For Crystal Growth & Design

Stereoelectronic effects of substituent groups in the solid state. Crystal chemistry of some cubanecarboxylic and phenylpropiolic acids

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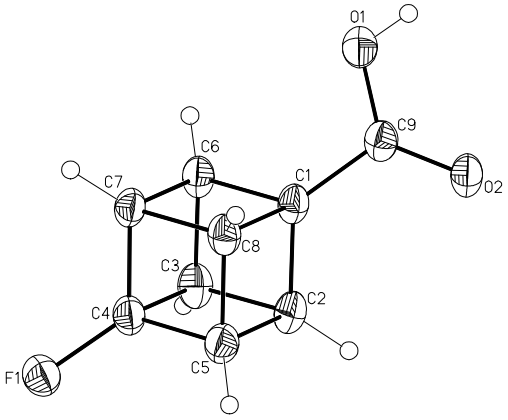
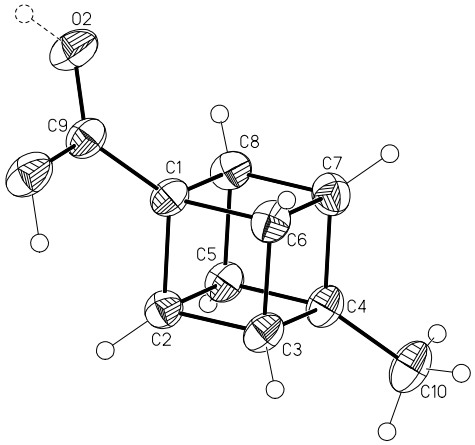
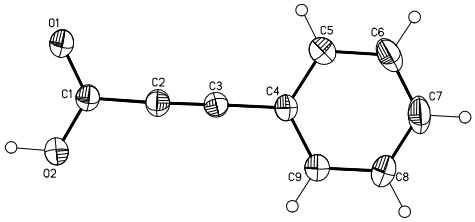
Supplementary Information
(42 pages)
Atomic coordinates
Bond lengths and angles
Anisotropic displacement parameters
For structures **1b, 1f, 2a, 2b, 2e** and **2f**



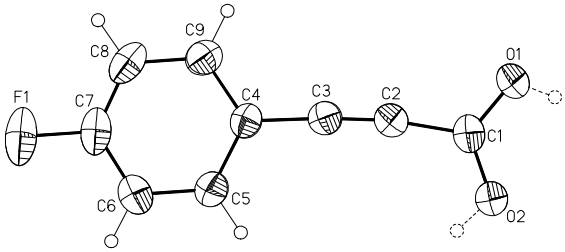
1b



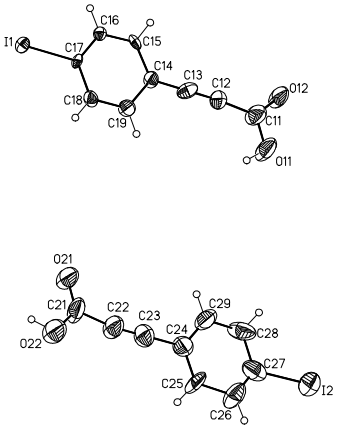
1f



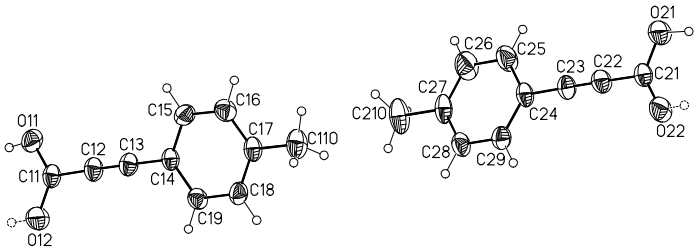
2a



2b



2e



2f

Table 1. Crystal data and structure refinement for **1b**.

Identification code	**1b**	
Empirical formula	$C_9 H_7 F O_2$	
Formula weight	166.15 Da	
Density (calculated)	1.546 g cm^{-3}	
F(000)	344	
Temperature	173(2) K	
Crystal size	0.31 x 0.28 x 0.05 mm	
Crystal color	colourless	
Crystal description	plate	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.529(2) Å	α = 90°
	b = 6.0556(15) Å	β = 105.810(4)°
	c = 12.861(3) Å	γ = 90°
Volume	714.0(3) $Å^3$	
Z	4	
Cell measurement reflections used	3164	
Cell measurement theta min/max	2.38° to 27.67°	
Diffractometer control software	Bruker AXS SMART Vers. 5.054 1997/98	
Diffractometer measurement device	Siemens SMART CCD area detector system	
Diffractometer measurement method	Full sphere data collection	
	in omega at 0.3° scan width	
	two runs with 720 frames, phi = 0°, 270°	
	and two runs with 436 frames, phi = 88°, 180°	
Theta range for data collection	2.22° to 28.30°	
Completeness to theta = 28.30°	99.1 %	
Index ranges	-12<=h<=12, -8<=k<=7, -17<=l<=17	
Computing data reduction	Bruker AXS SAINT program Vers. 6.02A	
Absorption coefficient	0.126 mm^{-1}	
Computing absorption correction	Bruker AXS SADABS program multiscan V2.03	
Absorption correction details	R.H. Blessing, Acta Cryst. (1995) A51 33-38	
Max. / min. transmission	1.00 / 0.86	
R(merg) before/after correction	0.0591 / 0.023520	
Computing structure solution	Bruker AXS SHELXTL Vers. 6.12 DOS/WIN95/NT/2000/ME	

