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Crystallographic Information. X-ray crystallographic data for **5a**, **5c**, **5d**, **5e**, and **7** were collected at room temperature on a Nonius KappaCCD diffractometer. Reflections were indexed and scaled using the Denzo-SMN software package (Otwinowski & Minor, 1997). The structure was solved with SHELXTL-PC (Sheldrick, 1990) and refined with SHELXL-93 (Sheldrick, 1993). Crystallographic data appear in Table 1. Hydrogen atoms were placed in calculated positions. Disorder was evident in one or more of the CO_2Et groups of **5a**, **5c**, **5e**, and **7**, but nothing was found that would call into question the stereochemistry of any of the materials.

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Otwinowski, Z. and Minor, W. (1997). *Methods of Enzymology*, Vol. 276: Macromolecular Crystallography, part A, edited by C. W. Carter, Jr. & R. M. Sweet pp.307-326. Academic Press.

Sheldrick, G. M. (1990). *SHELXTL-PC*, Release 4.1. Siemens Analytical Instruments, Inc., Madison, Wisconsin, USA

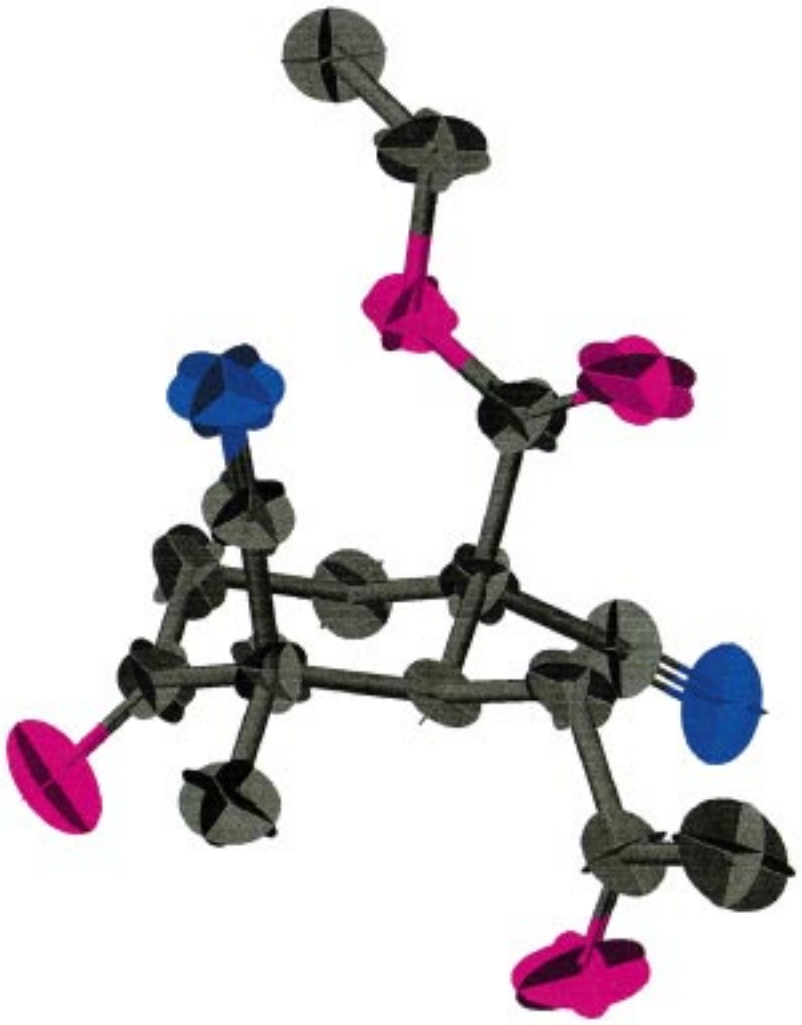
Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures.* University of Göttingen, Germany.

Table 1. Crystal data for **5a**, **5c**, **5d**, **5e**, and **7**.

	5a	**5c**	**5d**	**5e**	**7**
empirical formula	$C_{15}H_{18}N_2O_4$	$C_{17}H_{23}NO_6$	$C_{14}H_{16}N_2O_4$	$C_{16}H_{21}NO_6$	$C_{17}H_{23}NO_6$
fw	290.31	337.37	276.29	323.34	337.37
crystal system	triclinic	monoclinic	monoclinic	monoclinic	monoclinic
space group	*P*-1	$P2_1/n$	$P2_1/c$	$P2_1/n$	$P2_1/n$
a (Å)	7.6356(3)	14.363(9)	9.443(3)	9.8029(3)	12.073(4)
b (Å)	8.2260(3)	7.340(3)	10.795(3)	9.4637(3)	9.538(2)
c (Å)	12.8030(5)	17.147(1)	15.009(4)	18.7570(7)	15.908(5)
α (deg)	77.81(2)	90	90	90	90
β (deg)	75.73(2)	96.22(3)	100.53(3)	101.39(2)	107.30(3)
γ (deg)	88.45(3)	90	90	90	90
V (Å^3)	758.6(3)	1789.9(6)	1498.4(5)	1699.2(1)	1742.3(6)
Z	2	4	4	4	4
*D*calc(g/cm^3)	1.271	1.252	1.225	1.264	1.286
λ (Å)	0.7107	0.7107	0.7107	0.7107	0.7107
μ (mm^{-1})	0.093	0.095	0.091	0.097	0.095
temp (K)	295(2)	295(2)	295(2)	295(2)	295(2)
2θ range (deg)	8.0-50.0	6.0-50.0	5.6-50.0	6.2-50.0	8.0-55.8
$R(F_o^2)^a$	0.0513	0.0491	0.0424	0.0664	0.0541
$Rw(F_o^2)^b$	0.1384	0.1320	0.1079	0.1344	0.1482

$^aR = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $^bRw = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma wF_o^4]$–

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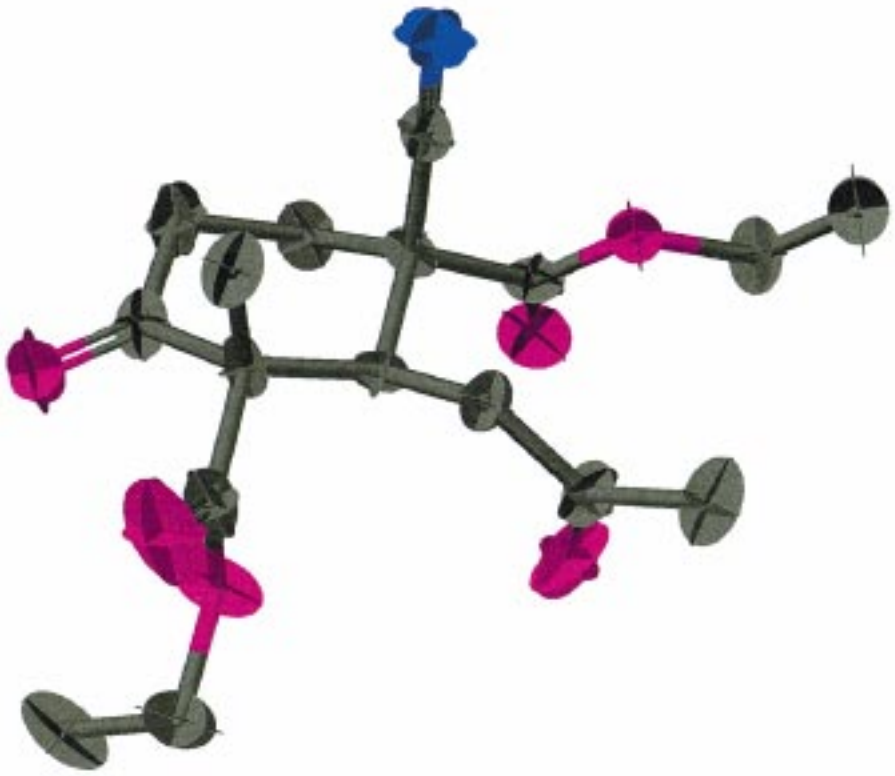
Thermal ellipsoid plot of **5a** (50% probability ellipsoids). Only the major conformer is shown.

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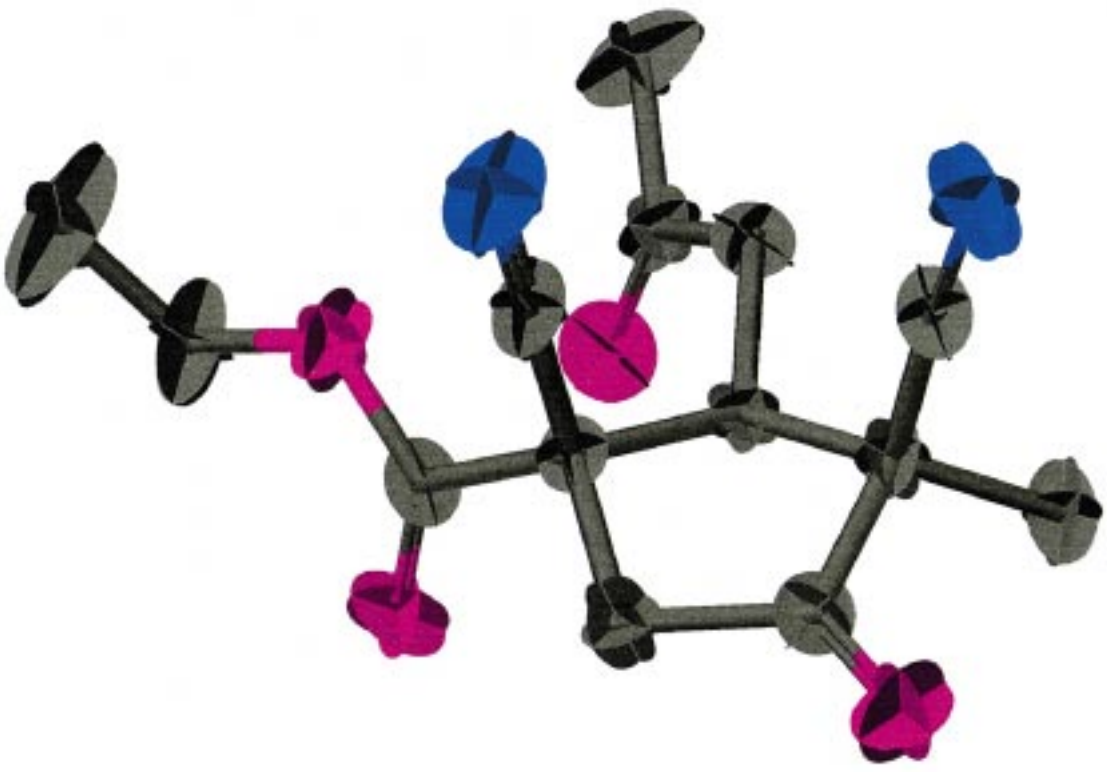
Thermal ellipsoid plot of **7** (50% probability ellipsoids). Only the major conformer is shown.

