Supporting Information

Lithiation of 1-Chloromethylbenzotriazole: Generation and Elaboration of Benzotriazolyloxiranes

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X-ray structures of **2g** and **3**

2g

3

X-ray structures of **5d**, **5e** and **5i**.

5d

5e

5i

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

Identification code	3hx	
Empirical formula	C ₂₁ H ₁₇ N ₃ O	
Formula weight	327.38	
Temperature	168(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.542(3) Å	α = 90°.
	b = 15.986(5) Å	β = 111.130(4)°.
	c = 12.161(4) Å	γ = 90°.
Volume	1730.4(10) Å ³	
Z	4	
Density (calculated)	1.257 Mg/m ³	
Absorption coefficient	0.079 mm ⁻¹	
F(000)	688	
Crystal size	0.79 x 0.65 x 0.15 mm ³	
Theta range for data collection	2.20 to 26.38°.	
Index ranges	-11 ≤ h ≤ 11, -19 ≤ k ≤ 19, -15 ≤ l ≤ 15	
Reflections collected	21827	
Independent reflections	3514 [R(int) = 0.0248]	
Completeness to theta = 26.38°	99.4 %	
Absorption correction	None	
Max. and min. transmission	0.9882 and 0.9399	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3514 / 0 / 227	
Goodness-of-fit on F ²	0.989	
Final R indices [I > 2σ(I)]	R1 = 0.0355, wR2 = 0.0880	
R indices (all data)	R1 = 0.0624, wR2 = 0.0958	
Largest diff. peak and hole	0.186 and -0.149 e.Å ⁻³	

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

	x	y	z	U(eq)
O(1)	6337(1)	1175(1)	1840(1)	45(1)
C(1)	7642(1)	1381(1)	1499(1)	37(1)
C(2)	6531(1)	2016(1)	1571(1)	42(1)
C(11)	7478(1)	1052(1)	302(1)	36(1)
C(12)	8717(1)	989(1)	-53(1)	43(1)
C(13)	8545(2)	706(1)	-1175(1)	48(1)
C(14)	7136(2)	478(1)	-1954(1)	48(1)
C(15)	5902(2)	535(1)	-1611(1)	46(1)
C(16)	6067(1)	820(1)	-491(1)	41(1)
C(21)	9140(1)	1327(1)	2475(1)	36(1)
C(22)	10127(1)	1999(1)	2737(1)	44(1)
C(23)	11533(2)	1936(1)	3614(1)	52(1)
C(24)	11988(2)	1205(1)	4254(1)	53(1)
C(25)	10977(2)	542(1)	4001(1)	55(1)
C(26)	9581(1)	595(1)	3121(1)	45(1)
C(27)	13532(2)	1125(1)	5199(1)	88(1)
N(31)	6825(1)	2579(1)	2543(1)	43(1)
N(32)	6783(1)	3418(1)	2312(1)	53(1)
N(33)	7081(1)	3827(1)	3297(1)	57(1)
C(34)	7654(2)	3386(1)	5403(1)	57(1)
C(35)	7835(2)	2691(1)	6102(1)	60(1)
C(36)	7688(2)	1885(1)	5623(1)	63(1)
C(37)	7347(2)	1740(1)	4441(1)	56(1)
C(38)	7164(1)	2448(1)	3730(1)	41(1)
C(39)	7314(1)	3252(1)	4193(1)	45(1)

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

O(1)-C(2)	1.4110(16)
O(1)-C(1)	1.4840(14)
C(1)-C(2)	1.4934(17)
C(1)-C(21)	1.4956(17)
C(1)-C(11)	1.5018(17)
C(2)-N(31)	1.4307(16)
C(11)-C(16)	1.3945(17)
C(11)-C(12)	1.4007(17)
C(12)-C(13)	1.3895(18)
C(13)-C(14)	1.3853(19)
C(14)-C(15)	1.3877(19)
C(15)-C(16)	1.3890(19)
C(21)-C(26)	1.3876(17)
C(21)-C(22)	1.3885(17)
C(22)-C(23)	1.3849(18)
C(23)-C(24)	1.385(2)
C(24)-C(25)	1.391(2)
C(24)-C(27)	1.512(2)
C(25)-C(26)	1.3780(17)
N(31)-N(32)	1.3679(15)
N(31)-C(38)	1.3766(17)
N(32)-N(33)	1.3022(16)
N(33)-C(39)	1.3804(18)
C(34)-C(35)	1.371(2)
C(34)-C(39)	1.404(2)
C(35)-C(36)	1.401(2)
C(36)-C(37)	1.374(2)
C(37)-C(38)	1.3971(19)
C(38)-C(39)	1.3907(18)
C(2)-O(1)-C(1)	62.05(7)
O(1)-C(1)-C(2)	56.57(7)
O(1)-C(1)-C(21)	115.07(10)
C(2)-C(1)-C(21)	119.21(11)
O(1)-C(1)-C(11)	112.89(9)
C(2)-C(1)-C(11)	117.85(10)

C(21)-C(1)-C(11)	118.99(10)
O(1)-C(2)-N(31)	114.29(10)
O(1)-C(2)-C(1)	61.38(8)
N(31)-C(2)-C(1)	122.99(11)
C(16)-C(11)-C(12)	118.64(12)
C(16)-C(11)-C(1)	120.05(11)
C(12)-C(11)-C(1)	121.30(11)
C(13)-C(12)-C(11)	120.76(12)
C(14)-C(13)-C(12)	120.00(12)
C(13)-C(14)-C(15)	119.71(13)
C(14)-C(15)-C(16)	120.54(12)
C(15)-C(16)-C(11)	120.35(12)
C(26)-C(21)-C(22)	118.75(12)
C(26)-C(21)-C(1)	120.40(11)
C(22)-C(21)-C(1)	120.83(11)
C(23)-C(22)-C(21)	120.61(13)
C(22)-C(23)-C(24)	120.96(13)
C(23)-C(24)-C(25)	117.86(12)
C(23)-C(24)-C(27)	121.35(15)
C(25)-C(24)-C(27)	120.79(15)
C(26)-C(25)-C(24)	121.62(14)
C(25)-C(26)-C(21)	120.16(13)
N(32)-N(31)-C(38)	110.06(11)
N(32)-N(31)-C(2)	117.71(11)
C(38)-N(31)-C(2)	132.22(11)
N(33)-N(32)-N(31)	108.82(11)
N(32)-N(33)-C(39)	108.18(12)
C(35)-C(34)-C(39)	117.17(14)
C(34)-C(35)-C(36)	121.03(15)
C(37)-C(36)-C(35)	122.80(15)
C(36)-C(37)-C(38)	116.11(14)
N(31)-C(38)-C(39)	103.58(11)
N(31)-C(38)-C(37)	134.63(13)
C(39)-C(38)-C(37)	121.79(13)
N(33)-C(39)-C(38)	109.36(12)
N(33)-C(39)-C(34)	129.55(14)
C(38)-C(39)-C(34)	121.09(13)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2g. 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
O(1)	40(1)	48(1)	49(1)	0(1)	20(1)	-6(1)
C(1)	32(1)	39(1)	41(1)	3(1)	14(1)	-3(1)
C(2)	36(1)	46(1)	43(1)	2(1)	15(1)	2(1)
C(11)	35(1)	36(1)	37(1)	6(1)	12(1)	1(1)
C(12)	35(1)	47(1)	44(1)	1(1)	12(1)	-1(1)
C(13)	48(1)	53(1)	47(1)	2(1)	23(1)	0(1)
C(14)	60(1)	47(1)	36(1)	2(1)	15(1)	-2(1)
C(15)	45(1)	48(1)	39(1)	5(1)	6(1)	-6(1)
C(16)	35(1)	45(1)	42(1)	5(1)	11(1)	-1(1)
C(21)	36(1)	39(1)	34(1)	-3(1)	14(1)	1(1)
C(22)	43(1)	42(1)	48(1)	0(1)	17(1)	-3(1)
C(23)	43(1)	65(1)	48(1)	-18(1)	16(1)	-11(1)
C(24)	42(1)	78(1)	35(1)	-13(1)	9(1)	9(1)
C(25)	60(1)	57(1)	43(1)	6(1)	13(1)	18(1)
C(26)	51(1)	38(1)	43(1)	-1(1)	14(1)	2(1)
C(27)	55(1)	140(2)	51(1)	-16(1)	-2(1)	17(1)
N(31)	40(1)	40(1)	51(1)	4(1)	19(1)	6(1)
N(32)	48(1)	43(1)	65(1)	7(1)	17(1)	8(1)
N(33)	52(1)	46(1)	70(1)	-2(1)	17(1)	7(1)
C(34)	40(1)	64(1)	69(1)	-22(1)	23(1)	-3(1)
C(35)	52(1)	87(1)	51(1)	-12(1)	29(1)	-3(1)
C(36)	77(1)	68(1)	56(1)	6(1)	38(1)	-4(1)
C(37)	75(1)	48(1)	56(1)	1(1)	36(1)	-3(1)
C(38)	35(1)	45(1)	48(1)	-2(1)	21(1)	1(1)
C(39)	31(1)	48(1)	60(1)	-3(1)	19(1)	3(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2g.

	x	y	z	U(eq)
H(2A)	5812	2224	798	50
H(12A)	9687	1142	479	51
H(13A)	9392	669	-1407	57
H(14A)	7016	283	-2721	57
H(15A)	4936	378	-2145	56
H(16A)	5215	856	-265	50
H(22A)	9834	2507	2310	53
H(23A)	12196	2402	3780	62
H(25A)	11256	40	4445	66
H(26A)	8919	129	2956	54
H(27A)	14168	1587	5127	132
H(27B)	13984	592	5105	132
H(27C)	13446	1144	5977	132
H(34A)	7754	3934	5723	68
H(35A)	8064	2758	6925	72
H(36A)	7830	1419	6136	76
H(37A)	7241	1189	4126	67

Table 6. Crystal data and structure refinement for 5d.