Computing structure refinement	Bruker AXS SHELXTL Vers. 6.12 DOS/WIN95/NT/2000/ME
Refinement method	Full-matrix least-squares on F^2
Reflections collected	8417
Independent reflections	1752 [R(int) = 0.0270]
Data / restraints / parameters	1300 / 0 / 109
Goodness-of-fit on F^2	1.074
Weighting details	$w = 1/[\sigma^2 (Fo^2)+ (0.0925*P)^2+0.1955*P]$ where $P = (Fo^2+2Fc^2)/3$
Final R indices [I>2sigma(I)]	$R1$ = 0.0596, $wR2$ = 0.1475
R indices (all data)	$R1$ = 0.0774, $wR2$ = 0.1653
Largest diff. peak and hole	0.362 and -0.205 eÅ^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1b**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	7249(2)	3546(3)	2414(2)	40(1)
C(2)	8468(2)	4878(3)	3217(2)	48(1)
C(3)	9342(2)	2678(3)	3573(2)	48(1)
C(4)	8520(2)	2363(3)	4455(2)	44(1)
C(5)	7664(2)	4554(3)	4127(2)	48(1)
C(6)	8102(2)	1339(3)	2768(2)	44(1)
C(7)	7302(2)	1006(3)	3674(2)	42(1)
C(8)	6438(2)	3206(3)	3328(1)	42(1)
C(9)	6408(2)	4170(3)	1316(1)	41(1)
F(1)	9202(1)	1746(2)	5550(1)	53(1)
O(1)	5654(2)	2543(2)	758(1)	52(1)
O(2)	6364(2)	6094(2)	980(1)	48(1)

Table 3. Bond lengths [Å] and angles [°] for **1b**.

C(1)-C(9)	1.470(3)
C(1)-C(2)	1.554(3)
C(1)-C(6)	1.566(2)
C(1)-C(8)	1.586(2)
C(2)-C(3)	1.572(3)
C(2)-C(5)	1.575(3)
C(3)-C(4)	1.555(3)
C(3)-C(6)	1.568(3)
C(4)-F(1)	1.431(2)
C(4)-C(7)	1.547(3)
C(4)-C(5)	1.555(3)
C(5)-C(8)	1.560(3)
C(6)-C(7)	1.570(3)
C(7)-C(8)	1.566(2)
C(9)-O(2)	1.240(2)
C(9)-O(1)	1.312(2)
C(9)-C(1)-C(2)	128.18(15)
C(9)-C(1)-C(6)	127.04(16)
C(2)-C(1)-C(6)	90.85(14)
C(9)-C(1)-C(8)	119.79(15)
C(2)-C(1)-C(8)	90.08(14)
C(6)-C(1)-C(8)	89.62(12)
C(1)-C(2)-C(3)	89.66(14)
C(1)-C(2)-C(5)	90.12(14)
C(3)-C(2)-C(5)	90.25(13)
C(4)-C(3)-C(6)	88.87(14)
C(4)-C(3)-C(2)	89.10(14)
C(6)-C(3)-C(2)	90.11(14)
F(1)-C(4)-C(7)	124.01(15)
F(1)-C(4)-C(5)	123.64(16)
C(7)-C(4)-C(5)	91.80(14)
F(1)-C(4)-C(3)	124.46(16)

C(7)-C(4)-C(3)	91.70(15)
C(5)-C(4)-C(3)	91.66(14)
C(4)-C(5)-C(8)	88.61(14)
C(4)-C(5)-C(2)	88.98(14)
C(8)-C(5)-C(2)	90.26(14)
C(1)-C(6)-C(3)	89.37(14)
C(1)-C(6)-C(7)	90.37(13)
C(3)-C(6)-C(7)	90.35(14)
C(4)-C(7)-C(8)	88.66(14)
C(4)-C(7)-C(6)	89.06(14)
C(8)-C(7)-C(6)	90.20(13)
C(5)-C(8)-C(7)	90.92(14)
C(5)-C(8)-C(1)	89.53(14)
C(7)-C(8)-C(1)	89.81(13)
O(2)-C(9)-O(1)	123.61(17)
O(2)-C(9)-C(1)	122.31(17)
O(1)-C(9)-C(1)	113.97(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1b**. 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
C(1)	50(1)	35(1)	41(1)	7(1)	21(1)	5(1)
C(2)	55(1)	39(1)	52(1)	11(1)	20(1)	-1(1)
C(3)	47(1)	50(1)	52(1)	12(1)	20(1)	6(1)
C(4)	54(1)	41(1)	39(1)	8(1)	15(1)	4(1)
C(5)	65(1)	38(1)	44(1)	4(1)	20(1)	7(1)
C(6)	55(1)	38(1)	42(1)	8(1)	21(1)	11(1)
C(7)	55(1)	35(1)	41(1)	7(1)	19(1)	0(1)
C(8)	48(1)	44(1)	41(1)	8(1)	22(1)	6(1)
C(9)	49(1)	40(1)	42(1)	6(1)	24(1)	7(1)
F(1)	61(1)	53(1)	44(1)	4(1)	14(1)	3(1)
O(1)	63(1)	45(1)	47(1)	7(1)	13(1)	4(1)
O(2)	60(1)	41(1)	46(1)	12(1)	20(1)	7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **1b**.