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Thermal ellipsoid plot of **5e** (50% probability ellipsoids). Only the major conformer is shown.

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Thermal ellipsoid plot of **5d** (50% probability ellipsoids).

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Thermal ellipsoid plot of **5e** (30% probability ellipsoids). Only the major conformer is shown.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5a**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(4)	2628(3)	-2670(2)	2955(2)	99(1)
O(11)	1147(3)	1604(2)	5348(1)	106(1)
N(8)	5749(3)	1666(3)	1102(2)	86(1)
N(9)	-2550(3)	3024(3)	3282(2)	91(1)
C(1)	460(3)	1850(2)	2249(2)	55(1)
C(2)	1622(2)	1404(2)	3121(2)	51(1)
C(3)	3206(3)	226(2)	2795(2)	57(1)
C(4)	2438(3)	-1277(2)	2475(2)	65(1)
C(5)	1438(3)	-864(3)	1600(2)	69(1)
C(6)	-121(3)	275(2)	1926(2)	63(1)
C(7)	4106(3)	-379(3)	3752(2)	78(1)
C(8)	4612(3)	1061(3)	1830(2)	62(1)
C(9)	-1221(3)	2559(3)	2817(2)	66(1)
C(10)	2226(3)	2928(2)	3468(2)	59(1)
C(11)	1963(3)	2755(3)	4689(2)	63(1)
C(12)	2789(5)	4079(3)	5046(2)	99(1)
C(13)	1353(3)	3239(3)	1262(2)	64(1)
O(13A)	1592(12)	4628(7)	1327(5)	121(2)
O(14A)	2090(7)	2708(10)	353(6)	76(1)
C(14A)	3156(7)	3900(5)	-600(3)	85(1)
C(15A)	3043(7)	3228(5)	-1594(3)	90(1)
O(13B)	1021(29)	4648(20)	1278(18)	116(7)
O(14B)	1582(29)	2689(32)	413(19)	76(1)
C(14B)	2285(17)	3918(19)	-592(12)	85(1)
C(15B)	3912(18)	3225(18)	-1317(12)	90(1)

Table 3. Bond lengths [A] and angles [deg] for **5a**.

O(4)-C(4)	1.205(2)
O(11)-C(11)	1.198(2)
N(8)-C(8)	1.140(3)
N(9)-C(9)	1.143(3)
C(1)-C(9)	1.480(3)
C(1)-C(13)	1.543(3)
C(1)-C(6)	1.548(3)
C(1)-C(2)	1.569(3)
C(2)-C(10)	1.533(3)
C(2)-C(3)	1.560(3)
C(2)-H(2)	0.980(2)
C(3)-C(8)	1.476(3)
C(3)-C(7)	1.536(3)
C(3)-C(4)	1.553(3)
C(4)-C(5)	1.483(3)
C(5)-C(6)	1.525(3)
C(5)-H(5A)	0.970(2)
C(5)-H(5B)	0.970(2)
C(6)-H(6A)	0.970(2)
C(6)-H(6B)	0.970(2)
C(7)-H(7A)	0.960(2)
C(7)-H(7B)	0.960(3)
C(7)-H(7C)	0.960(2)
C(10)-C(11)	1.502(3)
C(10)-H(10A)	0.970(2)
C(10)-H(10B)	0.970(2)
C(11)-C(12)	1.478(3)
C(12)-H(12A)	0.960(3)
C(12)-H(12B)	0.960(3)
C(12)-H(12C)	0.960(3)
C(13)-O(13B)	1.184(14)
C(13)-O(13A)	1.187(6)
C(13)-O(14B)	1.23(3)
C(13)-O(14A)	1.319(9)
O(14A)-C(14A)	1.472(4)
C(14A)-C(15A)	1.511(4)
C(14A)-H(14A)	0.970(5)
C(14A)-H(14B)	0.970(5)
C(15A)-H(15A)	0.960(4)
C(15A)-H(15B)	0.960(6)
C(15A)-H(15C)	0.960(4)
O(14B)-C(14B)	1.453(10)
C(14B)-C(15B)	1.530(5)
C(14B)-H(14C)	0.97(2)
C(14B)-H(14D)	0.97(2)
C(15B)-H(15D)	0.960(14)
C(15B)-H(15E)	0.96(2)
C(15B)-H(15F)	0.96(2)
C(9)-C(1)-C(13)	105.6(2)

C(9)-C(1)-C(6)	106.4(2)
C(13)-C(1)-C(6)	114.4(2)
C(9)-C(1)-C(2)	105.6(2)
C(13)-C(1)-C(2)	112.6(2)
C(6)-C(1)-C(2)	111.4(2)
C(10)-C(2)-C(3)	112.9(2)
C(10)-C(2)-C(1)	113.3(2)
C(3)-C(2)-C(1)	113.4(2)
C(10)-C(2)-H(2)	105.4(2)
C(3)-C(2)-H(2)	105.4(2)
C(1)-C(2)-H(2)	105.4(2)
C(8)-C(3)-C(7)	108.0(2)
C(8)-C(3)-C(4)	107.5(2)
C(7)-C(3)-C(4)	110.2(2)
C(8)-C(3)-C(2)	111.7(2)
C(7)-C(3)-C(2)	110.9(2)
C(4)-C(3)-C(2)	108.4(2)
O(4)-C(4)-C(5)	124.2(2)
O(4)-C(4)-C(3)	119.9(2)
C(5)-C(4)-C(3)	115.9(2)
C(4)-C(5)-C(6)	110.3(2)
C(4)-C(5)-H(5A)	109.6(2)
C(6)-C(5)-H(5A)	109.6(2)
C(4)-C(5)-H(5B)	109.6(2)
C(6)-C(5)-H(5B)	109.6(2)
H(5A)-C(5)-H(5B)	108.1(2)
C(5)-C(6)-C(1)	113.8(2)
C(5)-C(6)-H(6A)	108.8(2)
C(1)-C(6)-H(6A)	108.8(2)
C(5)-C(6)-H(6B)	108.8(2)
C(1)-C(6)-H(6B)	108.8(2)
H(6A)-C(6)-H(6B)	107.7(2)
C(3)-C(7)-H(7A)	109.5(2)
C(3)-C(7)-H(7B)	109.5(2)
H(7A)-C(7)-H(7B)	109.5(3)
C(3)-C(7)-H(7C)	109.5(2)
H(7A)-C(7)-H(7C)	109.5(2)
H(7B)-C(7)-H(7C)	109.5(2)
N(8)-C(8)-C(3)	177.2(2)
N(9)-C(9)-C(1)	176.4(2)
C(11)-C(10)-C(2)	114.8(2)
C(11)-C(10)-H(10A)	108.6(2)
C(2)-C(10)-H(10A)	108.6(2)
C(11)-C(10)-H(10B)	108.6(2)
C(2)-C(10)-H(10B)	108.6(2)
H(10A)-C(10)-H(10B)	107.5(2)
O(11)-C(11)-C(12)	121.0(2)
O(11)-C(11)-C(10)	122.6(2)
C(12)-C(11)-C(10)	116.4(2)
C(11)-C(12)-H(12A)	109.5(2)
C(11)-C(12)-H(12B)	109.5(2)
H(12A)-C(12)-H(12B)	109.5(3)
C(11)-C(12)-H(12C)	109.5(3)
H(12A)-C(12)-H(12C)	109.5(3)

H(12B)-C(12)-H(12C)	109.5(3)
O(13B)-C(13)-O(14B)	122(2)
O(13A)-C(13)-O(14A)	121.0(5)
O(13B)-C(13)-C(1)	120.3(11)
O(13A)-C(13)-C(1)	124.2(3)
O(14B)-C(13)-C(1)	108.2(9)
O(14A)-C(13)-C(1)	114.1(3)
C(13)-O(14A)-C(14A)	118.4(7)
O(14A)-C(14A)-C(15A)	105.0(5)
O(14A)-C(14A)-H(14A)	110.7(4)
C(15A)-C(14A)-H(14A)	110.7(5)
O(14A)-C(14A)-H(14B)	110.7(5)
C(15A)-C(14A)-H(14B)	110.7(4)
H(14A)-C(14A)-H(14B)	108.8(4)
C(14A)-C(15A)-H(15A)	109.5(4)
C(14A)-C(15A)-H(15B)	109.5(4)
H(15A)-C(15A)-H(15B)	109.5(5)
C(14A)-C(15A)-H(15C)	109.5(5)
H(15A)-C(15A)-H(15C)	109.5(4)
H(15B)-C(15A)-H(15C)	109.5(4)
C(13)-O(14B)-C(14B)	114(2)
O(14B)-C(14B)-C(15B)	110(2)
O(14B)-C(14B)-H(14C)	110(2)
C(15B)-C(14B)-H(14C)	109.7(13)
O(14B)-C(14B)-H(14D)	110(2)
C(15B)-C(14B)-H(14D)	109.7(14)
H(14C)-C(14B)-H(14D)	108.2(14)
C(14B)-C(15B)-H(15D)	109.5(11)
C(14B)-C(15B)-H(15E)	109.5(13)
H(15D)-C(15B)-H(15E)	110(2)
C(14B)-C(15B)-H(15F)	109.5(14)
H(15D)-C(15B)-H(15F)	109.5(14)
H(15E)-C(15B)-H(15F)	109.5(13)

