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Table 1. Crystal Data and Experimental Conditions for Structure Refinement

Empirical formula	C ₁₂ H ₂₅ B ₃
Molecular weight, M	201.8
Crystal system	monoclinic
Space group	P2 ₁ /c
a, Å	9.219(2)
b, Å	20.669(7)
c, Å	7.842(2)
β, deg.	111.97(2)
V, Å ³	1385.8(8)
Z	4
ρ _c (g cm ⁻³)	0.967
T(K)	120
Radiation	MoKα
μ (mm ⁻¹)	0.050
F(000)	448
Crystal size	cylinder diam. 0.3 mm
2θ range (deg)	3.0 to 90.0
Scan type	Wyckoff
Scan range (deg)	1.80 in ω
Refl. collected	8842
Unique refl.	6898
R _{merg}	0.033
Observed refl. (F ≥ 4σ)	5696
Number of parameters	237
R	0.056
R _w	0.075
Goodness of fit	1.18
Weight scheme	w ⁻¹ = σ ² (F) + 0.0021F ²
Largest difference peak/hole (e/Å ³)	0.31/ -0.21

Table 2. Atomic coordinates ($\times 10^5$) and equivalent isotropic displacement coefficients ($\text{\AA}^2 \times 10^4$)

	x	y	z	U(eq)
C(1)	-19189(8)	62445(3)	22488(11)	189(2)
C(1')	-32280(9)	59349(4)	6743(13)	241(2)
C(1'')	-29071(13)	52272(5)	3859(18)	359(3)
B(2)	-11083(9)	61350(4)	43879(13)	198(2)
C(2')	-14400(10)	56577(4)	57734(14)	264(2)
C(2'')	-31665(13)	55148(8)	52945(19)	427(4)
B(3)	-14928(9)	69282(4)	31424(12)	181(2)
C(3')	-23155(9)	76100(4)	27811(12)	214(2)
C(3'')	-40750(10)	75976(5)	16200(14)	298(3)
B(4)	-1114(9)	63359(4)	27541(13)	195(2)
C(4')	9894(9)	61476(5)	17064(14)	261(2)
C(4'')	27337(10)	62820(5)	27097(15)	293(3)
C(5)	1127(8)	66895(3)	46030(11)	184(2)
C(5')	14151(9)	70035(4)	61728(12)	236(2)
C(5'')	24820(11)	65166(5)	75501(14)	310(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 3. Anisotropic displacement coefficients ($\text{\AA}^2 \times 10^4$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	165(2)	166(2)	224(3)	-15(2)	61(2)	-10(2)
C(1')	215(3)	214(3)	253(3)	-45(2)	40(3)	-19(3)
C(1'')	342(4)	267(4)	450(6)	-56(3)	128(4)	-149(4)
B(2)	177(3)	176(3)	236(4)	-1(2)	70(3)	17(3)
C(2')	239(3)	248(3)	306(4)	3(3)	103(3)	83(3)
C(2'')	297(4)	579(8)	415(6)	-128(5)	146(4)	102(6)
B(3)	166(3)	165(3)	213(3)	-2(2)	73(2)	1(2)
C(3')	207(3)	178(3)	254(3)	19(2)	82(2)	2(2)
C(3'')	223(3)	343(4)	292(4)	81(3)	55(3)	-17(3)
B(4)	177(3)	174(3)	235(4)	5(2)	78(3)	-2(3)
C(4')	213(3)	293(4)	292(4)	9(3)	112(3)	-53(3)
C(4'')	200(3)	339(4)	361(5)	44(3)	128(3)	23(4)
C(5)	156(2)	173(2)	215(3)	-4(2)	59(2)	-7(2)
C(5')	190(3)	228(3)	257(3)	-26(2)	47(2)	-32(3)
C(5'')	231(3)	374(5)	263(4)	-12(3)	21(3)	40(3)

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2(h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12})$$

Table 4. Bond lengths (Å)

C(1)-C(1')	1.508 (1)	C(1)-B(2)	1.577 (1)
C(1)-B(3)	1.561 (1)	C(1)-B(4)	1.573 (1)
C(1')-C(1'')	1.526 (1)	B(2)-C(2')	1.580 (2)
B(2)-B(3)	1.873 (1)	B(2)-B(4)	1.882 (2)
B(2)-C(5)	1.571 (1)	C(2')-C(2'')	1.521 (2)
B(3)-C(3')	1.575 (1)	B(3)-B(4)	1.872 (1)
B(3)-C(5)	1.574 (1)	C(3')-C(3'')	1.535 (1)
B(4)-C(4')	1.575 (2)	B(4)-C(5)	1.567 (1)
C(4')-C(4'')	1.528 (1)	C(5)-C(5')	1.508 (1)
C(5')-C(5'')	1.534 (1)		