	x	y	z	U(eq)
H(2)	8895	6298	3049	57
H(3)	10413	2476	3680	58
H(5)	7511	5720	4636	57
H(6)	8259	163	2265	53
H(7)	6883	-413	3852	51
H(8)	5368	3401	3229	51
H(1)	4981	2973	191	78

Table 1. Crystal data and structure refinement for **1f**.

Identification code	**1f**	
Empirical formula	$C_{10}H_{10}O_2$	
Formula weight	162.18	
Density (calculated)	1.346 g/cm^3	
F(000)	688	
Temperature	293(2) K	
Crystal size	0.57 * 0.41 * 0.34 [mm]	
Crystal color	brown	
Crystal description	block	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	P*bcn*	
Unit cell dimensions	a = 7.3167(12) Å	α = 90°
	b = 8.5089(12) Å	β = 90°
	c = 25.704(3) Å	γ = 90°
Volume	1600.3(4) Å^3	
Z	8	
Cell measurement reflections used	100	
Cell measurement twotheta min/max	20/25 [°]	
Diffractometer control software	Siemens XSCANS Vers. 2.20 PC (1991-96)	
Diffractometer measurement device	Siemens P4 four circle diffractometer	
Diffractometer measurement method	Omega scan mode	
Theta range for data collection	3.17 to 28.51[°]	
Completeness to theta = 28.51°	99.1 %	
Index ranges	-9<=h<=9, -11<=k<=11, -34<=l<=33	
Computing data reduction	Siemens XSCANS Vers. 2.20 PC (1991-96)	
Absorption coefficient	0.093 mm^{-1}	
Computing structure solution	Bruker AXS SHELXTL Vers. 5.10 DOS/WIN95/NT	
Computing structure refinement	Bruker AXS SHELXTL Vers. 5.10 DOS/WIN95/NT	
Refinement method	Full-matrix least-squares on F^2	
Reflections collected	5700	
Independent reflections	2013 [R(int) = 0.0417]	
Data / restraints / parameters	1715 / 0 / 110	
Goodness-of-fit on F^2	1.099	

weighting details	$w = 1/[\sigma^2(Fo^2)+ (0.1058*P)^2+0.2023*P]$ where $P = (Fo^2+2Fc^2)/3$
Final R indices [I>2sigma(I)]	$R1$ = 0.0641, $wR2$ = 0.1687
R indices (all data)	$R1$ = 0.0703, $wR2$ = 0.1756
Extinction coefficient	0.031(6)
Largest diff. peak and hole	0.398 and -0.361 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **1f**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	1809(2)	9655(2)	2476(1)	63(1)
O(2)	4061(2)	8429(2)	2058(1)	64(1)
C(1)	1203(2)	8564(2)	1627(1)	44(1)
C(2)	-151(2)	9762(2)	1362(1)	45(1)
C(3)	-1701(2)	8489(2)	1359(1)	48(1)
C(4)	-1046(2)	7900(2)	806(1)	49(1)
C(5)	521(2)	9174(2)	812(1)	46(1)
C(6)	-381(2)	7279(2)	1627(1)	49(1)
C(7)	289(2)	6699(2)	1077(1)	53(1)
C(8)	1847(2)	7968(2)	1081(1)	48(1)
C(9)	2410(2)	8909(2)	2079(1)	49(1)
C(10)	-2289(3)	7541(3)	350(1)	67(1)

Table 3. Bond lengths [Å] and angles [°] for **1f**.

O(1)-C(9)	1.2784(19)
O(2)-C(9)	1.276(2)
C(1)-C(9)	1.4894(18)
C(1)-C(8)	1.5660(19)
C(1)-C(2)	1.5756(19)
C(1)-C(6)	1.593(2)
C(2)-C(3)	1.5682(19)
C(2)-C(5)	1.5783(19)
C(3)-C(6)	1.570(2)
C(3)-C(4)	1.582(2)
C(4)-C(10)	1.515(2)
C(4)-C(7)	1.576(2)
C(4)-C(5)	1.577(2)
C(5)-C(8)	1.572(2)
C(6)-C(7)	1.576(2)
C(7)-C(8)	1.570(2)
C(9)-C(1)-C(8)	125.83(12)
C(9)-C(1)-C(2)	125.67(13)
C(8)-C(1)-C(2)	90.62(10)
C(9)-C(1)-C(6)	124.47(12)
C(8)-C(1)-C(6)	89.84(10)
C(2)-C(1)-C(6)	89.24(10)
C(3)-C(2)-C(1)	90.58(10)
C(3)-C(2)-C(5)	90.11(10)
C(1)-C(2)-C(5)	89.24(10)
C(2)-C(3)-C(6)	90.33(10)
C(2)-C(3)-C(4)	90.21(10)
C(6)-C(3)-C(4)	90.07(11)
C(10)-C(4)-C(7)	125.73(14)
C(10)-C(4)-C(5)	125.62(13)
C(7)-C(4)-C(5)	89.47(11)
C(10)-C(4)-C(3)	125.27(14)
C(7)-C(4)-C(3)	89.71(11)