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Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **5a**. 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
O(4)	126(2)	45(1)	121(2)	-3(1)	-32(1)	3(1)
O(11)	144(2)	99(1)	64(1)	-14(1)	1(1)	-64(1)
N(8)	69(1)	92(1)	82(1)	-4(1)	-2(1)	-13(1)
N(9)	73(1)	94(2)	111(2)	-39(1)	-19(1)	15(1)
C(1)	54(1)	51(1)	59(1)	-13(1)	-11(1)	0(1)
C(2)	53(1)	42(1)	54(1)	-5(1)	-8(1)	-8(1)
C(3)	55(1)	47(1)	62(1)	-2(1)	-11(1)	-3(1)
C(4)	64(1)	45(1)	76(1)	-10(1)	-2(1)	0(1)
C(5)	77(1)	52(1)	78(1)	-22(1)	-10(1)	-8(1)
C(6)	61(1)	59(1)	69(1)	-18(1)	-13(1)	-9(1)
C(7)	79(2)	74(1)	77(2)	2(1)	-24(1)	5(1)
C(8)	55(1)	58(1)	69(1)	-7(1)	-13(1)	-2(1)
C(9)	63(1)	63(1)	77(1)	-20(1)	-20(1)	4(1)
C(10)	63(1)	47(1)	65(1)	-7(1)	-14(1)	-11(1)
C(11)	68(1)	54(1)	66(1)	-12(1)	-13(1)	-12(1)
C(12)	150(3)	69(2)	90(2)	-16(1)	-48(2)	-28(2)
C(13)	78(1)	54(1)	63(1)	-9(1)	-23(1)	-3(1)
O(13A)	228(7)	60(3)	68(2)	-5(2)	-25(3)	-43(3)
O(14A)	92(4)	60(1)	64(1)	-7(1)	2(2)	-15(3)
C(14A)	96(4)	75(2)	69(2)	5(1)	-9(3)	-29(3)
C(15A)	98(4)	86(2)	76(2)	-12(2)	-9(2)	-2(2)
O(13B)	132(10)	36(7)	147(13)	-3(6)	6(7)	38(7)
O(14B)	92(4)	60(1)	64(1)	-7(1)	2(2)	-15(3)
C(14B)	96(4)	75(2)	69(2)	5(1)	-9(3)	-29(3)
C(15B)	98(4)	86(2)	76(2)	-12(2)	-9(2)	-2(2)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5a**.

	x	y	z	U(eq)
H(2)	804	761	3785	62
H(5A)	968	-1877	1484	83
H(5B)	2255	-318	914	83
H(6A)	-1023	-344	2543	75
H(6B)	-681	612	1314	75
H(7A)	3215	-927	4390	118
H(7B)	4629	554	3918	118
H(7C)	5037	-1143	3546	118
H(10A)	3499	3158	3114	71
H(10B)	1561	3878	3198	71
H(12A)	2540	3846	5836	149
H(12B)	2290	5128	4793	149
H(12C)	4074	4123	4742	149
H(14A)	4402	3965	-555	101
H(14B)	2650	4998	-636	101
H(15A)	3716	3953	-2252	134
H(15B)	1801	3165	-1621	134
H(15C)	3542	2139	-1541	134
H(14C)	2648	4924	-411	101
H(14D)	1350	4195	-990	101
H(15D)	4371	4038	-1981	134
H(15E)	3545	2235	-1499	134
H(15F)	4841	2967	-924	134

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Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5c**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O6	1.09795(11)	0.0345(2)	0.44926(9)	0.0697(5)
*O7A	1.1171(2)	-0.3659(4)	0.3486(3)	0.0828(9)
O8	1.17045(9)	-0.1027(2)	0.30549(11)	0.0732(6)
O12	1.04749(13)	-0.0478(3)	0.10318(9)	0.0798(7)
O14	0.94334(9)	0.3258(2)	0.14739(8)	0.0607(5)
O15	0.82582(9)	0.1267(2)	0.12344(7)	0.0523(4)
N17	0.74741(12)	0.0106(3)	0.28930(11)	0.0646(6)
C1	1.01471(12)	-0.1026(2)	0.33635(10)	0.0415(5)
C2	0.98313(11)	-0.0282(2)	0.25256(9)	0.0359(5)
C3	0.90840(11)	0.1263(2)	0.25119(9)	0.0365(5)
C4	0.94425(15)	0.2776(2)	0.30870(12)	0.0484(6)
C5	0.9682(2)	0.2086(3)	0.39185(12)	0.0557(7)
C6	1.03490(13)	0.0501(3)	0.39695(11)	0.0491(6)
C7	1.10642(14)	-0.2081(3)	0.33223(12)	0.0552(7)
*C8A	1.2662(2)	-0.1693(6)	0.3054(3)	0.0903(13)
*C9A	1.3276(2)	-0.0525(7)	0.3576(3)	0.120(2)
C10	0.9426(2)	-0.2274(3)	0.36951(13)	0.0528(7)
C11	0.95537(13)	-0.1831(2)	0.19463(10)	0.0414(6)
C12	0.98761(14)	-0.1575(3)	0.11445(11)	0.0503(6)
C13	0.9428(2)	-0.2762(4)	0.05031(15)	0.0715(9)
C14	0.89477(11)	0.2072(2)	0.16797(10)	0.0414(5)
C15	0.8063(2)	0.1937(4)	0.04316(13)	0.0731(10)
C16	0.7340(2)	0.0752(5)	0.0019(2)	0.0929(14)
C17	0.81721(12)	0.0587(2)	0.27161(10)	0.0425(6)
*O7B	1.139(3)	-0.312(6)	0.381(2)	0.0828(9)
*C8B	1.265(2)	-0.196(6)	0.349(3)	0.0903(13)
*C9B	1.321(2)	-0.077(7)	0.301(3)	0.120(2)

Starred Atom sites have a S.O.F. less than 1.0

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Table 7. Bond lengths [A] and angles [deg] for **5c**.

O6-C6	1.207(2)
O7A-C7	1.196(4)
O7B-C7	1.19(4)
O8-C7	1.320(3)
O8-C8B	1.63(4)
O8-C8A	1.458(3)
O12-C12	1.207(3)
O14-C14	1.191(2)
O15-C15	1.458(3)
O15-C14	1.321(2)
N17-C17	1.133(2)
C1-C6	1.532(3)
C1-C7	1.534(3)
C1-C10	1.535(3)
C1-C2	1.556(2)
C2-C3	1.558(2)
C2-C11	1.532(2)
C3-C4	1.534(2)
C3-C14	1.536(2)
C3-C17	1.476(2)
C4-C5	1.515(3)
C5-C6	1.502(3)
C8-C9A	1.462(6)
C8-C9B	1.49(6)
C1-C12	1.507(3)
C1-C13	1.491(3)
C1-C16	1.473(4)
C2-H2	0.933(18)
C4-H4A	0.96(2)
C4-H4B	0.96(2)
C5-H5A	0.96(2)
C5-H5B	1.04(2)
C10-H10A	0.99(3)
C10-H10B	0.94(3)
C10-H10C	0.97(3)
C11-H11A	0.95(2)
C11-H11B	0.93(2)
C13-H13A	0.87(5)
C13-H13B	1.01(4)
C13-H13C	0.95(4)
C15-H15A	0.96(3)
C15-H15B	0.96(3)
C16-H16A	0.97(3)
C16-H16B	0.97(4)
C16-H16C	0.99(4)
C7-O8-C8A	119.7(2)
C7-O8-C8B	99.9(14)
C14-O15-C15	116.69(17)
C2-C1-C6	112.54(13)
C2-C1-C7	107.44(14)

C2-C1-C10	114.18(15)
C6-C1-C7	107.41(15)
C6-C1-C10	105.68(15)
C7-C1-C10	109.40(16)
C1-C2-C3	113.57(13)
C1-C2-C11	111.52(13)
C3-C2-C11	113.51(13)
C2-C3-C4	109.48(14)
C2-C3-C14	108.23(13)
C2-C3-C17	112.24(13)
C4-C3-C14	108.45(13)
C4-C3-C17	109.55(14)
C14-C3-C17	108.81(13)
C3-C4-C5	112.83(14)
C4-C5-C6	113.02(18)
O6-C6-C1	120.31(18)
O6-C6-C5	122.53(19)
C1-C6-C5	116.95(16)
O7A-C7-O8	124.8(2)
O7A-C7-C1	124.4(2)
O8-C7-C1	110.69(17)
O7B-C7-O8	113(2)
O7B-C7-C1	124(2)
H10A-C10-H10C	107(2)
H10B-C10-H10C	108(2)
C2-C11-H11A	111.2(12)
C2-C11-H11B	113.8(13)
C12-C11-H11A	103.4(12)
C12-C11-H11B	106.4(12)
H11A-C11-H11B	106.8(18)
C12-C13-H13A	113(3)
C12-C13-H13B	109(2)
C12-C13-H13C	111(2)
H13A-C13-H13B	107(4)
H13A-C13-H13C	121(3)
O8-C8A-C9A	108.0(3)
O8-C8B-C9B	88(3)
C2-C11-C12	114.44(15)
O12-C12-C11	121.49(18)
C11-C12-C13	116.62(19)
O12-C12-C13	121.9(2)
O14-C14-O15	125.50(16)
O14-C14-C3	122.44(15)
O15-C14-C3	112.04(13)
O15-C15-C16	107.9(2)
N17-C17-C3	177.77(19)
C1-C2-H2	106.7(11)
C3-C2-H2	104.5(10)
C11-C2-H2	106.3(10)
C3-C4-H4A	106.7(13)
C3-C4-H4B	109.4(13)
C5-C4-H4A	111.6(13)
C5-C4-H4B	111.1(12)
H4A-C4-H4B	104.8(18)

C4-C5-H5A	108.3(15)
C4-C5-H5B	109.3(12)
C6-C5-H5A	108.4(14)
C6-C5-H5B	106.9(12)
H5A-C5-H5B	110.9(19)
C1-C10-H10A	111.4(17)
C1-C10-H10B	108.5(16)
C1-C10-H10C	112.8(16)
H10A-C10-H10B	109(2)
H13B-C13-H13C	94(3)
O15-C15-H15A	104.1(17)
O15-C15-H15B	107.6(15)
C16-C15-H15A	113.6(17)
C16-C15-H15B	108.3(16)
H15A-C15-H15B	115(2)
C15-C16-H16A	112(2)
C15-C16-H16B	109(2)
C15-C16-H16C	116.7(18)
H16A-C16-H16B	106(3)
H16A-C16-H16C	112(3)
H16B-C16-H16C	100(3)