Identification code	3a	
Empirical formula	C ₂₆ H ₂₆ N ₄ O	
Formula weight	410.51	
Temperature	168(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 18.030(8) Å	α = 90°.
	b = 14.919(6) Å	β = 112.282(7)°.
	c = 17.376(8) Å	γ = 90°.
Volume	4325(3) Å ³	
Z	8	
Density (calculated)	1.261 Mg/m ³	
Absorption coefficient	0.079 mm ⁻¹	
F(000)	1744	
Crystal size	0.78 x 0.59 x 0.42 mm ³	
Theta range for data collection	2.36 to 24.00°.	
Index ranges	-20 ≤ h ≤ 20, -16 ≤ k ≤ 8, -19 ≤ l ≤ 18	
Reflections collected	13016	
Independent reflections	6440 [R(int) = 0.0287]	
Completeness to theta = 24.00°	95.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6440 / 0 / 565	
Goodness-of-fit on F ²	1.042	
Final R indices [I > 2σ(I)]	R1 = 0.0479, wR2 = 0.1081	
R indices (all data)	R1 = 0.0787, wR2 = 0.1180	
Largest diff. peak and hole	0.161 and -0.187 e.Å ⁻³	

Table 7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5d. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	3308(1)	4366(1)	2974(1)	40(1)
N(1)	1597(1)	3354(1)	1260(1)	36(1)
C(1)	2156(1)	3420(2)	2110(1)	31(1)
C(2)	2627(1)	4297(2)	2224(1)	32(1)
C(3)	3425(1)	4402(2)	2184(1)	34(1)
C(4)	3711(1)	5283(2)	1986(2)	40(1)
C(5)	3649(2)	5298(2)	1091(2)	46(1)
C(6)	4072(2)	4502(2)	892(2)	51(1)
C(7)	3778(2)	3623(2)	1108(2)	50(1)
C(8)	3857(1)	3612(2)	2010(2)	44(1)
C(11)	1796(1)	3365(1)	2769(1)	30(1)
C(12)	2254(1)	3029(2)	3548(2)	41(1)
C(13)	1961(2)	3045(2)	4180(2)	55(1)
C(14)	1218(2)	3402(2)	4039(2)	57(1)
C(15)	756(2)	3712(2)	3266(2)	49(1)
C(16)	1041(1)	3695(2)	2631(2)	38(1)
N(21)	2118(1)	5084(1)	2070(1)	30(1)
N(22)	1692(1)	5333(1)	1272(1)	35(1)
N(23)	1192(1)	5967(1)	1263(1)	41(1)
C(24)	871(1)	6734(2)	2389(2)	48(1)
C(25)	1078(2)	6735(2)	3224(2)	59(1)
C(26)	1691(2)	6180(2)	3753(2)	57(1)
C(27)	2102(2)	5591(2)	3456(2)	47(1)
C(28)	1879(1)	5576(2)	2599(2)	33(1)
C(29)	1285(1)	6133(2)	2075(2)	37(1)
C(31)	1057(1)	2647(2)	985(1)	31(1)
C(32)	1220(1)	1802(2)	1344(2)	40(1)
C(33)	685(2)	1102(2)	1041(2)	45(1)
C(34)	-20(2)	1230(2)	373(2)	47(1)
C(35)	-189(1)	2073(2)	11(2)	43(1)
C(36)	340(1)	2771(2)	310(1)	36(1)

O(1')	1817(1)	9385(1)	2570(1)	35(1)
N(1')	3784(1)	8505(1)	3899(1)	40(1)
C(1')	3044(1)	8448(1)	3181(1)	30(1)
C(2')	2644(1)	9361(1)	3055(1)	30(1)
C(3')	2090(1)	9645(2)	3451(1)	31(1)
C(4')	1861(1)	9016(2)	4001(1)	35(1)
C(5')	1010(1)	9201(2)	3936(2)	49(1)
C(6')	886(2)	10178(2)	4088(2)	56(1)
C(7')	1099(1)	10778(2)	3496(2)	50(1)
C(8')	1962(1)	10621(2)	3579(2)	40(1)
C(11')	3133(1)	8135(1)	2390(1)	29(1)
C(12')	2478(1)	7798(1)	1745(1)	33(1)
C(13')	2531(1)	7558(2)	1003(2)	42(1)
C(14')	3245(2)	7655(2)	895(2)	50(1)
C(15')	3901(2)	7971(2)	1537(2)	56(1)
C(16')	3854(1)	8210(2)	2283(2)	45(1)
N(21')	3104(1)	10049(1)	2856(1)	32(1)
N(22')	3704(1)	10462(1)	3489(1)	45(1)
N(23')	4121(1)	10949(1)	3179(2)	54(1)
C(24')	4052(2)	11213(2)	1733(2)	63(1)
C(25')	3617(2)	10983(2)	932(3)	77(1)
C(26')	2946(2)	10420(2)	714(2)	76(1)
C(27')	2695(2)	10053(2)	1296(2)	53(1)
C(28')	3147(1)	10279(2)	2111(2)	36(1)
C(29')	3800(2)	10857(2)	2332(2)	42(1)
C(31')	4202(1)	7762(2)	4324(1)	33(1)
C(32')	3970(1)	6897(2)	4053(2)	46(1)
C(33')	4389(2)	6182(2)	4513(2)	67(1)
C(34')	5043(2)	6311(2)	5235(2)	66(1)
C(35')	5281(1)	7168(2)	5502(2)	49(1)
C(36')	4866(1)	7892(2)	5052(2)	37(1)

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Table 8. Bond lengths [Å] and angles [°] for 5d.

O(1)-C(2)	1.416(3)
O(1)-C(3)	1.467(3)
N(1)-C(31)	1.391(3)
N(1)-C(1)	1.442(3)
C(1)-C(11)	1.517(3)
C(1)-C(2)	1.531(3)
C(2)-N(21)	1.452(3)
C(2)-C(3)	1.474(3)
C(3)-C(4)	1.499(3)
C(3)-C(8)	1.506(3)
C(4)-C(5)	1.517(3)
C(5)-C(6)	1.520(3)
C(6)-C(7)	1.514(3)
C(7)-C(8)	1.519(3)
C(11)-C(16)	1.381(3)
C(11)-C(12)	1.385(3)
C(12)-C(13)	1.387(3)
C(13)-C(14)	1.374(4)
C(14)-C(15)	1.366(4)
C(15)-C(16)	1.382(3)
N(21)-N(22)	1.358(2)
N(21)-C(28)	1.367(3)
N(22)-N(23)	1.302(2)
N(23)-C(29)	1.378(3)
C(24)-C(25)	1.354(4)
C(24)-C(29)	1.403(3)
C(25)-C(26)	1.407(4)
C(26)-C(27)	1.371(3)
C(27)-C(28)	1.388(3)
C(28)-C(29)	1.389(3)
C(31)-C(32)	1.388(3)
C(31)-C(36)	1.391(3)
C(32)-C(33)	1.383(3)
C(33)-C(34)	1.371(3)
C(34)-C(35)	1.387(3)
C(35)-C(36)	1.375(3)

O(1')-C(2')	1.407(2)
O(1')-C(3')	1.471(3)
N(1')-C(31')	1.386(3)
N(1')-C(1')	1.442(3)
C(1')-C(11')	1.516(3)
C(1')-C(2')	1.519(3)
C(2')-N(21')	1.442(3)
C(2')-C(3')	1.473(3)
C(3')-C(8')	1.504(3)
C(3')-C(4')	1.506(3)
C(4')-C(5')	1.520(3)
C(5')-C(6')	1.513(4)
C(6')-C(7')	1.519(3)
C(7')-C(8')	1.527(3)
C(11')-C(12')	1.380(3)
C(11')-C(16')	1.385(3)
C(12')-C(13')	1.376(3)
C(13')-C(14')	1.376(3)
C(14')-C(15')	1.366(4)
C(15')-C(16')	1.379(3)
N(21')-N(22')	1.363(2)
N(21')-C(28')	1.369(3)
N(22')-N(23')	1.301(3)
N(23')-C(29')	1.369(3)
C(24')-C(25')	1.358(4)
C(24')-C(29')	1.388(4)
C(25')-C(26')	1.401(4)
C(26')-C(27')	1.370(4)
C(27')-C(28')	1.382(3)
C(28')-C(29')	1.391(3)
C(31')-C(32')	1.383(3)
C(31')-C(36')	1.386(3)
C(32')-C(33')	1.375(4)
C(33')-C(34')	1.370(4)
C(34')-C(35')	1.373(4)
C(35')-C(36')	1.376(3)