C(5)-C(4)-C(3)	89.65(10)
C(8)-C(5)-C(4)	90.27(11)
C(8)-C(5)-C(2)	90.31(10)
C(4)-C(5)-C(2)	90.02(10)
C(3)-C(6)-C(7)	90.15(11)
C(3)-C(6)-C(1)	89.85(10)
C(7)-C(6)-C(1)	89.31(11)
C(8)-C(7)-C(6)	90.33(11)
C(8)-C(7)-C(4)	90.36(11)
C(6)-C(7)-C(4)	90.07(11)
C(1)-C(8)-C(7)	90.52(11)
C(1)-C(8)-C(5)	89.82(11)
C(7)-C(8)-C(5)	89.90(11)
O(2)-C(9)-O(1)	121.25(13)
O(2)-C(9)-C(1)	117.72(13)
O(1)-C(9)-C(1)	121.03(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1f**. 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)	54(1)	95(1)	40(1)	-9(1)	-5(1)	2(1)
O(2)	47(1)	94(1)	50(1)	-6(1)	-9(1)	7(1)
C(1)	43(1)	54(1)	36(1)	3(1)	-4(1)	-2(1)
C(2)	47(1)	50(1)	37(1)	0(1)	-3(1)	0(1)
C(3)	41(1)	63(1)	39(1)	0(1)	-2(1)	-3(1)
C(4)	50(1)	58(1)	38(1)	-2(1)	-4(1)	-7(1)
C(5)	49(1)	55(1)	34(1)	3(1)	-2(1)	-3(1)
C(6)	54(1)	54(1)	41(1)	6(1)	-2(1)	-7(1)
C(7)	62(1)	49(1)	48(1)	-4(1)	-2(1)	-1(1)
C(8)	44(1)	60(1)	41(1)	-2(1)	1(1)	3(1)
C(9)	48(1)	59(1)	39(1)	6(1)	-6(1)	-5(1)
C(10)	65(1)	90(1)	46(1)	-6(1)	-11(1)	-17(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1f**.

	x	y	z	U(eq)
H(1)	541	10030	2479	94
H(2)	4766	8613	2341	96
H(2A)	-309	10843	1459	54
H(3)	-2947	8669	1457	57
H(5)	836	9843	525	55
H(6)	-694	6613	1916	59
H(7)	443	5618	978	64
H(8)	3091	7789	980	58
H(10A)	-2919	8481	245	100
H(10B)	-3162	6755	450	100
H(10C)	-1571	7158	64	100

Table 1. Crystal data and structure refinement for **2a**.

Identification code	**2a**	
Empirical formula	$C_9 H_6 O_2$	
Formula weight	146.14 Da	
Density (calculated)	1.287 g cm^{-3}	
F(000)	304	
Temperature	203(2) K	
Crystal size	0.43 x 0.21 x 0.08 mm	
Crystal color	colourless	
Crystal description	plate	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 5.091(3) Å	α = 90°
	b = 14.988(9) Å	β = 91.180(11)°
	c = 9.886(6) Å	γ = 90°
Volume	754.3(8) $Å^3$	
Z	4	
Cell measurement reflections used	2613	
Cell measurement theta min/max	2.97° to 26.82°	
Diffractometer control software	Bruker AXS SMART Vers. 5.054 1997/98	
Diffractometer measurement device	Siemens SMART CCD area detector system	
Diffractometer measurement method	Full sphere data collection	
	in omega at 0.3° scan width	
	two runs with 720 frames, phi = 0°, 270°	
	and two runs with 436 frames, phi = 88°, 180°	
Theta range for data collection	2.47° to 28.40°	
Completeness to theta = 28.40°	98.9 %	
Index ranges	-6<=h<=6, -19<=k<=19, -13<=l<=13	
Computing data reduction	Bruker AXS SAINT program Vers. 6.02A	
Absorption coefficient	0.091 mm^{-1}	
Computing absorption correction	Bruker AXS SADABS program multiscan V2.03	
Absorption correction details	R.H. Blessing, Acta Cryst. (1995) A51 33-38	
Max. / min. transmission	1.00 / 0.86	
R(merg) before/after correction	0.0798 / 0.0324	
Computing structure solution	Bruker AXS SHELXTL Vers. 6.12 DOS/WIN95/NT/2000/ME	