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Table 8. Anisotropic displacement parameters (A^2 x 10^3) for **5c**. 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
O6	69(1)	80(1)	54(1)	-100(1)	-20(1)	1(1)
O7A	79(1)	52(1)	113(2)	12(1)	-9(1)	21(1)
O8	40(1)	72(1)	107(1)	6(1)	5(1)	11(1)
O12	92(1)	89(1)	64(1)	-6(1)	35(1)	-24(1)
O14	52(1)	62(1)	68(1)	24(1)	9(1)	-6(1)
O15	51(1)	61(1)	43(1)	3(1)	-4(1)	-3(1)
N17	44(1)	77(1)	76(1)	6(1)	17(1)	-6(1)
C1	43(1)	37(1)	43(1)	2(1)	-2(1)	1(1)
C2	34(1)	36(1)	38(1)	0(1)	4(1)	-3(1)
C3	33(1)	34(1)	42(1)	1(1)	3(1)	-2(1)
C4	53(1)	35(1)	55(1)	-5(1)	-3(1)	-2(1)
C5	69(1)	45(1)	50(1)	-15(1)	-4(1)	-1(1)
C6	53(1)	51(1)	42(1)	-1(1)	-3(1)	-7(1)
C7	54(1)	51(1)	58(1)	1(1)	-10(1)	9(1)
C8A	45(1)	106(2)	119(3)	-9(2)	4(2)	22(2)
C9A	50(0)	179(4)	124(4)	-10(3)	-22(2)	14(2)
C10	68(1)	44(1)	47(1)	6(1)	7(1)	-7(1)
C11	45(1)	37(1)	43(1)	-2(1)	5(1)	-0(1)
C12	61(1)	46(1)	45(1)	-0(1)	10(1)	7(1)
C13	110(2)	61(1)	44(1)	-7(1)	7(1)	2(1)
C14	36(1)	40(1)	48(1)	4(1)	6(1)	4(1)
C15	73(0)	102(0)	43(1)	10(1)	-2(1)	15(1)
C16	93(0)	114(0)	64(2)	-25(2)	-27(2)	32(2)
C17	39(1)	45(1)	43(1)	-1(1)	5(1)	1(1)
O7B	79(1)	52(1)	113(2)	12(1)	-9(1)	21(1)
C8B	45(1)	106(2)	119(3)	-9(2)	4(2)	22(2)
C9B	50(0)	179(4)	124(4)	-10(3)	-22(2)	14(2)

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Table 9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5c**.

	x	y	z	U(eq)
H2	1.0354(13)	0.028(2)	0.2351(10)	0.038(4)
H4A	0.9977(16)	0.331(3)	0.2884(12)	0.059(6)
H4B	0.8988(14)	0.374(3)	0.3069(12)	0.053(5)
H10B	0.9722(17)	-0.288(4)	0.4140(16)	0.080(8)
H10C	0.9169(18)	-0.319(4)	0.3319(16)	0.083(8)
H11A	0.9838(14)	-0.295(3)	0.2122(11)	0.051(5)
H11B	0.8914(14)	-0.204(3)	0.1866(11)	0.043(5)
H13A	0.950(3)	-0.235(5)	0.004(3)	0.140(14)
H13B	0.873(3)	-0.283(5)	0.054(2)	0.142(14)
H13C	0.953(3)	-0.401(6)	0.063(2)	0.135(13)
H15A	0.866(2)	0.187(4)	0.0224(17)	0.089(8)
H15B	0.7808(18)	0.315(4)	0.0457(15)	0.078(8)
H16A	0.714(2)	0.118(5)	-0.051(2)	0.123(11)
H16B	0.679(3)	0.078(6)	0.030(2)	0.141(15)
H16C	0.747(2)	-0.057(5)	0.0029(19)	0.111(11)
H5A	0.9966(17)	0.306(3)	0.4230(15)	0.077(7)
H5B	0.9073(16)	0.164(3)	0.4138(13)	0.066(6)
H10A	0.8890(18)	-0.157(4)	0.3851(15)	0.078(7)
*H81A	1.28470	-0.16510	0.25260	0.1080
*H82A	1.27050	-0.29450	0.32370	0.1080
*H91A	1.39120	-0.09390	0.35850	0.1800
*H92A	1.30890	-0.05800	0.40970	0.1800
*H93A	1.32310	0.07100	0.33890	0.1800
*H81B	1.27500	-0.17190	0.40500	0.1080
*H82B	1.27010	-0.32570	0.33840	0.1080
*H91B	1.38670	-0.10230	0.31370	0.1800
*H92B	1.30890	0.04850	0.31130	0.1800
*H93B	1.30390	-0.10200	0.24590	0.1800

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Table 10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5d**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	1876(1)	2311(1)	6414(1)	72(1)
O(7)	7241(1)	440(1)	4986(1)	65(1)
O(10)	6106(1)	-680(1)	6716(1)	62(1)
O(11)	7929(1)	656(1)	7105(1)	60(1)
N(9)	6906(2)	3298(1)	7722(1)	78(1)
N(14)	4373(2)	5011(1)	6110(1)	70(1)
C(1)	3104(2)	2111(1)	6362(1)	45(1)
C(2)	3879(2)	2700(1)	5638(1)	42(1)
C(3)	5247(1)	1896(1)	5702(1)	39(1)
C(4)	5609(2)	1505(1)	6726(1)	41(1)
C(5)	4117(2)	1264(2)	6956(1)	49(1)
C(6)	6465(2)	2456(2)	5307(1)	51(1)
C(7)	7505(2)	1533(2)	5036(1)	51(1)
C(8)	8864(3)	2058(4)	4808(2)	90(1)
C(9)	6344(2)	2513(1)	7289(1)	50(1)
C(10)	6563(2)	342(1)	6851(1)	44(1)
C(11)	9008(2)	-329(2)	7235(2)	78(1)
C(12)	10173(4)	76(5)	7954(3)	137(2)
C(13)	2909(2)	2709(2)	4698(1)	58(1)
C(14)	4198(2)	3998(1)	5914(1)	48(1)

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Table 11. Bond lengths [A] and angles [deg] for **5d**.

O(1)-C(1)	1.194(2)
O(7)-C(7)	1.204(2)
O(10)-C(10)	1.187(2)
O(11)-C(10)	1.319(2)
O(11)-C(11)	1.459(2)
N(9)-C(9)	1.137(2)
N(14)-C(14)	1.135(2)
C(1)-C(5)	1.492(2)
C(1)-C(2)	1.551(2)
C(2)-C(14)	1.476(2)
C(2)-C(13)	1.533(2)
C(2)-C(3)	1.542(2)
C(3)-C(6)	1.512(2)
C(3)-C(4)	1.568(2)
C(3)-H(3)	0.95(2)
C(4)-C(9)	1.470(2)
C(4)-C(5)	1.530(2)
C(4)-C(10)	1.534(2)
C(5)-H(5A)	0.96(2)
C(5)-H(5B)	0.93(2)
C(6)-C(7)	1.504(2)
C(6)-H(6A)	0.95(2)
C(6)-H(6B)	0.96(2)
C(7)-C(8)	1.496(3)
C(8)-H(8A)	0.90(3)
C(8)-H(8B)	0.95(4)
C(8)-H(8C)	0.96(4)
C(11)-C(12)	1.459(4)
C(11)-H(11A)	1.01(3)
C(11)-H(11B)	0.95(3)
C(12)-H(12A)	0.88(4)
C(12)-H(12B)	0.96(5)
C(12)-H(12C)	1.00(5)
C(13)-H(13A)	0.92(2)
C(13)-H(13B)	0.98(2)
C(13)-H(13C)	1.01(2)

C(10)-O(11)-C(11)	118.2(2)
O(1)-C(1)-C(5)	126.45(14)
O(1)-C(1)-C(2)	123.94(13)
C(5)-C(1)-C(2)	109.60(12)
C(14)-C(2)-C(13)	107.98(12)
C(14)-C(2)-C(3)	112.94(12)
C(13)-C(2)-C(3)	114.42(12)
C(14)-C(2)-C(1)	106.80(11)
C(13)-C(2)-C(1)	111.60(13)
C(3)-C(2)-C(1)	102.82(10)
C(6)-C(3)-C(2)	115.97(12)
C(6)-C(3)-C(4)	116.52(12)
C(2)-C(3)-C(4)	104.07(10)
C(6)-C(3)-H(3)	110.4(8)

