4
C11B
C11C
C11A
C9
C3
C11
C10
C1
C2


C2
C1
C10
C3
C11
C9
C11A
C11C
C4
C11B
C8
C4A
C7A
C6A
C5
N7
C6
C12
C13