Computing structure refinement	Bruker AXS SHELXTL Vers. 6.12 DOS/WIN95/NT/2000/ME
Refinement method	Full-matrix least-squares on F^2
Reflections collected	9198
Independent reflections	1872 [*R*(int) = 0.0449]
Data / restraints / parameters	1178 / 0 / 100
Goodness-of-fit on F^2	1.037
Weighting details	$w = 1/[\sigma^2 (Fo^2)+ (0.1281*P)^2+0.0366*P]$ where $P = (Fo^2+2Fc^2)/3$
Final R indices [I>2sigma(I)]	*R*1 = 0.0714, *wR*2 = 0.1863
R indices (all data)	*R*1 = 0.1036, *wR*2 = 0.2116
Largest diff. peak and hole	0.341 and -0.180 eÅ^{-3}

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

	x	y	z	U(eq)
O(1)	2028(3)	9452(1)	3991(2)	68(1)
O(2)	1666(3)	9335(1)	6227(2)	63(1)
C(1)	2703(4)	9130(1)	5102(2)	46(1)
C(2)	4758(4)	8470(1)	5168(2)	49(1)
C(3)	6425(4)	7908(1)	5170(2)	45(1)
C(4)	8421(4)	7229(1)	5192(2)	43(1)
C(5)	9391(5)	6903(1)	3987(2)	59(1)
C(6)	11295(5)	6252(2)	4034(3)	79(1)
C(7)	12222(6)	5938(2)	5258(3)	84(1)
C(8)	11261(5)	6255(2)	6448(3)	75(1)
C(9)	9370(4)	6900(1)	6419(2)	57(1)

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

O(1)-C(1)	1.242(2)
O(2)-C(1)	1.278(3)
C(1)-C(2)	1.440(3)
C(2)-C(3)	1.196(3)
C(3)-C(4)	1.437(3)
C(4)-C(9)	1.387(3)
C(4)-C(5)	1.388(3)
C(5)-C(6)	1.375(3)
C(6)-C(7)	1.373(4)
C(7)-C(8)	1.368(4)
C(8)-C(9)	1.365(3)
O(1)-C(1)-O(2)	124.33(18)
O(1)-C(1)-C(2)	119.63(18)
O(2)-C(1)-C(2)	116.03(17)
C(3)-C(2)-C(1)	177.1(2)
C(2)-C(3)-C(4)	179.2(2)
C(9)-C(4)-C(5)	120.10(18)
C(9)-C(4)-C(3)	119.89(18)
C(5)-C(4)-C(3)	120.01(18)
C(6)-C(5)-C(4)	119.0(2)
C(7)-C(6)-C(5)	120.1(2)
C(8)-C(7)-C(6)	121.1(2)
C(9)-C(8)-C(7)	119.5(2)
C(8)-C(9)-C(4)	120.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2a**. 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)	75(1)	71(1)	58(1)	10(1)	8(1)	31(1)
O(2)	65(1)	68(1)	55(1)	-3(1)	1(1)	25(1)
C(1)	44(1)	43(1)	51(1)	-1(1)	-2(1)	3(1)
C(2)	46(1)	48(1)	53(1)	-1(1)	0(1)	5(1)
C(3)	45(1)	46(1)	45(1)	-2(1)	0(1)	3(1)
C(4)	40(1)	38(1)	50(1)	-1(1)	1(1)	1(1)
C(5)	63(1)	61(1)	53(1)	-4(1)	7(1)	8(1)
C(6)	84(2)	74(2)	81(2)	-15(1)	24(1)	26(1)
C(7)	80(2)	67(2)	105(2)	0(1)	10(2)	37(1)
C(8)	78(2)	72(2)	74(2)	11(1)	-2(1)	32(1)
C(9)	61(1)	59(1)	52(1)	2(1)	3(1)	15(1)

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

	x	y	z	U(eq)
H(2)	352	9767	6172	94
H(5)	8756	7123	3153	71
H(6)	11963	6022	3226	95
H(7)	13540	5499	5279	101
H(8)	11897	6028	7279	90
H(9)	8708	7122	7233	69

Table 1. Crystal data and structure refinement for **2b**.

Identification code	**2b**	
Empirical formula	$C_9 H_5 F O_2$	
Formula weight	164.13 Da	
Density (calculated)	1.419 g cm^{-3}	
F(000)	336	
Temperature	203(2) K	
Crystal size	0.42 x 0.21 x 0.07 mm	
Crystal color	colourless	
Crystal description	plate	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 3.849(8) Å	α = 90°
	b = 6.349(13) Å	β = 92.83(4)°
	c = 31.47(7) Å	γ = 90°
Volume	768(3) $Å^3$	
Z	4	
Cell measurement reflections used	1554	
Cell measurement theta min/max	3.24° to 27.78°	
Diffractometer control software	Bruker AXS SMART Vers. 5.054 1997/98	
Diffractometer measurement device	Siemens SMART CCD area detector system	
Diffractometer measurement method	Full sphere data collection	
	in omega at 0.3° scan width	
	two runs with 720 frames, phi = 0°, 270°	
	and two runs with 436 frames, phi = 88°, 180°	
Theta range for data collection	2.59° to 28.87°	
Completeness to theta = 28.87°	87.5 %	
Index ranges	-5<=h<=4, -8<=k<=8, -42<=l<=39	
Computing data reduction	Bruker AXS SAINT program Vers. 6.02A	
Absorption coefficient	0.116 mm^{-1}	
Absorption correction	Empirical	
Computing absorption correction	Bruker AXS SADABS program multiscan V2.03	
Absorption correction details	R.H. Blessing, Acta Cryst. (1995) A51 33-38	
Max. / min. transmission	1.00 / 0.54	
R(merg) before/after correction	0.0945 / 0.0526	