C(2)-C(3)-H(3)	104.0(8)
C(4)-C(3)-H(3)	104.6(8)
C(9)-C(4)-C(5)	110.67(12)
C(9)-C(4)-C(10)	109.26(11)
C(5)-C(4)-C(10)	112.19(12)
C(9)-C(4)-C(3)	110.96(11)
C(5)-C(4)-C(3)	102.76(11)
C(10)-C(4)-C(3)	110.91(11)
C(1)-C(5)-C(4)	106.09(12)
C(1)-C(5)-H(5A)	107.5(11)
C(4)-C(5)-H(5A)	108.1(11)
C(1)-C(5)-H(5B)	111.6(11)
C(4)-C(5)-H(5B)	113.4(11)
H(5A)-C(5)-H(5B)	110(2)
C(7)-C(6)-C(3)	114.90(13)
C(7)-C(6)-H(6A)	105.2(11)
C(3)-C(6)-H(6A)	108.9(11)
C(7)-C(6)-H(6B)	110.3(11)
C(3)-C(6)-H(6B)	111.8(11)
H(6A)-C(6)-H(6B)	105(2)
O(7)-C(7)-C(8)	122.2(2)
O(7)-C(7)-C(6)	121.79(14)
C(8)-C(7)-C(6)	116.0(2)
C(7)-C(8)-H(8A)	111(2)
C(7)-C(8)-H(8B)	106(2)
H(8A)-C(8)-H(8B)	112(3)
C(7)-C(8)-H(8C)	111(2)
H(8A)-C(8)-H(8C)	115(3)
H(8B)-C(8)-H(8C)	101(3)
N(9)-C(9)-C(4)	179.6(2)
O(10)-C(10)-O(11)	126.35(13)
O(10)-C(10)-C(4)	123.39(14)
O(11)-C(10)-C(4)	110.25(12)
C(12)-C(11)-O(11)	107.1(2)
C(12)-C(11)-H(11A)	116(2)
O(11)-C(11)-H(11A)	109(2)
C(12)-C(11)-H(11B)	98(2)
O(11)-C(11)-H(11B)	106(2)
H(11A)-C(11)-H(11B)	119(3)
C(11)-C(12)-H(12A)	107(2)
C(11)-C(12)-H(12B)	91(3)
H(12A)-C(12)-H(12B)	110(4)
C(11)-C(12)-H(12C)	117(3)
H(12A)-C(12)-H(12C)	122(4)
H(12B)-C(12)-H(12C)	105(4)
C(2)-C(13)-H(13A)	108.1(13)
C(2)-C(13)-H(13B)	109.8(12)
H(13A)-C(13)-H(13B)	114(2)
C(2)-C(13)-H(13C)	109.8(11)
H(13A)-C(13)-H(13C)	106(2)
H(13B)-C(13)-H(13C)	109(2)
N(14)-C(14)-C(2)	176.6(2)

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Table 12. Anisotropic displacement parameters (A^2 x 10^3) for **5d**. 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
O(1)	48(1)	88(1)	81(1)	10(1)	15(1)	13(1)
O(7)	70(1)	61(1)	70(1)	-1(1)	25(1)	9(1)
O(10)	71(1)	38(1)	80(1)	2(1)	21(1)	5(1)
O(11)	50(1)	53(1)	72(1)	-3(1)	-4(1)	15(1)
N(9)	82(1)	61(1)	79(1)	-25(1)	-17(1)	12(1)
N(14)	107(1)	38(1)	60(1)	-2(1)	0(1)	5(1)
C(1)	44(1)	43(1)	49(1)	-4(1)	6(1)	2(1)
C(2)	47(1)	35(1)	40(1)	-1(1)	1(1)	3(1)
C(3)	45(1)	32(1)	39(1)	0(1)	5(1)	0(1)
C(4)	45(1)	36(1)	38(1)	0(1)	3(1)	3(1)
C(5)	52(1)	50(1)	48(1)	7(1)	15(1)	5(1)
C(6)	57(1)	46(1)	52(1)	6(1)	13(1)	-5(1)
C(7)	45(1)	68(1)	39(1)	1(1)	6(1)	-4(1)
C(8)	55(1)	129(2)	89(2)	-18(2)	23(1)	-23(1)
C(9)	54(1)	46(1)	47(1)	-5(1)	-3(1)	12(1)
C(10)	51(1)	42(1)	38(1)	3(1)	8(1)	7(1)
C(11)	63(1)	79(1)	88(2)	1(1)	1(1)	35(1)
C(12)	80(2)	144(3)	163(4)	-17(3)	-41(2)	51(2)
C(13)	63(1)	56(1)	47(1)	-3(1)	-7(1)	10(1)
C(14)	61(1)	40(1)	41(1)	3(1)	3(1)	7(1)

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Table 13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5d**.

	x	y	z	U(eq)
H(3)	4913(14)	1157(14)	5389(9)	38(3)
H(5A)	3842(20)	425(18)	6781(13)	69(5)
H(5B)	4082(18)	1382(16)	7563(13)	66(5)
H(6A)	6072(19)	2884(17)	4764(13)	69(5)
H(6B)	6973(20)	3075(18)	5696(13)	69(5)
H(8A)	9328(35)	1495(32)	4524(22)	140(12)
H(8B)	9422(34)	2322(28)	5371(24)	134(10)
H(8C)	8681(40)	2836(37)	4503(26)	168(16)
H(11A)	8527(31)	-1139(29)	7339(19)	125(10)
H(11B)	9503(36)	-266(29)	6739(22)	141(12)
H(12A)	10853(43)	-499(33)	8015(24)	154(12)
H(12B)	9581(60)	-38(51)	8402(37)	226(27)
H(12C)	10413(52)	982(53)	7973(34)	222(22)
H(13A)	2654(22)	1903(22)	4542(14)	84(6)
H(13B)	3402(21)	3129(19)	4263(15)	78(6)
H(13C)	1984(22)	3164(19)	4727(13)	77(5)

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Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5e**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	7794(2)	-1957(2)	6959(1)	69(1)
O(7)	2546(2)	752(2)	6831(1)	63(1)
O(9)	6427(2)	-3039(2)	8329(1)	59(1)
O(10)	5712(2)	-1998(2)	9263(1)	62(1)
O(12)	5420(2)	1333(2)	9017(1)	61(1)
O(13)	7585(2)	549(2)	9384(1)	83(1)
N(15)	4208(3)	-3235(2)	6587(1)	71(1)
C(1)	7115(2)	-1247(2)	7291(1)	46(1)
C(2)	5546(2)	-920(2)	7020(1)	40(1)
C(3)	5079(2)	-232(2)	7688(1)	36(1)
C(4)	6298(2)	-521(2)	8346(1)	40(1)
C(5)	7591(2)	-518(2)	8000(1)	45(1)
C(6)	3654(2)	-683(2)	7821(1)	42(1)
C(7)	2437(2)	-200(2)	7246(1)	44(1)
C(8)	1094(3)	-951(3)	7228(2)	66(1)
C(9)	6161(2)	-2003(2)	8642(1)	44(1)
C(10)	5645(3)	-3352(3)	9626(2)	69(1)
C(11)	6987(4)	-3683(4)	10092(2)	96(1)
C(12)	6347(2)	570(3)	8945(1)	50(1)
C(13A)	7666(7)	1559(12)	10000(4)	77(3)
C(14A)	9128(7)	1435(7)	10426(4)	96(2)
C(13B)	7623(22)	763(18)	10202(11)	77(3)
C(14B)	8448(23)	2131(19)	10158(12)	96(2)
C(13C)	8109(25)	1844(32)	9829(10)	77(3)
C(14C)	7868(19)	1191(18)	10537(8)	96(2)
C(15)	4805(2)	-2231(3)	6783(1)	45(1)
C(16)	5426(3)	80(3)	6363(1)	61(1)

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Table 15. Bond lengths [A] and angles [deg] for **5e**.

O(1)-C(1)	1.201(3)
O(7)-C(7)	1.207(3)
O(9)-C(9)	1.197(3)
O(10)-C(9)	1.321(3)
O(10)-C(10)	1.457(3)
O(12)-C(12)	1.187(3)
O(13)-C(12)	1.323(3)
O(13)-C(13A)	1.487(9)
O(13)-C(13C)	1.51(3)
O(13)-C(13B)	1.54(2)
N(15)-C(15)	1.137(3)
C(1)-C(5)	1.487(3)
C(1)-C(2)	1.550(3)
C(2)-C(15)	1.460(3)
C(2)-C(16)	1.538(3)
C(2)-C(3)	1.556(3)
C(3)-C(6)	1.525(3)
C(3)-C(4)	1.562(3)
C(3)-H(3)	0.980(2)
C(4)-C(12)	1.518(3)
C(4)-C(9)	1.522(3)
C(4)-C(5)	1.532(3)
C(5)-H(5A)	0.970(2)
C(5)-H(5B)	0.970(2)
C(6)-C(7)	1.510(3)
C(6)-H(6A)	0.970(2)
C(6)-H(6B)	0.970(2)
C(7)-C(8)	1.489(3)
C(8)-H(8A)	0.960(3)
C(8)-H(8B)	0.960(3)
C(8)-H(8C)	0.960(3)
C(10)-C(11)	1.460(4)
C(10)-H(10A)	0.970(3)
C(10)-H(10B)	0.970(3)
C(11)-H(11A)	0.960(3)
C(11)-H(11B)	0.960(4)
C(11)-H(11C)	0.960(4)
C(13A)-C(14A)	1.500(7)
C(13A)-H(13A)	0.970(9)
C(13A)-H(13B)	0.970(11)
C(14A)-H(14A)	0.960(6)
C(14A)-H(14B)	0.960(8)
C(14A)-H(14C)	0.960(7)
C(13B)-C(14B)	1.536(10)
C(13B)-H(13C)	0.97(2)
C(13B)-H(13D)	0.97(2)
C(14B)-H(14D)	0.96(2)
C(14B)-H(14E)	0.96(2)
C(14B)-H(14F)	0.96(2)
C(13C)-C(14C)	1.523(10)

C(13C)-H(13E)	0.97(3)
C(13C)-H(13F)	0.97(2)
C(14C)-H(14G)	0.96(2)
C(14C)-H(14H)	0.96(2)
C(14C)-H(14I)	0.96(2)
C(16)-H(16A)	0.960(3)
C(16)-H(16B)	0.960(3)
C(16)-H(16C)	0.960(3)