C(2)-O(1)-C(3)	61.47(13)
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C(31)-N(1)-C(1)	121.94(19)
N(1)-C(1)-C(11)	115.94(18)
N(1)-C(1)-C(2)	109.16(18)
C(11)-C(1)-C(2)	108.91(18)
O(1)-C(2)-N(21)	112.14(18)
O(1)-C(2)-C(3)	60.99(13)
N(21)-C(2)-C(3)	117.69(19)
O(1)-C(2)-C(1)	115.24(18)
N(21)-C(2)-C(1)	112.74(17)
C(3)-C(2)-C(1)	126.06(19)
O(1)-C(3)-C(2)	57.54(12)
O(1)-C(3)-C(4)	115.50(19)
C(2)-C(3)-C(4)	122.11(19)
O(1)-C(3)-C(8)	115.37(19)
C(2)-C(3)-C(8)	121.0(2)
C(4)-C(3)-C(8)	112.99(18)
C(3)-C(4)-C(5)	110.5(2)
C(4)-C(5)-C(6)	112.0(2)
C(7)-C(6)-C(5)	111.51(19)
C(6)-C(7)-C(8)	111.1(2)
C(3)-C(8)-C(7)	110.2(2)
C(16)-C(11)-C(12)	118.8(2)
C(16)-C(11)-C(1)	121.7(2)
C(12)-C(11)-C(1)	119.38(19)
C(11)-C(12)-C(13)	120.2(2)
C(14)-C(13)-C(12)	120.2(3)
C(15)-C(14)-C(13)	119.8(2)
C(14)-C(15)-C(16)	120.4(2)
C(11)-C(16)-C(15)	120.6(2)
N(22)-N(21)-C(28)	109.82(17)
N(22)-N(21)-C(2)	118.87(17)
C(28)-N(21)-C(2)	130.45(19)
N(23)-N(22)-N(21)	109.36(18)
N(22)-N(23)-C(29)	107.68(19)
C(25)-C(24)-C(29)	116.6(3)
C(24)-C(25)-C(26)	121.9(2)
C(27)-C(26)-C(25)	122.3(3)
C(26)-C(27)-C(28)	115.9(3)

N(21)-C(28)-C(27)	133.9(2)
N(21)-C(28)-C(29)	104.0(2)
C(27)-C(28)-C(29)	122.1(2)
N(23)-C(29)-C(28)	109.13(19)
N(23)-C(29)-C(24)	129.6(2)
C(28)-C(29)-C(24)	121.2(2)
C(32)-C(31)-C(36)	118.1(2)
C(32)-C(31)-N(1)	122.3(2)
C(36)-C(31)-N(1)	119.6(2)
C(33)-C(32)-C(31)	121.2(2)
C(34)-C(33)-C(32)	120.3(2)
C(33)-C(34)-C(35)	119.0(2)
C(36)-C(35)-C(34)	120.9(2)
C(35)-C(36)-C(31)	120.5(2)
C(2')-O(1')-C(3')	61.52(13)
C(31')-N(1')-C(1')	123.49(19)
N(1')-C(1')-C(11')	114.88(17)
N(1')-C(1')-C(2')	107.75(18)
C(11')-C(1')-C(2')	110.67(18)
O(1')-C(2')-N(21')	114.49(18)
O(1')-C(2')-C(3')	61.35(13)
N(21')-C(2')-C(3')	117.46(18)
O(1')-C(2')-C(1')	116.51(18)
N(21')-C(2')-C(1')	112.82(16)
C(3')-C(2')-C(1')	124.02(18)
O(1')-C(3')-C(2')	57.12(13)
O(1')-C(3')-C(8')	113.59(18)
C(2')-C(3')-C(8')	121.10(18)
O(1')-C(3')-C(4')	115.61(18)
C(2')-C(3')-C(4')	121.04(19)
C(8')-C(3')-C(4')	114.50(18)
C(3')-C(4')-C(5')	110.59(19)
C(6')-C(5')-C(4')	111.9(2)
C(5')-C(6')-C(7')	111.0(2)
C(6')-C(7')-C(8')	110.8(2)
C(3')-C(8')-C(7')	110.08(19)
C(12')-C(11')-C(16')	118.5(2)
C(12')-C(11')-C(1')	119.80(17)

C(16')-C(11')-C(1')	121.6(2)
C(13')-C(12')-C(11')	120.9(2)
C(14')-C(13')-C(12')	120.1(2)
C(15')-C(14')-C(13')	119.4(2)
C(14')-C(15')-C(16')	120.9(2)
C(15')-C(16')-C(11')	120.1(2)
N(22')-N(21')-C(28')	109.74(18)
N(22')-N(21')-C(2')	118.74(18)
C(28')-N(21')-C(2')	130.48(19)
N(23')-N(22')-N(21')	108.9(2)
N(22')-N(23')-C(29')	108.3(2)
C(25')-C(24')-C(29')	116.5(3)
C(24')-C(25')-C(26')	122.2(3)
C(27')-C(26')-C(25')	122.2(3)
C(26')-C(27')-C(28')	115.3(3)
N(21')-C(28')-C(27')	133.2(2)
N(21')-C(28')-C(29')	103.9(2)
C(27')-C(28')-C(29')	122.9(2)
N(23')-C(29')-C(24')	130.0(3)
N(23')-C(29')-C(28')	109.1(2)
C(24')-C(29')-C(28')	120.9(3)
C(32')-C(31')-N(1')	122.1(2)
C(32')-C(31')-C(36')	119.1(2)
N(1')-C(31')-C(36')	118.8(2)
C(33')-C(32')-C(31')	119.8(3)
C(34')-C(33')-C(32')	121.0(3)
C(33')-C(34')-C(35')	119.3(3)
C(34')-C(35')-C(36')	120.4(3)
C(35')-C(36')-C(31')	120.3(2)

Table 9. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5d. 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
O(1)	29(1)	58(1)	29(1)	2(1)	7(1)	0(1)
N(1)	46(1)	35(1)	24(1)	2(1)	8(1)	1(1)
C(1)	30(1)	37(1)	26(2)	3(1)	9(1)	5(1)
C(2)	25(1)	44(2)	22(2)	1(1)	5(1)	4(1)
C(3)	24(1)	48(2)	27(2)	5(1)	6(1)	4(1)
C(4)	32(1)	45(2)	44(2)	0(1)	15(1)	-3(1)
C(5)	51(2)	45(2)	50(2)	10(1)	26(1)	3(1)
C(6)	54(2)	55(2)	53(2)	7(1)	32(2)	8(1)
C(7)	55(2)	47(2)	57(2)	4(1)	33(2)	13(1)
C(8)	34(1)	49(2)	53(2)	12(1)	20(1)	11(1)
C(11)	29(1)	30(1)	27(2)	0(1)	7(1)	-5(1)
C(12)	42(1)	41(2)	38(2)	3(1)	12(1)	-6(1)
C(13)	77(2)	56(2)	33(2)	3(1)	21(2)	-17(2)
C(14)	74(2)	60(2)	52(2)	-8(2)	43(2)	-20(2)
C(15)	49(2)	53(2)	55(2)	-12(2)	30(2)	-17(1)
C(16)	33(1)	44(2)	39(2)	-5(1)	15(1)	-6(1)
N(21)	26(1)	36(1)	26(1)	4(1)	9(1)	4(1)
N(22)	29(1)	37(1)	36(1)	4(1)	8(1)	4(1)
N(23)	33(1)	38(1)	50(2)	6(1)	12(1)	5(1)
C(24)	40(1)	36(2)	78(2)	-5(2)	32(2)	-4(1)
C(25)	64(2)	38(2)	96(3)	-19(2)	56(2)	-10(2)
C(26)	73(2)	55(2)	58(2)	-23(2)	43(2)	-20(2)
C(27)	52(2)	51(2)	44(2)	-4(1)	24(1)	-5(1)
C(28)	31(1)	32(1)	42(2)	-4(1)	20(1)	-7(1)
C(29)	30(1)	30(1)	55(2)	-4(1)	21(1)	-5(1)
C(31)	35(1)	34(1)	26(2)	-4(1)	14(1)	2(1)
C(32)	46(1)	38(2)	33(2)	-1(1)	11(1)	4(1)
C(33)	56(2)	36(2)	45(2)	-2(1)	21(2)	-1(1)
C(34)	47(2)	45(2)	55(2)	-12(1)	26(2)	-9(1)
C(35)	31(1)	58(2)	39(2)	-8(1)	13(1)	4(1)
C(36)	37(1)	38(2)	34(2)	-1(1)	15(1)	6(1)
O(1')	30(1)	45(1)	27(1)	-2(1)	8(1)	2(1)
N(1')	36(1)	33(1)	36(1)	-4(1)	-1(1)	-1(1)