Bond angles (°)

C(1')-C(1)-B(2)	136.5(1)	C(1')-C(1)-B(3)	137.8(1)
B(2)-C(1)-B(3)	73.3(1)	C(1')-C(1)-B(4)	134.8(1)
B(2)-C(1)-B(4)	73.4(1)	B(3)-C(1)-B(4)	73.3(1)
C(1)-C(1')-C(1'')	112.8(1)	C(1)-B(2)-C(2')	133.2(1)
C(1)-B(2)-B(3)	53.0(1)	C(2')-B(2)-B(3)	149.1(1)
C(1)-B(2)-B(4)	53.2(1)	C(2')-B(2)-B(4)	151.1(1)
B(3)-B(2)-B(4)	59.8(1)	C(1)-B(2)-C(5)	92.6(1)
C(2')-B(2)-C(5)	134.2(1)	B(3)-B(2)-C(5)	53.5(1)
B(4)-B(2)-C(5)	53.1(1)	B(2)-C(2')-C(2'')	113.9(1)
C(1)-B(3)-B(2)	53.7(1)	C(1)-B(3)-C(3')	134.9(1)
B(2)-B(3)-C(3')	149.5(1)	C(1)-B(3)-B(4)	53.6(1)
B(2)-B(3)-B(4)	60.3(1)	C(3')-B(3)-B(4)	150.1(1)
C(1)-B(3)-C(5)	93.0(1)	B(2)-B(3)-C(5)	53.4(1)
C(3')-B(3)-C(5)	132.1(1)	B(4)-B(3)-C(5)	53.2(1)
B(3)-C(3')-C(3'')	115.0(1)	C(1)-B(4)-B(2)	53.4(1)
C(1)-B(4)-B(3)	53.0(1)	B(2)-B(4)-B(3)	59.9(1)
C(1)-B(4)-C(4')	131.9(1)	B(2)-B(4)-C(4')	151.0(1)
B(3)-B(4)-C(4')	149.0(1)	C(1)-B(4)-C(5)	92.8(1)
B(2)-B(4)-C(5)	53.2(1)	B(3)-B(4)-C(5)	53.6(1)
C(4')-B(4)-C(5)	135.3(1)	B(4)-C(4')-C(4'')	116.5(1)
B(2)-C(5)-B(3)	73.1(1)	B(2)-C(5)-B(4)	73.7(1)
B(3)-C(5)-B(4)	73.2(1)	B(2)-C(5)-C(5')	136.2(1)
B(3)-C(5)-C(5')	134.8(1)	B(4)-C(5)-C(5')	138.2(1)
C(5)-C(5')-C(5'')	113.4(1)		

Table5. H-Atom coordinates ($\times 10^4$) and isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

	x	y	z	U
H(1'A)	-3429(21)	6163(8)	-503(27)	55(5)
H(1'B)	-4225(17)	5974(7)	952(21)	37(4)
H(1"A)	-3720(19)	5021(8)	-568(24)	44(4)
H(1"B)	-1962(19)	5199(9)	36(23)	49(4)
H(1"C)	-2733(23)	4980(9)	1538(29)	64(6)
H(2'A)	-942(20)	5835(8)	7133(24)	50(4)
H(2'B)	-861(20)	5290(9)	5832(27)	57(5)
H(2"A)	-3341(19)	5211(9)	6228(25)	53(5)
H(2"B)	-3798(26)	5934(11)	5193(31)	77(6)
H(2"C)	-3636(28)	5306(12)	4086(37)	90(7)
H(3'A)	-1792(18)	7889(8)	2192(21)	43(4)
H(3'B)	-2116(17)	7825(7)	3987(21)	36(4)
H(3"A)	-4526(18)	8040(8)	1525(21)	44(4)
H(3"B)	-4250(19)	7420(7)	396(22)	37(4)
H(3"C)	-4659(18)	7310(8)	2164(22)	39(4)
H(4'A)	645(19)	6372(8)	466(23)	49(4)
H(4'B)	840(19)	5672(8)	1359(22)	45(4)
H(4"A)	3351(18)	6167(7)	1958(21)	39(4)
H(4"B)	2967(20)	6754(9)	3117(23)	54(5)
H(4"C)	3137(20)	6041(9)	3881(25)	51(5)
H(5'A)	952(18)	7312(7)	6889(22)	38(4)
H(5'B)	2038(16)	7279(7)	5612(19)	30(3)
H(5"A)	3376(20)	6727(9)	8652(24)	58(5)
H(5"B)	1853(18)	6236(8)	8141(22)	46(4)
H(5"C)	2969(19)	6198(8)	6885(24)	50(5)