C(9)-O(10)-C(10)	117.5(2)
C(12)-O(13)-C(13A)	112.0(3)
C(12)-O(13)-C(13C)	120.0(10)
C(12)-O(13)-C(13B)	117.1(8)
O(1)-C(1)-C(5)	127.8(2)
O(1)-C(1)-C(2)	123.8(2)
C(5)-C(1)-C(2)	108.4(2)
C(15)-C(2)-C(16)	108.9(2)
C(15)-C(2)-C(1)	109.3(2)
C(16)-C(2)-C(1)	107.4(2)
C(15)-C(2)-C(3)	113.0(2)
C(16)-C(2)-C(3)	113.5(2)
C(1)-C(2)-C(3)	104.5(2)
C(6)-C(3)-C(2)	116.0(2)
C(6)-C(3)-C(4)	113.8(2)
C(2)-C(3)-C(4)	105.1(2)
C(6)-C(3)-H(3)	107.1(2)
C(2)-C(3)-H(3)	107.1(2)
C(4)-C(3)-H(3)	107.1(2)
C(12)-C(4)-C(9)	110.3(2)
C(12)-C(4)-C(5)	113.8(2)
C(9)-C(4)-C(5)	107.2(2)
C(12)-C(4)-C(3)	111.9(2)
C(9)-C(4)-C(3)	109.9(2)
C(5)-C(4)-C(3)	103.4(2)
C(1)-C(5)-C(4)	103.7(2)
C(1)-C(5)-H(5A)	111.0(2)
C(4)-C(5)-H(5A)	111.0(2)
C(1)-C(5)-H(5B)	111.0(2)
C(4)-C(5)-H(5B)	111.0(2)
H(5A)-C(5)-H(5B)	109.0(2)
C(7)-C(6)-C(3)	114.7(2)
C(7)-C(6)-H(6A)	108.6(2)
C(3)-C(6)-H(6A)	108.6(2)
C(7)-C(6)-H(6B)	108.6(2)
C(3)-C(6)-H(6B)	108.6(2)
H(6A)-C(6)-H(6B)	107.6(2)
O(7)-C(7)-C(8)	122.1(2)
O(7)-C(7)-C(6)	121.8(2)
C(8)-C(7)-C(6)	116.2(2)
C(7)-C(8)-H(8A)	109.5(3)
C(7)-C(8)-H(8B)	109.5(2)
H(8A)-C(8)-H(8B)	109.5(3)
C(7)-C(8)-H(8C)	109.5(2)
H(8A)-C(8)-H(8C)	109.5(3)

H(8B)-C(8)-H(8C)	109.5(3)
O(9)-C(9)-O(10)	125.2(2)
O(9)-C(9)-C(4)	122.0(2)
O(10)-C(9)-C(4)	112.7(2)
O(10)-C(10)-C(11)	110.4(3)
O(10)-C(10)-H(10A)	109.6(2)
C(11)-C(10)-H(10A)	109.6(3)
O(10)-C(10)-H(10B)	109.6(3)
C(11)-C(10)-H(10B)	109.6(3)
H(10A)-C(10)-H(10B)	108.1(3)
C(10)-C(11)-H(11A)	109.5(3)
C(10)-C(11)-H(11B)	109.5(3)
H(11A)-C(11)-H(11B)	109.5(3)
C(10)-C(11)-H(11C)	109.5(3)
H(11A)-C(11)-H(11C)	109.5(4)
H(11B)-C(11)-H(11C)	109.5(4)
O(12)-C(12)-O(13)	124.5(2)
O(12)-C(12)-C(4)	125.6(2)
O(13)-C(12)-C(4)	109.9(2)
O(13)-C(13A)-C(14A)	105.2(6)
O(13)-C(13A)-H(13A)	110.7(7)
C(14A)-C(13A)-H(13A)	110.7(7)
O(13)-C(13A)-H(13B)	110.7(6)
C(14A)-C(13A)-H(13B)	110.7(7)
H(13A)-C(13A)-H(13B)	108.8(9)
C(13A)-C(14A)-H(14A)	109.5(7)
C(13A)-C(14A)-H(14B)	109.5(6)
H(14A)-C(14A)-H(14B)	109.5(6)
C(13A)-C(14A)-H(14C)	109.5(7)
H(14A)-C(14A)-H(14C)	109.5(7)
H(14B)-C(14A)-H(14C)	109.5(7)
C(14B)-C(13B)-O(13)	88.1(13)
C(14B)-C(13B)-H(13C)	114(2)
O(13)-C(13B)-H(13C)	114(2)
C(14B)-C(13B)-H(13D)	114(2)
O(13)-C(13B)-H(13D)	114(2)
H(13C)-C(13B)-H(13D)	111(2)
C(13B)-C(14B)-H(14D)	110(2)
C(13B)-C(14B)-H(14E)	110(2)
H(14D)-C(14B)-H(14E)	110(2)
C(13B)-C(14B)-H(14F)	110(2)
H(14D)-C(14B)-H(14F)	110(2)
H(14E)-C(14B)-H(14F)	110(2)
O(13)-C(13C)-C(14C)	93(2)
O(13)-C(13C)-H(13E)	113(2)
C(14C)-C(13C)-H(13E)	113(2)
O(13)-C(13C)-H(13F)	113(2)
C(14C)-C(13C)-H(13F)	113(2)
H(13E)-C(13C)-H(13F)	110(3)
C(13C)-C(14C)-H(14G)	110(2)
C(13C)-C(14C)-H(14H)	110(2)
H(14G)-C(14C)-H(14H)	110(2)
C(13C)-C(14C)-H(14I)	110(2)
H(14G)-C(14C)-H(14I)	110(2)

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H(14H)-C(14C)-H(14I)	110(2)
N(15)-C(15)-C(2)	178.5(3)
C(2)-C(16)-H(16A)	109.5(2)
C(2)-C(16)-H(16B)	109.5(2)
H(16A)-C(16)-H(16B)	109.5(3)
C(2)-C(16)-H(16C)	109.5(2)
H(16A)-C(16)-H(16C)	109.5(3)
H(16B)-C(16)-H(16C)	109.5(3)

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Table 16. Anisotropic displacement parameters (A^2 x 10^3) for **5e**. 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
O(1)	48(1)	77(1)	89(1)	-32(1)	25(1)	0(1)
O(7)	50(1)	61(1)	73(1)	18(1)	1(1)	3(1)
O(9)	74(1)	38(1)	64(1)	1(1)	11(1)	5(1)
O(10)	74(1)	59(1)	59(1)	14(1)	23(1)	11(1)
O(12)	64(1)	58(1)	62(1)	-13(1)	13(1)	13(1)
O(13)	64(1)	100(2)	72(1)	-42(1)	-20(1)	19(1)
N(15)	70(2)	56(1)	81(2)	-15(1)	-2(1)	-13(1)
C(1)	38(1)	42(1)	60(1)	-7(1)	15(1)	-5(1)
C(2)	38(1)	36(1)	45(1)	-1(1)	9(1)	-5(1)
C(3)	34(1)	30(1)	44(1)	2(1)	6(1)	1(1)
C(4)	34(1)	36(1)	47(1)	-3(1)	3(1)	2(1)
C(5)	33(1)	41(1)	61(1)	-8(1)	6(1)	-3(1)
C(6)	35(1)	43(1)	49(1)	0(1)	9(1)	1(1)
C(7)	37(1)	40(1)	55(1)	-5(1)	7(1)	3(1)
C(8)	39(1)	62(2)	93(2)	3(2)	2(1)	-5(1)
C(9)	35(1)	42(1)	50(1)	2(1)	-2(1)	5(1)
C(10)	76(2)	65(2)	68(2)	23(1)	19(2)	0(1)
C(11)	99(3)	100(3)	82(2)	42(2)	-3(2)	4(2)
C(12)	49(1)	48(1)	51(1)	-5(1)	4(1)	4(1)
C(13A)	75(4)	81(6)	65(5)	-35(5)	-15(3)	1(6)
C(14A)	98(4)	86(4)	81(4)	-25(3)	-35(3)	-1(3)
C(13B)	75(4)	81(6)	65(5)	-35(5)	-15(3)	1(6)
C(14B)	98(4)	86(4)	81(4)	-25(3)	-35(3)	-1(3)
C(13C)	75(4)	81(6)	65(5)	-35(5)	-15(3)	1(6)
C(14C)	98(4)	86(4)	81(4)	-25(3)	-35(3)	-1(3)
C(15)	41(1)	45(1)	48(1)	-6(1)	4(1)	-2(1)
C(16)	68(2)	60(2)	56(2)	9(1)	18(1)	-4(1)

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Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(3)	5042	792	7606	43
H(5A)	7891	441	7927	54
H(5B)	8354	-1027	8301	54
H(6A)	3632	-1707	7850	51
H(6B)	3539	-311	8288	51
H(8A)	394	-566	6845	100
H(8B)	811	-830	7687	100
H(8C)	1210	-1940	7141	100
H(10A)	5396	-4092	9265	83
H(10B)	4931	-3314	9919	83
H(11A)	6928	-4576	10327	145
H(11B)	7227	-2956	10453	145
H(11C)	7690	-3733	9800	145
H(13A)	6999	1311	10299	93
H(13B)	7478	2517	9820	93
H(14A)	9252	2066	10836	143
H(14B)	9772	1678	10121	143
H(14C)	9296	480	10596	143
H(13C)	6714	913	10322	93
H(13D)	8141	40	10510	93
H(14D)	8658	2569	10629	143
H(14E)	7902	2766	9816	143
H(14F)	9300	1912	10000	143
H(13E)	7543	2677	9685	93
H(13F)	9083	2046	9834	93
H(14G)	8139	1853	10928	143
H(14H)	8414	345	10638	143
H(14I)	6899	964	10491	143
H(16A)	5911	946	6514	91
H(16B)	4462	282	6173	91
H(16C)	5830	-362	5992	91

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Table 18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(5)	9180(1)	-3913(1)	7980(1)	83(1)
O(8)	10412(1)	-1656(2)	9554(1)	65(1)
O(12)	9525(1)	-1392(2)	5510(1)	83(1)
O(13)	8389(1)	328(1)	5724(1)	58(1)
N(16)	7111(2)	-2368(2)	6154(1)	86(1)
C(1)	9198(1)	-149(1)	7570(1)	39(1)
C(2)	9973(1)	-316(2)	6952(1)	45(1)
C(3)	10818(1)	-1548(2)	7296(1)	57(1)
C(4)	10681(1)	-2162(2)	8154(1)	53(1)
C(5)	9461(1)	-2712(2)	7943(1)	54(1)
C(6)	8547(1)	-1527(2)	7635(1)	44(1)
C(7)	10004(1)	193(2)	8492(1)	45(1)
C(8)	10824(1)	-1047(2)	8879(1)	51(1)
C(9)	10655(1)	1058(2)	6957(1)	54(1)
C(12)	9276(1)	-543(2)	5977(1)	52(1)
C(13)	7654(2)	196(2)	4818(1)	76(1)
C(15)	12078(2)	-575(2)	9259(1)	73(1)
C(16)	7743(1)	-1975(2)	6787(1)	57(1)
C(17)	7814(1)	-1401(2)	8279(1)	57(1)
O(9A)	11705(5)	1013(6)	7074(4)	81(2)
O(10A)	9978(4)	2174(3)	6822(5)	81(2)
C(10A)	10422(3)	3632(4)	6903(3)	66(1)
C(11A)	9872(7)	4186(9)	5998(4)	132(3)
O(9B)	11577(11)	1273(12)	6884(8)	56(2)
O(10B)	10011(7)	2164(5)	6992(9)	46(2)
C(10B)	10695(8)	3253(9)	6703(8)	91(3)
C(11B)	9960(6)	4251(10)	6049(7)	57(3)
C(14A)	6560(3)	983(5)	4727(2)	99(1)
C(14B)	7136(13)	1589(7)	4509(7)	106(4)

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Table 19. Bond lengths [A] and angles [deg] for **7**.