Computing structure solution	Bruker AXS SHELXTL Vers. 5.10 DOS/WIN95/NT
Computing structure refinement	Bruker AXS SHELXTL Vers. 5.10 DOS/WIN95/NT
Refinement method	Full-matrix least-squares on F^2
Reflections collected	3286
Independent reflections	1764 [R(int) = 0.0312]
Data / restraints / parameters	1028 / 0 / 117
Goodness-of-fit on F^2	0.919
Weighting details	$w = 1/[\sigma^2 (Fo^2)+ (0.077*P)^2]$
	where $P = (Fo^2+2Fc^2)/3$
Final R indices [I>2sigma(I)]	$R1$ = 0.0585, $wR2$ = 0.1267
R indices (all data)	$R1$ = 0.0960, $wR2$ = 0.1419
Largest diff. peak and hole	0.306 and -0.186 eÅ^{-3}
Disorder	Hydrogen atoms H(1) and H(2)
	disordered over two sites with occupancies 0.5

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

	x	y	z	U(eq)
O(1)	4406(4)	907(2)	4627(1)	61(1)
O(2)	1724(5)	3228(3)	5018(1)	61(1)
F(1)	-3741(4)	10989(2)	2848(1)	80(1)
C(1)	2692(6)	2583(3)	4663(1)	48(1)
C(2)	1820(5)	3806(3)	4290(1)	46(1)
C(3)	882(5)	4993(3)	4011(1)	42(1)
C(4)	-319(5)	6502(3)	3701(1)	38(1)
C(5)	-1792(5)	8382(3)	3841(1)	43(1)
C(6)	-2939(5)	9902(3)	3553(1)	49(1)
C(7)	-2592(5)	9501(3)	3132(1)	51(1)
C(8)	-1184(6)	7669(4)	2982(1)	54(1)
C(9)	-14(5)	6154(3)	3270(1)	46(1)

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

O(1)-C(1)	1.260(3)
O(2)-C(1)	1.263(3)
F(1)-C(7)	1.360(3)
C(1)-C(2)	1.433(3)
C(2)-C(3)	1.198(3)
C(3)-C(4)	1.428(3)
C(4)-C(9)	1.386(4)
C(4)-C(5)	1.402(3)
C(5)-C(6)	1.382(3)
C(6)-C(7)	1.361(4)
C(7)-C(8)	1.377(4)
C(8)-C(9)	1.382(3)
O(1)-C(1)-O(2)	122.05(18)
O(1)-C(1)-C(2)	119.2(2)
O(2)-C(1)-C(2)	118.7(2)
C(3)-C(2)-C(1)	171.9(2)
C(2)-C(3)-C(4)	176.1(2)
C(9)-C(4)-C(5)	119.92(16)
C(9)-C(4)-C(3)	121.5(2)
C(5)-C(4)-C(3)	118.6(2)
C(6)-C(5)-C(4)	120.6(2)
C(7)-C(6)-C(5)	117.6(2)
F(1)-C(7)-C(6)	117.7(2)
F(1)-C(7)-C(8)	118.8(2)
C(6)-C(7)-C(8)	123.52(18)
C(7)-C(8)-C(9)	118.9(2)
C(8)-C(9)-C(4)	119.4(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2b**. 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)	84(1)	54(1)	46(1)	6(1)	7(1)	33(1)
O(2)	87(1)	55(1)	40(1)	4(1)	4(1)	30(1)
F(1)	79(1)	88(1)	70(1)	41(1)	-12(1)	5(1)
C(1)	54(1)	46(1)	44(1)	7(1)	-3(1)	8(1)
C(2)	51(1)	44(1)	43(1)	1(1)	4(1)	11(1)
C(3)	43(1)	42(1)	40(1)	0(1)	1(1)	4(1)
C(4)	36(1)	43(1)	35(1)	4(1)	0(1)	-1(1)
C(5)	46(1)	46(1)	38(1)	1(1)	-1(1)	2(1)
C(6)	46(1)	43(1)	57(1)	6(1)	0(1)	5(1)
C(7)	44(1)	58(1)	52(1)	22(1)	-6(1)	-4(1)
C(8)	53(1)	75(1)	32(1)	6(1)	-1(1)	-5(1)
C(9)	47(1)	51(1)	40(1)	-2(1)	2(1)	0(1)

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

	x	y	z	U(eq)
H(1)	4630(120)	420(70)	4863(14)	53(14)
H(2)	1040(110)	4540(80)	5003(15)	55(15)
H(5)	-2004	8616	4138	52
H(6)	-3950	11194	3646	58
H(8)	-988	7451	2684	64
H(9)	997	4870	3172	55

Table 1. Crystal data and structure refinement for **2e**.