C(1')	26(1)	32(1)	30(2)	-2(1)	10(1)	-3(1)
C(2')	26(1)	35(1)	27(1)	0(1)	7(1)	-3(1)
C(3')	27(1)	37(1)	25(2)	-2(1)	6(1)	1(1)
C(4')	32(1)	41(1)	31(2)	-2(1)	12(1)	-3(1)
C(5')	37(1)	64(2)	53(2)	0(1)	25(1)	0(1)
C(6')	46(2)	79(2)	53(2)	-1(2)	28(1)	16(2)
C(7')	49(2)	51(2)	48(2)	-4(1)	16(1)	18(1)
C(8')	39(1)	41(2)	39(2)	1(1)	14(1)	6(1)
C(11')	26(1)	29(1)	30(2)	1(1)	11(1)	2(1)
C(12')	28(1)	34(1)	35(2)	-4(1)	12(1)	-4(1)
C(13')	43(1)	43(2)	37(2)	-7(1)	14(1)	-2(1)
C(14')	61(2)	55(2)	43(2)	-3(1)	30(2)	7(1)
C(15')	42(2)	83(2)	55(2)	-7(2)	31(2)	-2(2)
C(16')	28(1)	61(2)	47(2)	-7(1)	16(1)	-4(1)
N(21')	35(1)	32(1)	29(1)	-1(1)	11(1)	-3(1)
N(22')	48(1)	43(1)	39(1)	-3(1)	10(1)	-11(1)
N(23')	49(1)	46(1)	65(2)	11(1)	20(1)	-12(1)
C(24')	71(2)	50(2)	87(3)	20(2)	51(2)	6(2)
C(25')	121(3)	58(2)	85(3)	25(2)	74(3)	17(2)
C(26')	136(3)	56(2)	45(2)	8(2)	46(2)	7(2)
C(27')	82(2)	39(2)	39(2)	5(1)	25(2)	5(1)
C(28')	46(1)	33(1)	33(2)	5(1)	20(1)	6(1)
C(29')	45(2)	36(2)	53(2)	13(1)	26(1)	6(1)
C(31')	31(1)	41(2)	30(2)	6(1)	16(1)	8(1)
C(32')	46(2)	40(2)	46(2)	-2(1)	10(1)	12(1)
C(33')	83(2)	44(2)	62(2)	-3(2)	14(2)	20(2)
C(34')	78(2)	58(2)	59(2)	12(2)	21(2)	37(2)
C(35')	36(1)	73(2)	38(2)	11(2)	14(1)	14(1)
C(36')	29(1)	50(2)	33(2)	2(1)	14(1)	-2(1)

Table 10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5d.

	x	y	z	U(eq)
H(1)	1416(15)	3853(17)	1051(16)	55
H(1A)	2547	2915	2211	38
H(4A)	4276	5381	2363	48
H(4B)	3384	5774	2076	48
H(5A)	3889	5859	988	56
H(5B)	3077	5291	715	56
H(6A)	3976	4508	292	61
H(6B)	4657	4555	1208	61
H(7A)	4093	3123	1011	60
H(7B)	3209	3533	741	60
H(8A)	3628	3049	2126	53
H(8B)	4431	3635	2380	53
H(12A)	2770	2787	3651	50
H(13A)	2276	2809	4712	66
H(14A)	1027	3432	4478	68
H(15A)	235	3942	3163	59
H(16A)	714	3912	2095	46
H(24A)	466	7120	2035	58
H(25A)	802	7122	3460	70
H(26A)	1824	6215	4336	68
H(27A)	2515	5217	3815	57
H(32A)	1707	1702	1805	48
H(33A)	807	529	1297	54
H(34A)	-387	749	162	56
H(35A)	-677	2168	-451	51
H(36A)	214	3343	53	43
H(1')	3953(15)	8988(18)	4082(17)	59
H(1'A)	2687	8012	3312	36
H(4'A)	2236	9092	4585	42
H(4'B)	1901	8389	3835	42

H(5'A)	629	9028	3375	59
H(5'B)	893	8828	4348	59
H(6'A)	1225	10336	4669	68
H(6'B)	319	10277	4010	68
H(7'A)	1030	11414	3620	60
H(7'B)	731	10654	2917	60
H(8'A)	2077	10985	3161	48
H(8'B)	2335	10810	4138	48
H(12B)	1983	7730	1813	39
H(13B)	2075	7326	564	50
H(14B)	3281	7503	379	60
H(15B)	4397	8028	1468	68
H(16B)	4316	8426	2725	54
H(24B)	4504	11597	1877	76
H(25B)	3772	11211	505	93
H(26B)	2656	10290	143	91
H(27B)	2242	9669	1149	63
H(32B)	3523	6797	3550	55
H(33B)	4223	5589	4328	80
H(34B)	5328	5812	5548	79
H(35B)	5735	7262	6000	58
H(36B)	5035	8483	5241	44

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Table 11. Crystal data and structure refinement for 5e.

Identification code	3hw	
Empirical formula	C ₂₇ H ₂₁ N ₃ O ₂	
Formula weight	419.47	
Temperature	168(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.726(2) Å	α = 98.152(3)°.
	b = 13.433(3) Å	β = 94.144(3)°.
	c = 15.136(3) Å	γ = 108.549(3)°.
Volume	2219.8(8) Å ³	
Z	4	
Density (calculated)	1.255 Mg/m ³	
Absorption coefficient	0.081 mm ⁻¹	
F(000)	880	
Crystal size	0.76 x 0.51 x 0.26 mm ³	
Theta range for data collection	2.16 to 26.39°.	
Index ranges	-6 ≤ h ≤ 14, -16 ≤ k ≤ 13, -18 ≤ l ≤ 18	
Reflections collected	17724	
Independent reflections	8857 [R(int) = 0.0181]	
Completeness to theta = 26.39°	97.4 %	
Absorption correction	None	
Max. and min. transmission	0.9793 and 0.9413	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	8857 / 0 / 584	
Goodness-of-fit on F ²	0.931	
Final R indices [I > 2σ(I)]	R1 = 0.0362, wR2 = 0.0844	
R indices (all data)	R1 = 0.0586, wR2 = 0.0906	
Extinction coefficient	0.0039(5)	
Largest diff. peak and hole	0.215 and -0.180 e.Å ⁻³	

Table 12. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5e. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	5628(1)	1171(1)	4891(1)	35(1)
O(2)	8594(1)	855(1)	5404(1)	33(1)
C(1)	6893(1)	1569(1)	5165(1)	31(1)
C(2)	7388(1)	640(1)	5021(1)	29(1)
C(3)	7641(1)	63(1)	5745(1)	30(1)
C(11)	7506(1)	2387(1)	4611(1)	32(1)
C(12)	6957(1)	2433(1)	3783(1)	42(1)
C(13)	7573(2)	3147(1)	3258(1)	56(1)
C(14)	8735(2)	3802(1)	3555(1)	59(1)
C(15)	9294(1)	3766(1)	4377(1)	54(1)
C(16)	8675(1)	3070(1)	4909(1)	43(1)
N(21)	7153(1)	72(1)	4105(1)	28(1)
N(22)	6127(1)	-780(1)	3825(1)	32(1)
N(23)	6175(1)	-1221(1)	3011(1)	37(1)
C(24)	7766(1)	-832(1)	1949(1)	41(1)
C(25)	8891(1)	-151(1)	1891(1)	45(1)
C(26)	9520(1)	696(1)	2593(1)	44(1)
C(27)	9046(1)	885(1)	3378(1)	38(1)
C(28)	7900(1)	175(1)	3441(1)	30(1)
C(29)	7264(1)	-656(1)	2750(1)	32(1)
C(31)	7630(1)	-1067(1)	5500(1)	31(1)
C(32)	6766(1)	-1898(1)	5781(1)	46(1)
C(33)	6742(2)	-2939(1)	5534(1)	53(1)
C(34)	7581(1)	-3159(1)	5019(1)	46(1)
C(35)	8449(1)	-2338(1)	4750(1)	41(1)
C(36)	8472(1)	-1294(1)	4984(1)	36(1)
C(41)	7466(1)	420(1)	6698(1)	32(1)
C(42)	8474(1)	920(1)	7332(1)	41(1)
C(43)	8331(2)	1212(1)	8224(1)	49(1)
C(44)	7187(1)	1013(1)	8482(1)	46(1)
C(45)	6187(1)	530(1)	7850(1)	42(1)

C(46)	6316(1)	227(1)	6961(1)	35(1)
O(1')	515(1)	5466(1)	1067(1)	39(1)
O(2')	3601(1)	5724(1)	539(1)	30(1)
C(1')	1791(1)	5921(1)	1215(1)	31(1)
C(2')	2332(1)	5308(1)	532(1)	28(1)
C(3')	2840(1)	5686(1)	-280(1)	28(1)
C(11')	2264(1)	5859(1)	2155(1)	30(1)
C(12')	1663(1)	5024(1)	2578(1)	38(1)
C(13')	2156(1)	4917(1)	3403(1)	46(1)
C(14')	3248(1)	5648(1)	3817(1)	46(1)
C(15')	3850(1)	6485(1)	3406(1)	41(1)
C(16')	3359(1)	6593(1)	2578(1)	35(1)
N(21')	1911(1)	4161(1)	506(1)	29(1)
N(22')	911(1)	3520(1)	-55(1)	35(1)
N(23')	762(1)	2527(1)	3(1)	41(1)
C(24')	1931(1)	1649(1)	910(1)	46(1)
C(25')	2919(1)	1883(1)	1528(1)	51(1)
C(26')	3674(1)	2944(1)	1849(1)	46(1)
C(27')	3460(1)	3803(1)	1567(1)	37(1)
C(28')	2437(1)	3554(1)	935(1)	30(1)
C(29')	1686(1)	2513(1)	608(1)	35(1)
C(31')	2890(1)	4895(1)	-1071(1)	29(1)
C(32')	2144(1)	4741(1)	-1862(1)	47(1)
C(33')	2200(2)	4038(1)	-2603(1)	61(1)
C(34')	3007(1)	3483(1)	-2566(1)	51(1)
C(35')	3743(1)	3629(1)	-1781(1)	42(1)
C(36')	3684(1)	4324(1)	-1033(1)	35(1)
C(41')	2914(1)	6768(1)	-477(1)	30(1)
C(42')	4050(1)	7524(1)	-454(1)	41(1)
C(43')	4153(1)	8502(1)	-701(1)	51(1)
C(44')	3135(2)	8732(1)	-967(1)	50(1)
C(45')	2009(1)	7995(1)	-981(1)	44(1)
C(46')	1892(1)	7008(1)	-742(1)	37(1)

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Table 13. Bond lengths [Å] and angles [°] for 5e.