O(5)-C(5)	1.199(2)
O(8)-C(8)	1.432(2)
O(12)-C(12)	1.195(2)
O(13)-C(12)	1.319(2)
O(13)-C(13)	1.455(2)
N(16)-C(16)	1.130(2)
C(1)-C(7)	1.533(2)
C(1)-C(6)	1.549(2)
C(1)-C(2)	1.553(2)
C(2)-C(12)	1.542(2)
C(2)-C(9)	1.544(2)
C(2)-C(3)	1.544(2)
C(3)-C(4)	1.537(2)
C(4)-C(5)	1.503(2)
C(4)-C(8)	1.538(2)
C(5)-C(6)	1.552(2)
C(6)-C(16)	1.470(2)
C(6)-C(17)	1.542(2)
C(7)-C(8)	1.546(2)
C(8)-C(15)	1.520(2)
C(9)-O(9B)	1.169(12)
C(9)-O(9A)	1.224(6)
C(9)-O(10A)	1.319(2)
C(9)-O(10B)	1.320(2)
C(13)-C(14B)	1.486(3)
C(13)-C(14A)	1.487(3)
O(10A)-C(10A)	1.480(3)
C(10A)-C(11A)	1.491(4)
O(10B)-C(10B)	1.481(3)
C(10B)-C(11B)	1.490(4)
C(12)-O(13)-C(13)	116.56(13)
C(7)-C(1)-C(6)	107.85(10)
C(7)-C(1)-C(2)	107.21(9)
C(6)-C(1)-C(2)	111.58(11)
C(12)-C(2)-C(9)	104.75(11)
C(12)-C(2)-C(3)	110.72(12)
C(9)-C(2)-C(3)	110.38(12)
C(12)-C(2)-C(1)	113.49(10)
C(9)-C(2)-C(1)	109.25(11)
C(3)-C(2)-C(1)	108.21(11)
C(4)-C(3)-C(2)	111.67(11)
C(5)-C(4)-C(3)	106.97(12)
C(5)-C(4)-C(8)	106.95(12)
C(3)-C(4)-C(8)	112.61(13)
O(5)-C(5)-C(4)	126.4(2)
O(5)-C(5)-C(6)	121.7(2)
C(4)-C(5)-C(6)	111.88(12)
C(16)-C(6)-C(17)	106.23(12)
C(16)-C(6)-C(1)	113.15(11)
C(17)-C(6)-C(1)	112.33(11)

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C(16)-C(6)-C(5)	106.91(12)
C(17)-C(6)-C(5)	109.93(12)
C(1)-C(6)-C(5)	108.15(11)
C(1)-C(7)-C(8)	111.50(11)
O(8)-C(8)-C(15)	110.34(13)
O(8)-C(8)-C(4)	107.18(13)
C(15)-C(8)-C(4)	112.24(14)
O(8)-C(8)-C(7)	106.53(12)
C(15)-C(8)-C(7)	112.00(14)
C(4)-C(8)-C(7)	108.28(11)
O(9A)-C(9)-O(10A)	127.9(4)
O(9B)-C(9)-O(10B)	116.9(7)
O(9B)-C(9)-C(2)	131.9(6)
O(9A)-C(9)-C(2)	119.7(3)
O(10A)-C(9)-C(2)	112.3(2)
O(10B)-C(9)-C(2)	111.0(4)
O(12)-C(12)-O(13)	124.57(14)
O(12)-C(12)-C(2)	123.81(14)
O(13)-C(12)-C(2)	111.61(12)
O(13)-C(13)-C(14B)	108.8(4)
O(13)-C(13)-C(14A)	108.3(2)
N(16)-C(16)-C(6)	176.9(2)
C(9)-O(10A)-C(10A)	123.5(3)
O(10A)-C(10A)-C(11A)	101.7(5)
C(9)-O(10B)-C(10B)	99.1(5)
O(10B)-C(10B)-C(11B)	113.2(8)

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Table 20. Anisotropic displacement parameters (A^2 x 10^3) for **7**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

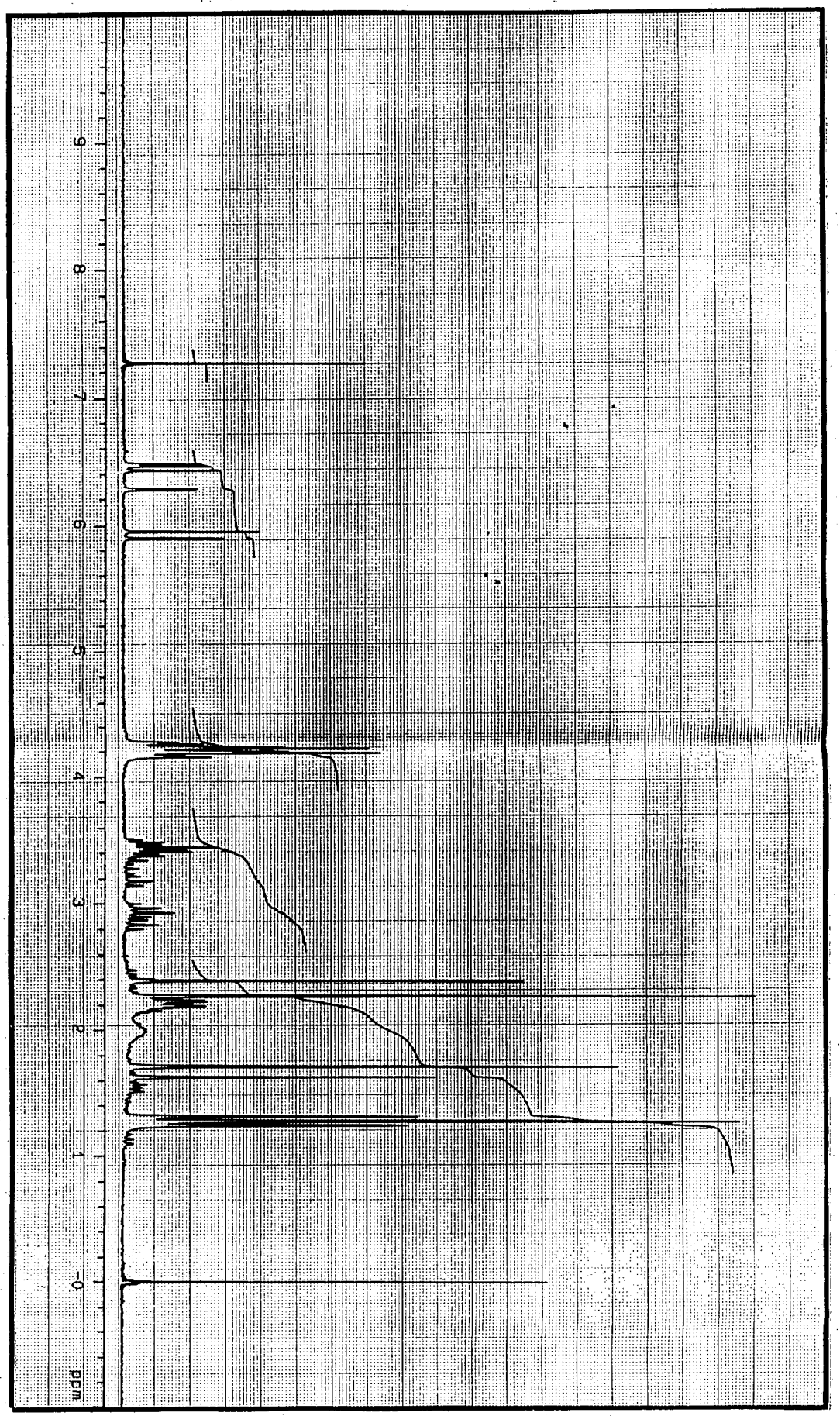
	U11	U22	U33	U23	U13	U12
O(5)	93(1)	49(1)	96(1)	4(1)	13(1)	-3(1)
O(8)	60(1)	89(1)	41(1)	15(1)	6(1)	7(1)
O(12)	93(1)	104(1)	49(1)	-21(1)	16(1)	26(1)
O(13)	59(1)	73(1)	36(1)	-3(1)	4(1)	7(1)
N(16)	87(1)	103(1)	54(1)	-10(1)	-2(1)	-38(1)
C(1)	37(1)	45(1)	34(1)	-2(1)	8(1)	2(1)
C(2)	41(1)	57(1)	38(1)	-3(1)	12(1)	3(1)
C(3)	53(1)	70(1)	51(1)	-1(1)	18(1)	18(1)
C(4)	51(1)	55(1)	48(1)	2(1)	9(1)	16(1)
C(5)	63(1)	48(1)	45(1)	-1(1)	8(1)	4(1)
C(6)	43(1)	50(1)	36(1)	-1(1)	6(1)	-2(1)
C(7)	45(1)	51(1)	37(1)	-7(1)	7(1)	-1(1)
C(8)	43(1)	66(1)	38(1)	0(1)	4(1)	5(1)
C(9)	44(1)	73(1)	45(1)	1(1)	14(1)	-7(1)
C(12)	55(1)	65(1)	39(1)	-2(1)	16(1)	2(1)
C(13)	86(1)	94(1)	36(1)	-4(1)	-1(1)	10(1)
C(15)	46(1)	98(1)	63(1)	-4(1)	0(1)	-1(1)
C(16)	57(1)	61(1)	46(1)	-1(1)	6(1)	-14(1)
C(17)	53(1)	69(1)	53(1)	5(1)	20(1)	-6(1)
O(9A)	42(1)	101(3)	99(3)	14(2)	20(2)	-9(2)
O(10A)	57(2)	70(2)	105(4)	29(2)	9(2)	-14(2)
C(10A)	56(2)	52(2)	87(2)	1(1)	16(1)	-3(1)
C(11A)	179(6)	122(6)	107(6)	40(4)	59(5)	-11(5)
O(9B)	49(4)	62(3)	66(4)	-4(4)	30(3)	6(2)
O(10B)	40(3)	42(3)	54(3)	4(2)	13(2)	2(2)
C(10B)	79(6)	45(4)	152(10)	17(5)	38(6)	-15(4)
C(11B)	31(2)	51(4)	86(7)	17(4)	12(3)	0(3)
C(14A)	87(2)	126(3)	59(2)	-14(2)	-17(2)	25(2)
C(14B)	121(9)	103(8)	62(6)	10(5)	-22(6)	35(7)