Identification code	**2e**	
Empirical formula	$C_9 H_5 I O_2$	
Formula weight	272.03 Da	
Density (calculated)	2.063 g cm^{-3}	
F(000)	512	
Temperature	183(2) K	
Crystal size	0.75 x 0.55 x 0.12 mm	
Crystal color	colorless	
Crystal description	plate	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 4.1162(14) Å	α = 90°
	b = 6.013(2) Å	β = 90.958(6)°
	c = 35.398(12) Å	γ = 90°
Volume	876.1(5) $Å^3$	
Z	4	
Cell measurement reflections used	4121	
Cell measurement theta min/max	2.32° to 28.36°	
Diffractometer control software	Bruker AXS SMART Vers. 5.054 1997/98	
Diffractometer measurement device	Siemens SMART CCD area detector system	
Diffractometer measurement method	Full sphere data collection	
	in omega at 0.3° scan width	
	two runs with 720 frames, phi = 0°, 270°	
	and two runs with 436 frames, phi = 88°, 180°	
Theta range for data collection	3.44° to 28.46°	
Completeness to theta = 28.46°	96.1 %	
Index ranges	-5<=h<=5, -7<=k<=8, -47<=l<=47	
Computing data reduction	Bruker AXS SAINT program Vers. 6.02A	
Absorption coefficient	3.608 mm^{-1}	
Computing absorption correction	Bruker AXS SADABS program multiscan V2.03	
Absorption correction details	R.H. Blessing, Acta Cryst. (1995) A51 33-38	
Max. / min. transmission	1.00 / 0.54	
R(merg) before/after correction	0.1691 / 0.0617	
Computing structure solution	Bruker AXS SHELXTL Vers. 6.10 DOS/WIN95/NT/2000	

Computing structure refinement	Bruker AXS SHELXTL Vers. 6.10 DOS/WIN95/NT/2000
Refinement method	Full-matrix least-squares on F^2
Reflections collected	9460
Independent reflections	4136 [*R*(int) = 0.0439]
Data / restraints / parameters	3861 / 1 / 219
Goodness-of-fit on F^2	1.449
Weighting details	$w = 1/[\sigma^2 (Fo^2)+ (0.0691*P)^2+0.35*P]$ where $P = (Fo^2+2Fc^2)/3$
Final R indices [I>2sigma(I)]	*R*1 = 0.0570, *wR*2 = 0.1560
R indices (all data)	*R*1 = 0.0604, *wR*2 = 0.1584
Absolute structure parameter	0.43(8)
Extinction coefficient	0.0085(16)
Largest diff. peak and hole	1.859 and -1.965 $eÅ^{-3}$

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

	x	y	z	U(eq)
I(1)	1045(1)	5254(1)	348(1)	25(1)
O(11)	6840(30)	13540(20)	2514(3)	71(3)
O(12)	9690(30)	15789(19)	2169(3)	83(5)
C(11)	7870(40)	14150(30)	2185(4)	62(4)
C(12)	7040(30)	12830(20)	1859(3)	49(3)
C(13)	6190(20)	11650(20)	1615(3)	40(2)
C(14)	5029(17)	10270(30)	1329(2)	31(2)
C(15)	5400(20)	10697(11)	940(2)	28(2)
C(16)	4353(18)	9297(15)	681(2)	23(1)
C(17)	2762(16)	7347(14)	776(2)	19(1)
C(18)	2270(20)	6807(16)	1153(3)	30(2)
C(19)	3430(30)	8230(20)	1425(3)	38(2)
I(2)	9014(3)	8199(2)	4649(1)	74(1)
O(21)	3300(40)	20(30)	2479(3)	93(5)
O(22)	530(30)	-2270(20)	2831(3)	82(4)
C(21)	2180(40)	-580(30)	2782(4)	71(5)
C(22)	3130(40)	660(30)	3121(4)	69(5)
C(23)	4040(30)	1860(30)	3357(4)	58(3)
C(24)	5160(40)	3380(30)	3654(4)	56(3)
C(25)	4830(50)	2820(30)	4014(4)	96(7)
C(26)	5830(30)	4270(30)	4330(4)	68(4)
C(27)	7350(40)	6000(20)	4239(5)	64(4)
C(28)	7700(40)	6650(30)	3854(5)	76(5)
C(29)	6860(30)	5300(50)	3566(3)	68(3)

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

I(1)-C(17)	2.084(7)
O(11)-C(11)	1.298(18)
O(12)-C(11)	1.242(18)
C(11)-C(12)	1.436(19)
C(12)-C(13)	1.165(16)
C(13)-C(14)	1.389(16)
C(14)-C(15)	1.409(12)
C(14)-C(19)	1.441(19)
C(15)-C(16)	1.313(11)
C(16)-C(17)	1.387(11)
C(17)-C(18)	1.392(12)
C(18)-C(19)	1.365(14)
I(2)-C(27)	2.072(17)
O(21)-C(21)	1.229(17)
O(22)-C(21)	1.24(2)
C(21)-C(22)	1.462(19)
C(22)-C(23)	1.157(19)
C(23)-C(24)	1.46(2)
C(24)-C(25)	1.33(2)
C(24)-C(29)	1.39(3)
C(25)-C(26)	1.47(2)
C(26)-C(27)	1.26(2)
C(27)-C(28)	1.43(2)
C(28)-C(29)	1.34(2)
O(12)-C(11)-O(11)	118.1(14)
O(12)-C(11)-C(12)	122.4(14)
O(11)-C(11)-C(12)	119.3(14)
C(13)-C(12)-C(11)	173.8(14)
C(12)-C(13)-C(14)	177.3(12)
C(13)-C(14)-C(15)	124.2(13)
C(13)-C(14)-C(19)	119.5(9)
C(15)-C(14)-C(19)	116.3(10)
C(16)-C(15)-C(14)	121.8(9)