O(1)-C(1)	1.4146(14)
O(2)-C(2)	1.4131(14)
O(2)-C(3)	1.4594(15)
C(1)-C(11)	1.5076(18)
C(1)-C(2)	1.5306(16)
C(2)-N(21)	1.4455(16)
C(2)-C(3)	1.4936(17)
C(3)-C(41)	1.5037(17)
C(3)-C(31)	1.5064(17)
C(11)-C(16)	1.3844(18)
C(11)-C(12)	1.3856(18)
C(12)-C(13)	1.390(2)
C(13)-C(14)	1.368(2)
C(14)-C(15)	1.379(2)
C(15)-C(16)	1.385(2)
N(21)-N(22)	1.3610(14)
N(21)-C(28)	1.3737(15)
N(22)-N(23)	1.3013(14)
N(23)-C(29)	1.3808(16)
C(24)-C(25)	1.3625(19)
C(24)-C(29)	1.4080(18)
C(25)-C(26)	1.406(2)
C(26)-C(27)	1.3724(18)
C(27)-C(28)	1.3978(17)
C(28)-C(29)	1.3858(17)
C(31)-C(36)	1.3832(17)
C(31)-C(32)	1.3898(18)
C(32)-C(33)	1.3858(19)
C(33)-C(34)	1.376(2)
C(34)-C(35)	1.374(2)
C(35)-C(36)	1.3883(18)
C(41)-C(42)	1.3845(18)
C(41)-C(46)	1.3889(18)
C(42)-C(43)	1.390(2)
C(43)-C(44)	1.377(2)
C(44)-C(45)	1.375(2)

C(45)-C(46)	1.3820(18)
O(1')-C(1')	1.4116(14)
O(2')-C(2')	1.4123(14)
O(2')-C(3')	1.4592(14)
C(1')-C(11')	1.5117(17)
C(1')-C(2')	1.5279(16)
C(2')-N(21')	1.4540(15)
C(2')-C(3')	1.4877(17)
C(3')-C(41')	1.5018(17)
C(3')-C(31')	1.5024(17)
C(11')-C(16')	1.3880(17)
C(11')-C(12')	1.3896(18)
C(12')-C(13')	1.3832(19)
C(13')-C(14')	1.380(2)
C(14')-C(15')	1.380(2)
C(15')-C(16')	1.3879(18)
N(21')-N(22')	1.3579(14)
N(21')-C(28')	1.3704(15)
N(22')-N(23')	1.3059(14)
N(23')-C(29')	1.3734(16)
C(24')-C(25')	1.359(2)
C(24')-C(29')	1.4084(18)
C(25')-C(26')	1.410(2)
C(26')-C(27')	1.3729(18)
C(27')-C(28')	1.3986(17)
C(28')-C(29')	1.3906(18)
C(31')-C(32')	1.3803(18)
C(31')-C(36')	1.3844(17)
C(32')-C(33')	1.3809(19)
C(33')-C(34')	1.380(2)
C(34')-C(35')	1.368(2)
C(35')-C(36')	1.3825(18)
C(41')-C(46')	1.3842(17)
C(41')-C(42')	1.3890(18)
C(42')-C(43')	1.3872(19)
C(43')-C(44')	1.373(2)
C(44')-C(45')	1.372(2)
C(45')-C(46')	1.3912(18)

C(2)-O(2)-C(3)	62.63(8)
O(1)-C(1)-C(11)	110.09(10)
O(1)-C(1)-C(2)	108.56(10)
C(11)-C(1)-C(2)	109.06(10)
O(2)-C(2)-N(21)	112.17(9)
O(2)-C(2)-C(3)	60.20(7)
N(21)-C(2)-C(3)	117.20(10)
O(2)-C(2)-C(1)	116.15(10)
N(21)-C(2)-C(1)	114.36(10)
C(3)-C(2)-C(1)	124.32(10)
O(2)-C(3)-C(2)	57.16(7)
O(2)-C(3)-C(41)	113.40(10)
C(2)-C(3)-C(41)	120.00(10)
O(2)-C(3)-C(31)	114.67(10)
C(2)-C(3)-C(31)	119.56(10)
C(41)-C(3)-C(31)	116.91(10)
C(16)-C(11)-C(12)	118.86(13)
C(16)-C(11)-C(1)	119.42(12)
C(12)-C(11)-C(1)	121.62(12)
C(11)-C(12)-C(13)	120.56(14)
C(14)-C(13)-C(12)	119.84(15)
C(13)-C(14)-C(15)	120.29(15)
C(14)-C(15)-C(16)	119.97(15)
C(11)-C(16)-C(15)	120.45(14)
N(22)-N(21)-C(28)	109.65(10)
N(22)-N(21)-C(2)	120.56(10)
C(28)-N(21)-C(2)	129.35(10)
N(23)-N(22)-N(21)	109.30(10)
N(22)-N(23)-C(29)	107.87(10)
C(25)-C(24)-C(29)	116.92(13)
C(24)-C(25)-C(26)	121.69(13)
C(27)-C(26)-C(25)	122.37(13)
C(26)-C(27)-C(28)	115.76(13)
N(21)-C(28)-C(29)	104.04(11)
N(21)-C(28)-C(27)	133.47(12)
C(29)-C(28)-C(27)	122.49(12)
N(23)-C(29)-C(28)	109.13(11)

N(23)-C(29)-C(24)	130.08(12)
C(28)-C(29)-C(24)	120.76(12)
C(36)-C(31)-C(32)	118.99(12)
C(36)-C(31)-C(3)	120.50(12)
C(32)-C(31)-C(3)	120.50(11)
C(33)-C(32)-C(31)	120.26(13)
C(34)-C(33)-C(32)	120.37(15)
C(35)-C(34)-C(33)	119.65(13)
C(34)-C(35)-C(36)	120.43(13)
C(31)-C(36)-C(35)	120.28(13)
C(42)-C(41)-C(46)	119.36(12)
C(42)-C(41)-C(3)	119.21(11)
C(46)-C(41)-C(3)	121.39(11)
C(41)-C(42)-C(43)	120.04(14)
C(44)-C(43)-C(42)	120.27(14)
C(43)-C(44)-C(45)	119.66(14)
C(44)-C(45)-C(46)	120.68(14)
C(45)-C(46)-C(41)	119.98(13)
C(2')-O(2')-C(3')	62.38(7)
O(1')-C(1')-C(11')	110.48(10)
O(1')-C(1')-C(2')	108.93(10)
C(11')-C(1')-C(2')	109.17(9)
O(2')-C(2')-N(21')	111.93(9)
O(2')-C(2')-C(3')	60.35(7)
N(21')-C(2')-C(3')	116.41(10)
O(2')-C(2')-C(1')	115.98(10)
N(21')-C(2')-C(1')	114.24(10)
C(3')-C(2')-C(1')	125.41(10)
O(2')-C(3')-C(2')	57.27(7)
O(2')-C(3')-C(41')	113.55(10)
C(2')-C(3')-C(41')	121.34(10)
O(2')-C(3')-C(31')	114.79(9)
C(2')-C(3')-C(31')	120.02(10)
C(41')-C(3')-C(31')	115.40(10)
C(16')-C(11')-C(12')	119.02(12)
C(16')-C(11')-C(1')	120.10(12)
C(12')-C(11')-C(1')	120.68(12)
C(13')-C(12')-C(11')	120.50(13)

C(14')-C(13')-C(12')	120.08(14)
C(13')-C(14')-C(15')	119.99(13)
C(14')-C(15')-C(16')	120.04(13)
C(15')-C(16')-C(11')	120.35(13)
N(22')-N(21')-C(28')	109.89(10)
N(22')-N(21')-C(2')	120.59(9)
C(28')-N(21')-C(2')	129.32(10)
N(23')-N(22')-N(21')	109.10(9)
N(22')-N(23')-C(29')	107.97(10)
C(25')-C(24')-C(29')	117.06(13)
C(24')-C(25')-C(26')	121.59(13)
C(27')-C(26')-C(25')	122.73(13)
C(26')-C(27')-C(28')	115.28(13)
N(21')-C(28')-C(29')	103.90(11)
N(21')-C(28')-C(27')	133.32(12)
C(29')-C(28')-C(27')	122.78(11)
N(23')-C(29')-C(28')	109.14(11)
N(23')-C(29')-C(24')	130.29(13)
C(28')-C(29')-C(24')	120.57(12)
C(32')-C(31')-C(36')	118.86(12)
C(32')-C(31')-C(3')	119.61(11)
C(36')-C(31')-C(3')	121.52(11)
C(33')-C(32')-C(31')	120.32(13)
C(34')-C(33')-C(32')	120.56(14)
C(35')-C(34')-C(33')	119.24(13)
C(34')-C(35')-C(36')	120.60(12)
C(35')-C(36')-C(31')	120.40(12)
C(46')-C(41')-C(42')	119.09(12)
C(46')-C(41')-C(3')	122.06(11)
C(42')-C(41')-C(3')	118.69(11)
C(43')-C(42')-C(41')	120.21(13)
C(44')-C(43')-C(42')	120.36(14)
C(45')-C(44')-C(43')	119.82(14)
C(44')-C(45')-C(46')	120.45(13)
C(41')-C(46')-C(45')	120.07(13)