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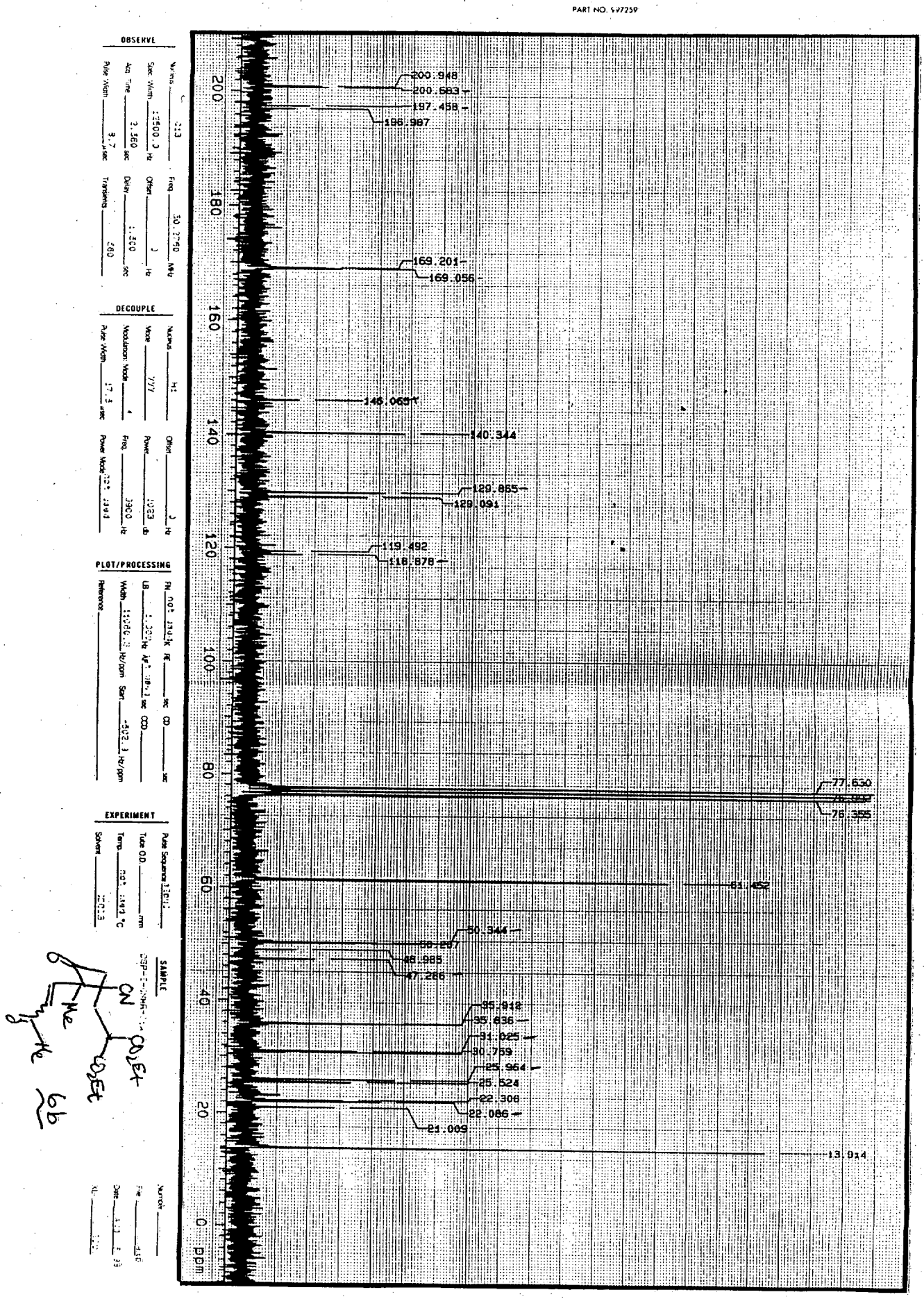
Table 21. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7**.

	x	y	z	U(eq)
H(8)	11011(20)	-2077(25)	9904(17)	89(7)
H(1)	8640	616	7361	47
H(3A)	10673	-2278	6850	69
H(3B)	11610	-1223	7400	69
H(4)	11238	-2926	8365	63
H(7A)	9540	410	8880	55
H(7B)	10463	1016	8459	55
H(13A)	7483	-785	4673	92
H(13B)	8050	576	4418	92
H(15A)	12127	117	9708	109
H(15B)	12344	-177	8799	109
H(15C)	12554	-1367	9510	109
H(17A)	8302	-1109	8847	86
H(17B)	7473	-2296	8332	86
H(17C)	7210	-721	8059	86
H(10A)	11263	3652	7055	79
H(10B)	10177	4156	7340	79
H(11A)	10085	5152	5971	199
H(11B)	9042	4113	5857	199
H(11C)	10132	3649	5581	199
H(10C)	11235	2799	6444	110
H(10D)	11145	3777	7214	110
H(11D)	10446	4948	5900	86
H(11E)	9418	4701	6298	86
H(11F)	9543	3748	5527	86
H(14A)	6059	897	4133	148
H(14B)	6736	1955	4861	148
H(14C)	6177	604	5127	148
H(14D)	6633	1508	3916	159
H(14E)	7743	2249	4526	159
H(14F)	6696	1908	4886	159

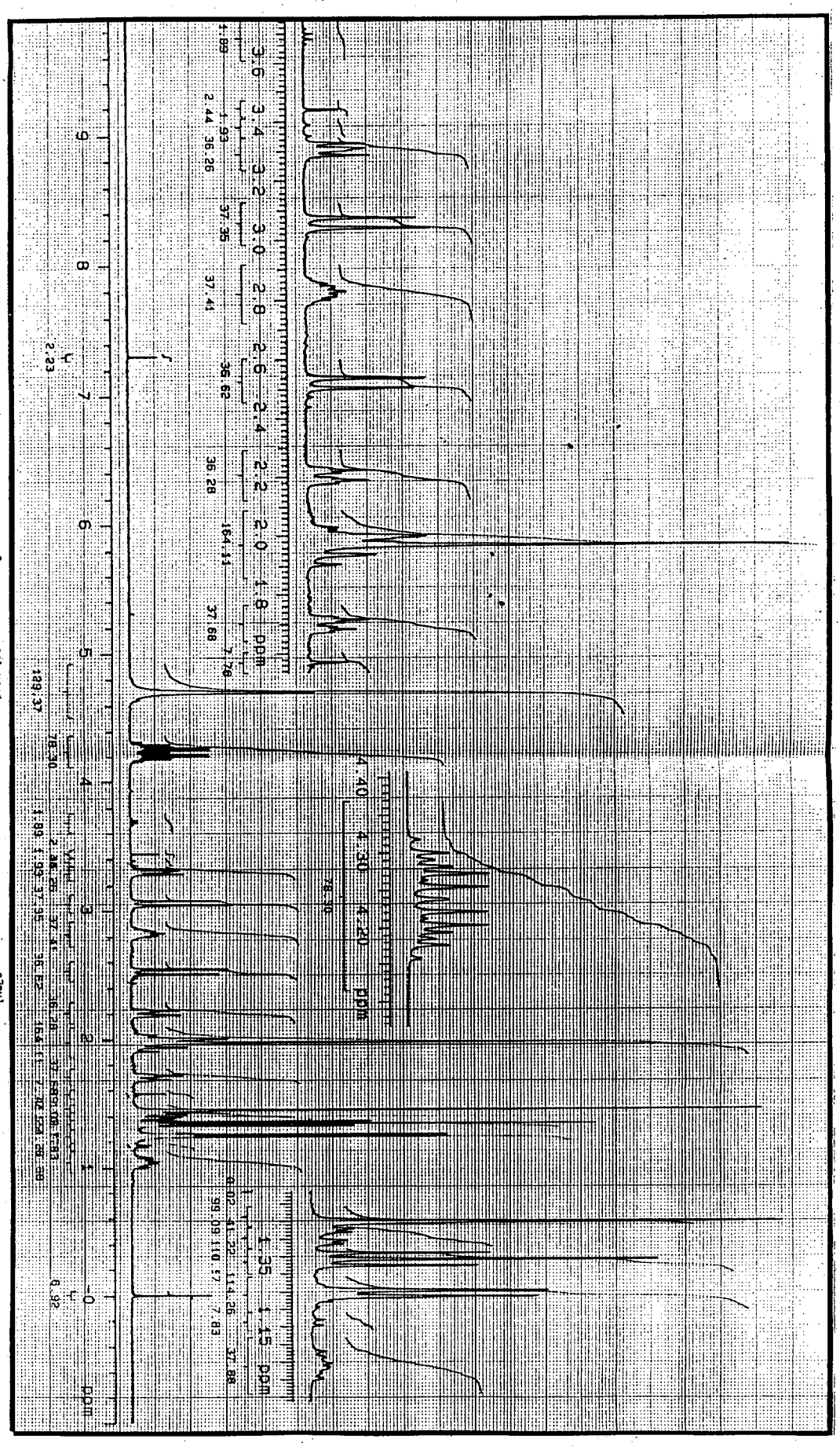
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