Table 14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5e. 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
O(1)	29(1)	42(1)	39(1)	11(1)	10(1)	13(1)
O(2)	28(1)	35(1)	36(1)	7(1)	4(1)	10(1)
C(1)	30(1)	31(1)	31(1)	4(1)	6(1)	11(1)
C(2)	25(1)	30(1)	30(1)	5(1)	4(1)	8(1)
C(3)	26(1)	32(1)	33(1)	8(1)	5(1)	10(1)
C(11)	34(1)	27(1)	38(1)	6(1)	10(1)	14(1)
C(12)	40(1)	45(1)	44(1)	15(1)	10(1)	13(1)
C(13)	59(1)	59(1)	57(1)	31(1)	18(1)	20(1)
C(14)	58(1)	51(1)	79(1)	34(1)	30(1)	17(1)
C(15)	38(1)	38(1)	82(1)	12(1)	17(1)	6(1)
C(16)	38(1)	35(1)	54(1)	6(1)	7(1)	11(1)
N(21)	28(1)	29(1)	29(1)	6(1)	5(1)	10(1)
N(22)	31(1)	29(1)	37(1)	5(1)	5(1)	10(1)
N(23)	39(1)	34(1)	36(1)	3(1)	7(1)	13(1)
C(24)	52(1)	43(1)	34(1)	5(1)	10(1)	22(1)
C(25)	53(1)	56(1)	36(1)	13(1)	18(1)	27(1)
C(26)	38(1)	55(1)	46(1)	20(1)	16(1)	17(1)
C(27)	35(1)	39(1)	39(1)	8(1)	7(1)	10(1)
C(28)	32(1)	33(1)	30(1)	10(1)	9(1)	16(1)
C(29)	36(1)	33(1)	32(1)	6(1)	6(1)	17(1)
C(31)	31(1)	36(1)	28(1)	6(1)	0(1)	15(1)
C(32)	57(1)	41(1)	49(1)	17(1)	22(1)	24(1)
C(33)	74(1)	37(1)	56(1)	20(1)	24(1)	21(1)
C(34)	68(1)	39(1)	38(1)	6(1)	3(1)	29(1)
C(35)	42(1)	44(1)	39(1)	0(1)	2(1)	22(1)
C(36)	31(1)	38(1)	38(1)	3(1)	1(1)	12(1)
C(41)	39(1)	30(1)	30(1)	7(1)	4(1)	16(1)
C(42)	41(1)	41(1)	39(1)	4(1)	-1(1)	16(1)
C(43)	65(1)	42(1)	37(1)	-1(1)	-11(1)	20(1)
C(44)	74(1)	39(1)	32(1)	7(1)	9(1)	29(1)
C(45)	56(1)	41(1)	38(1)	14(1)	16(1)	25(1)
C(46)	39(1)	37(1)	34(1)	10(1)	5(1)	17(1)
O(1')	32(1)	45(1)	47(1)	16(1)	6(1)	20(1)

O(2')	28(1)	32(1)	33(1)	8(1)	3(1)	11(1)
C(1')	32(1)	28(1)	37(1)	10(1)	7(1)	13(1)
C(2')	27(1)	27(1)	31(1)	7(1)	2(1)	11(1)
C(3')	28(1)	30(1)	29(1)	8(1)	3(1)	12(1)
C(11')	35(1)	31(1)	30(1)	7(1)	10(1)	18(1)
C(12')	35(1)	44(1)	39(1)	14(1)	10(1)	14(1)
C(13')	50(1)	53(1)	42(1)	24(1)	14(1)	20(1)
C(14')	56(1)	57(1)	31(1)	11(1)	3(1)	27(1)
C(15')	45(1)	39(1)	38(1)	0(1)	0(1)	17(1)
C(16')	42(1)	30(1)	35(1)	6(1)	8(1)	15(1)
N(21')	29(1)	26(1)	33(1)	9(1)	3(1)	11(1)
N(22')	32(1)	31(1)	41(1)	6(1)	-1(1)	11(1)
N(23')	38(1)	31(1)	52(1)	7(1)	0(1)	10(1)
C(24')	53(1)	31(1)	59(1)	15(1)	12(1)	17(1)
C(25')	62(1)	44(1)	60(1)	25(1)	12(1)	30(1)
C(26')	48(1)	52(1)	48(1)	18(1)	2(1)	26(1)
C(27')	37(1)	37(1)	40(1)	11(1)	3(1)	15(1)
C(28')	32(1)	30(1)	33(1)	12(1)	10(1)	15(1)
C(29')	36(1)	30(1)	41(1)	9(1)	7(1)	13(1)
C(31')	32(1)	26(1)	32(1)	8(1)	8(1)	10(1)
C(32')	66(1)	52(1)	36(1)	4(1)	-1(1)	39(1)
C(33')	89(1)	70(1)	35(1)	-4(1)	-10(1)	54(1)
C(34')	72(1)	48(1)	39(1)	-3(1)	5(1)	34(1)
C(35')	40(1)	38(1)	49(1)	-1(1)	5(1)	21(1)
C(36')	30(1)	34(1)	41(1)	2(1)	-1(1)	12(1)
C(41')	38(1)	29(1)	26(1)	7(1)	9(1)	14(1)
C(42')	41(1)	36(1)	51(1)	14(1)	14(1)	16(1)
C(43')	58(1)	35(1)	64(1)	19(1)	25(1)	13(1)
C(44')	75(1)	36(1)	51(1)	21(1)	23(1)	26(1)
C(45')	60(1)	43(1)	41(1)	17(1)	10(1)	30(1)
C(46')	42(1)	37(1)	36(1)	12(1)	9(1)	18(1)

Table 15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5e.

	x	y	z	U(eq)
H(1)	5226(13)	1086(12)	5369(10)	53
H(1A)	7056	1901	5816	37
H(12A)	6153	1972	3573	51
H(13A)	7187	3179	2694	67
H(14A)	9160	4285	3192	71
H(15A)	10104	4219	4579	64
H(16A)	9054	3061	5483	51
H(24A)	7340	-1400	1471	50
H(25A)	9260	-251	1362	54
H(26A)	10300	1154	2521	53
H(27A)	9471	1461	3848	45
H(32A)	6191	-1752	6144	55
H(33A)	6142	-3505	5722	63
H(34A)	7560	-3873	4850	55
H(35A)	9036	-2487	4402	49
H(36A)	9068	-733	4788	43
H(42A)	9265	1063	7157	49
H(43A)	9024	1551	8659	59
H(44A)	7091	1208	9093	55
H(45A)	5398	402	8025	50
H(46A)	5619	-113	6531	42
H(1')	217(14)	5845(12)	767(10)	58
H(1'A)	2034	6684	1136	37
H(12B)	908	4522	2298	46
H(13B)	1742	4340	3685	55
H(14B)	3584	5574	4384	55
H(15B)	4602	6987	3691	49
H(16B)	3774	7171	2298	42
H(24B)	1427	933	691	55
H(25B)	3106	1319	1750	61

H(26B)	4359	3070	2278	55
H(27B)	3971	4516	1785	44
H(32B)	1588	5122	-1897	57
H(33B)	1680	3934	-3144	73
H(34B)	3049	3004	-3078	61
H(35B)	4300	3250	-1750	50
H(36B)	4191	4411	-490	42
H(42B)	4758	7371	-268	49
H(43B)	4933	9014	-686	61
H(44B)	3210	9401	-1140	60
H(45B)	1304	8160	-1155	53
H(46B)	1109	6498	-761	44

Table 16. Crystal data and structure refinement for 5i.

Identification code	3hy	
Empirical formula	C23 H19 N3 O2	
Formula weight	369.41	
Temperature	168(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.756(3) Å	$\alpha = 77.049(4)^\circ$.
	b = 14.397(4) Å	$\beta = 76.607(4)^\circ$.
	c = 16.125(5) Å	$\gamma = 87.885(4)^\circ$.
Volume	1926.9(10) Å ³	
Z	4	
Density (calculated)	1.273 Mg/m ³	
Absorption coefficient	0.083 mm ⁻¹	
F(000)	776	
Crystal size	0.42 x 0.38 x 0.24 mm ³	
Theta range for data collection	2.18 to 26.47°.	
Index ranges	-10 ≤ h ≤ 10, -17 ≤ k ≤ 17, -20 ≤ l ≤ 20	
Reflections collected	25183	
Independent reflections	7738 [R(int) = 0.0307]	
Completeness to theta = 26.47°	97.4 %	
Absorption correction	None	
Max. and min. transmission	0.9803 and 0.9659	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7738 / 0 / 505	
Goodness-of-fit on F ²	0.868	
Final R indices [I > 2σ(I)]	R1 = 0.0355, wR2 = 0.0747	
R indices (all data)	R1 = 0.0683, wR2 = 0.0807	
Largest diff. peak and hole	0.154 and -0.169 e.Å ⁻³	

Table 17. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5i. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6931(1)	5277(1)	4117(1)	40(1)
O(2)	6082(1)	4198(1)	3062(1)	33(1)
C(1)	7958(2)	4804(1)	3764(1)	29(1)
C(2)	7477(1)	4009(1)	3379(1)	29(1)
C(3)	7553(1)	4144(1)	2426(1)	32(1)
C(11)	9651(1)	4963(1)	3698(1)	28(1)
C(12)	10813(2)	4388(1)	3333(1)	37(1)
C(13)	12376(2)	4550(1)	3316(1)	44(1)
C(14)	12781(2)	5296(1)	3639(1)	42(1)
C(15)	11638(2)	5890(1)	3974(1)	41(1)
C(16)	10073(2)	5716(1)	4016(1)	34(1)
N(21)	7529(1)	3080(1)	3940(1)	30(1)
N(22)	8707(1)	2441(1)	3759(1)	37(1)
N(23)	8592(1)	1739(1)	4443(1)	39(1)
C(24)	6766(2)	1395(1)	5943(1)	45(1)
C(25)	5508(2)	1766(1)	6438(1)	49(1)
C(26)	4806(2)	2627(1)	6107(1)	42(1)
C(27)	5356(2)	3153(1)	5271(1)	34(1)
C(28)	6652(1)	2773(1)	4778(1)	29(1)
C(29)	7344(2)	1917(1)	5092(1)	34(1)
C(31)	8192(2)	5096(1)	1880(1)	35(1)
C(32)	9629(2)	5148(1)	1280(1)	51(1)
C(33)	10272(2)	6039(2)	836(1)	67(1)
C(34)	9516(2)	6864(1)	982(1)	68(1)
C(35)	8082(2)	6820(1)	1557(1)	56(1)
C(36)	7417(2)	5935(1)	2005(1)	41(1)
C(41)	7626(2)	3309(1)	1996(1)	40(1)
C(42)	6532(2)	3444(1)	1363(1)	53(1)
O(1')	14378(1)	-17(1)	1546(1)	51(1)
O(2')	11901(1)	511(1)	766(1)	39(1)
C(1')	13604(2)	634(1)	1785(1)	36(1)

C(2')	12363(2)	1090(1)	1281(1)	34(1)
C(3')	10715(2)	732(1)	1491(1)	34(1)
C(11')	13798(2)	1006(1)	2547(1)	35(1)
C(12')	12663(2)	1557(1)	2963(1)	39(1)
C(13')	12813(2)	1798(1)	3729(1)	45(1)
C(14')	14108(2)	1504(1)	4078(1)	48(1)
C(15')	15264(2)	981(1)	3656(1)	48(1)
C(16')	15119(2)	730(1)	2895(1)	41(1)
N(21')	12785(1)	2057(1)	814(1)	35(1)
N(22')	12173(1)	2836(1)	1135(1)	42(1)
N(23')	12929(1)	3597(1)	640(1)	44(1)
C(24')	15169(2)	3868(1)	-703(1)	50(1)
C(25')	16121(2)	3383(1)	-1258(1)	58(1)
C(26')	16003(2)	2389(1)	-1152(1)	56(1)
C(27')	14941(2)	1836(1)	-475(1)	45(1)
C(28')	13983(2)	2335(1)	89(1)	34(1)
C(29')	14056(2)	3321(1)	-15(1)	38(1)
C(31')	10238(2)	-102(1)	2254(1)	33(1)
C(32')	10412(2)	-1032(1)	2146(1)	43(1)
C(33')	9915(2)	-1787(1)	2851(1)	51(1)
C(34')	9269(2)	-1614(1)	3667(1)	50(1)
C(35')	9094(2)	-688(1)	3783(1)	47(1)
C(36')	9564(2)	66(1)	3079(1)	39(1)
C(41')	9396(2)	1343(1)	1218(1)	40(1)
C(42')	8441(2)	829(1)	769(1)	53(1)

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Table 18. Bond lengths [Å] and angles [°] for 5i.

O(1)-C(1)	1.2198(14)
O(2)-C(2)	1.4254(14)
O(2)-C(3)	1.4604(14)
C(1)-C(11)	1.4844(17)
C(1)-C(2)	1.5317(18)
C(2)-N(21)	1.4426(16)
C(2)-C(3)	1.4908(18)
C(3)-C(31)	1.5019(18)
C(3)-C(41)	1.5103(18)
C(11)-C(16)	1.3937(17)
C(11)-C(12)	1.3943(17)
C(12)-C(13)	1.3894(19)
C(13)-C(14)	1.3829(19)
C(14)-C(15)	1.3850(19)
C(15)-C(16)	1.3855(18)
N(21)-C(28)	1.3735(15)
N(21)-N(22)	1.3807(14)
N(22)-N(23)	1.3056(14)
N(23)-C(29)	1.3878(16)
C(24)-C(25)	1.3702(19)
C(24)-C(29)	1.3958(18)
C(25)-C(26)	1.414(2)
C(26)-C(27)	1.3755(18)
C(27)-C(28)	1.3963(17)
C(28)-C(29)	1.3956(17)
C(31)-C(32)	1.3901(19)
C(31)-C(36)	1.3946(18)
C(32)-C(33)	1.390(2)
C(33)-C(34)	1.378(2)
C(34)-C(35)	1.371(2)
C(35)-C(36)	1.390(2)
C(41)-C(42)	1.5319(19)
O(1')-C(1')	1.2163(15)
O(2')-C(2')	1.4281(15)
O(2')-C(3')	1.4591(15)
C(1')-C(11')	1.4926(19)

C(1')-C(2')	1.5459(19)
C(2')-N(21')	1.4423(16)
C(2')-C(3')	1.4870(18)
C(3')-C(31')	1.5055(18)
C(3')-C(41')	1.5131(18)
C(11')-C(12')	1.3925(18)
C(11')-C(16')	1.4064(19)
C(12')-C(13')	1.3901(19)
C(13')-C(14')	1.392(2)
C(14')-C(15')	1.382(2)
C(15')-C(16')	1.386(2)
N(21')-C(28')	1.3703(16)
N(21')-N(22')	1.3790(15)
N(22')-N(23')	1.3010(15)
N(23')-C(29')	1.3866(17)
C(24')-C(25')	1.370(2)
C(24')-C(29')	1.4016(19)
C(25')-C(26')	1.408(2)
C(26')-C(27')	1.372(2)
C(27')-C(28')	1.3942(19)
C(28')-C(29')	1.3944(19)
C(31')-C(32')	1.3882(18)
C(31')-C(36')	1.3939(18)
C(32')-C(33')	1.3842(19)
C(33')-C(34')	1.380(2)
C(34')-C(35')	1.386(2)
C(35')-C(36')	1.3794(19)
C(41')-C(42')	1.5292(19)

C(2)-O(2)-C(3)	62.19(8)
O(1)-C(1)-C(11)	122.68(12)
O(1)-C(1)-C(2)	118.59(11)
C(11)-C(1)-C(2)	118.72(11)
O(2)-C(2)-N(21)	115.22(10)
O(2)-C(2)-C(3)	60.06(7)
N(21)-C(2)-C(3)	122.41(11)
O(2)-C(2)-C(1)	113.91(10)
N(21)-C(2)-C(1)	112.01(10)

C(3)-C(2)-C(1)	121.80(11)
O(2)-C(3)-C(2)	57.75(7)
O(2)-C(3)-C(31)	113.80(11)
C(2)-C(3)-C(31)	114.92(11)
O(2)-C(3)-C(41)	113.98(10)
C(2)-C(3)-C(41)	121.76(11)
C(31)-C(3)-C(41)	119.02(11)
C(16)-C(11)-C(12)	119.65(12)
C(16)-C(11)-C(1)	117.98(11)
C(12)-C(11)-C(1)	122.38(12)
C(13)-C(12)-C(11)	119.80(13)
C(14)-C(13)-C(12)	120.08(13)
C(13)-C(14)-C(15)	120.37(13)
C(14)-C(15)-C(16)	119.87(13)
C(15)-C(16)-C(11)	120.17(13)
C(28)-N(21)-N(22)	109.94(10)
C(28)-N(21)-C(2)	126.33(10)
N(22)-N(21)-C(2)	122.64(10)
N(23)-N(22)-N(21)	108.68(10)
N(22)-N(23)-C(29)	108.23(11)
C(25)-C(24)-C(29)	116.68(13)
C(24)-C(25)-C(26)	122.11(14)
C(27)-C(26)-C(25)	122.17(13)
C(26)-C(27)-C(28)	115.03(13)
N(21)-C(28)-C(29)	104.00(11)
N(21)-C(28)-C(27)	132.54(12)
C(29)-C(28)-C(27)	123.46(12)
N(23)-C(29)-C(24)	130.33(13)
N(23)-C(29)-C(28)	109.14(12)
C(24)-C(29)-C(28)	120.53(13)
C(32)-C(31)-C(36)	119.42(13)
C(32)-C(31)-C(3)	119.54(13)
C(36)-C(31)-C(3)	120.90(12)
C(31)-C(32)-C(33)	118.88(16)
C(34)-C(33)-C(32)	121.21(16)
C(35)-C(34)-C(33)	120.32(16)
C(34)-C(35)-C(36)	119.27(17)
C(35)-C(36)-C(31)	120.86(14)

C(3)-C(41)-C(42)	111.30(11)
C(2')-O(2')-C(3')	61.99(8)
O(1')-C(1')-C(11')	122.62(13)
O(1')-C(1')-C(2')	118.70(12)
C(11')-C(1')-C(2')	118.68(12)
O(2')-C(2')-N(21')	113.95(11)
O(2')-C(2')-C(3')	60.03(8)
N(21')-C(2')-C(3')	121.29(11)
O(2')-C(2')-C(1')	114.15(11)
N(21')-C(2')-C(1')	111.96(11)
C(3')-C(2')-C(1')	123.49(11)
O(2')-C(3')-C(2')	57.99(8)
O(2')-C(3')-C(31')	114.06(11)
C(2')-C(3')-C(31')	117.50(11)
O(2')-C(3')-C(41')	114.31(11)
C(2')-C(3')-C(41')	122.61(11)
C(31')-C(3')-C(41')	116.14(11)
C(12')-C(11')-C(16')	118.98(13)
C(12')-C(11')-C(1')	122.25(13)
C(16')-C(11')-C(1')	118.59(13)
C(13')-C(12')-C(11')	120.15(14)
C(12')-C(13')-C(14')	120.35(14)
C(15')-C(14')-C(13')	119.90(14)
C(14')-C(15')-C(16')	120.16(14)
C(15')-C(16')-C(11')	120.41(14)
C(28')-N(21')-N(22')	110.42(10)
C(28')-N(21')-C(2')	126.27(11)
N(22')-N(21')-C(2')	122.56(10)
N(23')-N(22')-N(21')	108.58(11)
N(22')-N(23')-C(29')	108.03(11)
C(25')-C(24')-C(29')	116.44(15)
C(24')-C(25')-C(26')	122.37(15)
C(27')-C(26')-C(25')	122.28(15)
C(26')-C(27')-C(28')	114.93(14)
N(21')-C(28')-C(29')	103.39(12)
N(21')-C(28')-C(27')	132.82(13)
C(29')-C(28')-C(27')	123.76(13)
N(23')-C(29')-C(28')	109.58(12)

N(23')-C(29')-C(24')	130.23(14)
C(28')-C(29')-C(24')	120.19(14)
C(32')-C(31')-C(36')	119.49(13)
C(32')-C(31')-C(3')	121.17(12)
C(36')-C(31')-C(3')	119.31(12)
C(33')-C(32')-C(31')	120.18(14)
C(34')-C(33')-C(32')	119.87(14)
C(33')-C(34')-C(35')	120.46(14)
C(36')-C(35')-C(34')	119.77(14)
C(35')-C(36')-C(31')	120.22(13)
C(3')-C(41')-C(42')	111.50(11)

Table 19. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5i. 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
O(1)	32(1)	42(1)	48(1)	-19(1)	-9(1)	8(1)
O(2)	23(1)	40(1)	39(1)	-9(1)	-9(1)	2(1)
C(1)	30(1)	28(1)	27(1)	-4(1)	-8(1)	4(1)
C(2)	19(1)	33(1)	35(1)	-8(1)	-6(1)	4(1)
C(3)	22(1)	40(1)	35(1)	-12(1)	-6(1)	3(1)
C(11)	29(1)	29(1)	26(1)	-3(1)	-8(1)	0(1)
C(12)	31(1)	37(1)	47(1)	-15(1)	-9(1)	-1(1)
C(13)	29(1)	45(1)	57(1)	-13(1)	-8(1)	1(1)
C(14)	30(1)	48(1)	46(1)	-4(1)	-12(1)	-8(1)
C(15)	44(1)	40(1)	42(1)	-9(1)	-14(1)	-11(1)
C(16)	36(1)	33(1)	34(1)	-7(1)	-8(1)	0(1)
N(21)	27(1)	28(1)	36(1)	-9(1)	-7(1)	3(1)
N(22)	30(1)	34(1)	46(1)	-12(1)	-8(1)	5(1)
N(23)	35(1)	34(1)	48(1)	-7(1)	-11(1)	3(1)
C(24)	49(1)	36(1)	48(1)	-1(1)	-13(1)	-1(1)
C(25)	54(1)	45(1)	41(1)	-1(1)	-2(1)	-9(1)
C(26)	40(1)	41(1)	42(1)	-13(1)	1(1)	-6(1)
C(27)	31(1)	32(1)	41(1)	-12(1)	-7(1)	-2(1)
C(28)	26(1)	29(1)	34(1)	-10(1)	-8(1)	-4(1)
C(29)	29(1)	32(1)	42(1)	-9(1)	-10(1)	-1(1)
C(31)	32(1)	44(1)	30(1)	-7(1)	-11(1)	-4(1)
C(32)	42(1)	70(1)	39(1)	-13(1)	-6(1)	-7(1)
C(33)	57(1)	97(2)	40(1)	-7(1)	-1(1)	-34(1)
C(34)	89(2)	68(1)	43(1)	8(1)	-23(1)	-38(1)
C(35)	79(1)	46(1)	47(1)	2(1)	-31(1)	-10(1)
C(36)	44(1)	43(1)	38(1)	-3(1)	-17(1)	-3(1)
C(41)	39(1)	44(1)	42(1)	-16(1)	-12(1)	2(1)
C(42)	56(1)	63(1)	53(1)	-27(1)	-24(1)	5(1)
O(1')	53(1)	51(1)	56(1)	-22(1)	-18(1)	17(1)
O(2')	41(1)	41(1)	35(1)	-14(1)	-5(1)	-1(1)
C(1')	35(1)	32(1)	36(1)	-6(1)	-2(1)	-2(1)
C(2')	39(1)	30(1)	33(1)	-8(1)	-5(1)	0(1)
C(3')	36(1)	34(1)	31(1)	-12(1)	-5(1)	3(1)

C(11')	31(1)	33(1)	37(1)	-4(1)	-5(1)	-5(1)
C(12')	35(1)	42(1)	41(1)	-9(1)	-9(1)	-1(1)
C(13')	37(1)	52(1)	48(1)	-18(1)	-6(1)	-1(1)
C(14')	43(1)	59(1)	49(1)	-19(1)	-12(1)	-11(1)
C(15')	35(1)	56(1)	58(1)	-13(1)	-18(1)	-6(1)
C(16')	32(1)	40(1)	49(1)	-10(1)	-7(1)	-3(1)
N(21')	37(1)	33(1)	34(1)	-8(1)	-5(1)	1(1)
N(22')	48(1)	35(1)	43(1)	-10(1)	-8(1)	3(1)
N(23')	52(1)	36(1)	46(1)	-7(1)	-16(1)	-1(1)
C(24')	45(1)	49(1)	52(1)	7(1)	-21(1)	-11(1)
C(25')	40(1)	74(1)	48(1)	9(1)	-8(1)	-8(1)
C(26')	40(1)	77(1)	45(1)	-7(1)	-2(1)	10(1)
C(27')	41(1)	50(1)	40(1)	-7(1)	-8(1)	7(1)
C(28')	31(1)	40(1)	31(1)	-4(1)	-10(1)	0(1)
C(29')	35(1)	42(1)	38(1)	-4(1)	-16(1)	-3(1)
C(31')	31(1)	32(1)	36(1)	-8(1)	-9(1)	2(1)
C(32')	52(1)	39(1)	40(1)	-13(1)	-11(1)	5(1)
C(33')	69(1)	31(1)	56(1)	-8(1)	-18(1)	1(1)
C(34')	54(1)	42(1)	48(1)	3(1)	-11(1)	-5(1)
C(35')	46(1)	49(1)	39(1)	-7(1)	-1(1)	-2(1)
C(36')	40(1)	34(1)	43(1)	-10(1)	-4(1)	0(1)
C(41')	41(1)	37(1)	40(1)	-6(1)	-10(1)	3(1)
C(42')	49(1)	56(1)	61(1)	-14(1)	-24(1)	3(1)

Table 20. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5i.

	x	y	z	U(eq)
H(12A)	10538	3887	3097	45
H(13A)	13166	4149	3083	52
H(14A)	13849	5402	3630	50
H(15A)	11926	6415	4175	49
H(16A)	9285	6111	4262	41
H(24A)	7223	812	6167	54
H(25A)	5093	1433	7023	59
H(26A)	3926	2849	6474	50
H(27A)	4888	3731	5045	41
H(32A)	10161	4584	1176	61
H(33A)	11251	6081	424	80
H(34A)	9990	7466	684	81
H(35A)	7548	7388	1648	67
H(36A)	6420	5900	2401	49
H(41A)	7321	2717	2451	48
H(41B)	8717	3238	1673	48
H(42A)	6600	2891	1096	80
H(42B)	6847	4021	905	80
H(42C)	5449	3506	1683	80
H(12B)	11784	1769	2723	47
H(13B)	12027	2166	4015	54
H(14B)	14197	1662	4607	58
H(15B)	16161	793	3886	58
H(16B)	15917	370	2608	49
H(24B)	15257	4540	-780	60
H(25B)	16890	3731	-1732	69
H(26B)	16682	2090	-1562	68
H(27B)	14864	1164	-398	53
H(32B)	10873	-1151	1586	52
H(33B)	10019	-2424	2774	62

H(34B)	8942	-2134	4152	60
H(35B)	8651	-573	4347	56
H(36B)	9427	701	3155	47
H(41C)	9841	1944	812	48
H(41D)	8696	1509	1739	48
H(42D)	7600	1243	599	80
H(42E)	7981	241	1173	80
H(42F)	9128	673	247	80

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