C(15)-C(16)-C(17)	121.6(7)
C(16)-C(17)-C(18)	120.4(7)
C(16)-C(17)-I(1)	119.4(5)
C(18)-C(17)-I(1)	120.2(6)
C(19)-C(18)-C(17)	118.4(8)
C(18)-C(19)-C(14)	121.5(8)
O(21)-C(21)-O(22)	125.4(14)
O(21)-C(21)-C(22)	117.9(13)
O(22)-C(21)-C(22)	116.4(14)
C(23)-C(22)-C(21)	170.9(17)
C(22)-C(23)-C(24)	179.6(19)
C(25)-C(24)-C(29)	118.9(15)
C(25)-C(24)-C(23)	119.9(16)
C(29)-C(24)-C(23)	120.9(13)
C(24)-C(25)-C(26)	123.4(19)
C(27)-C(26)-C(25)	115.3(15)
C(26)-C(27)-C(28)	122.0(16)
C(26)-C(27)-I(2)	120.5(13)
C(28)-C(27)-I(2)	117.1(11)
C(29)-C(28)-C(27)	122.0(15)
C(28)-C(29)-C(24)	117.2(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2e**. 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
I(1)	19(1)	31(1)	24(1)	-4(1)	-3(1)	-5(1)
O(11)	90(8)	87(9)	36(4)	-17(5)	1(4)	-38(6)
O(12)	143(11)	71(10)	36(4)	-13(5)	11(6)	-73(8)
C(11)	80(10)	67(9)	38(6)	-3(6)	-8(6)	-28(8)
C(12)	70(8)	39(7)	38(6)	-4(5)	-2(5)	-12(5)
C(13)	34(5)	57(7)	28(4)	5(4)	6(4)	0(4)
C(14)	32(3)	30(3)	31(3)	-5(7)	5(3)	-13(6)
C(15)	41(4)	10(5)	33(4)	0(2)	3(3)	-3(2)
C(16)	25(3)	22(3)	21(3)	-2(3)	-1(3)	-3(3)
C(17)	18(3)	23(3)	15(3)	-7(3)	-7(2)	-2(3)
C(18)	34(4)	24(4)	34(4)	-2(3)	10(3)	-8(3)
C(19)	45(5)	36(5)	33(5)	0(5)	2(4)	-18(4)
I(2)	95(1)	71(1)	56(1)	-10(1)	-10(1)	0(1)
O(21)	158(11)	77(9)	44(4)	-8(6)	6(5)	-76(10)
O(22)	107(10)	81(9)	59(6)	-7(6)	5(6)	-47(8)
C(21)	94(11)	68(9)	50(7)	-27(7)	17(7)	-38(8)
C(22)	91(10)	66(14)	50(7)	-11(7)	6(6)	-40(9)
C(23)	60(8)	51(7)	62(8)	-5(6)	-1(6)	-12(6)
C(24)	67(8)	48(7)	53(7)	2(7)	-14(6)	-2(6)
C(25)	180(20)	87(14)	21(5)	-14(7)	-27(8)	21(12)
C(26)	62(8)	97(11)	46(7)	-20(7)	19(6)	-13(8)
C(27)	66(9)	49(7)	77(9)	16(6)	18(7)	12(6)
C(28)	88(11)	68(10)	71(9)	33(8)	-27(7)	-40(8)
C(29)	93(8)	78(8)	32(5)	-5(11)	-3(5)	21(13)

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

	x	y	z	U(eq)
H(1)	5954	12282	2496	106
H(15)	6441	12034	866	34
H(16)	4670	9635	422	27
H(18)	1185	5473	1220	36
H(19)	3122	7870	1684	46
H(22)	957	-2988	2612	123
H(25)	4163	1350	4073	115
H(26)	5224	3949	4582	82
H(28)	8622	8055	3797	91
H(29)	7332	5667	3312	81

Table 1. Crystal data and structure refinement for **2f**.

Identification code	**2f**	
Empirical formula	$C_{10}\ H_8\ O_2$	
Formula weight	160.16 Da	
Density (calculated)	1.270 g cm^{-3}	
F(000)	672	
Temperature	203(2) K	
Crystal size	0.53 x 0.17 x 0.13 mm	
Crystal color	colourless	
Crystal description	rod	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.862(2) Å	α = 90°
	b = 12.442(4) Å	β = 90°
	c = 19.621(7) Å	γ = 90°
Volume	1675.1(10) $Å^3$	
Z	8	
Cell measurement reflections used	5589	
Cell measurement theta min/max	2.64° to 28.28°	
Diffractometer control software	Bruker AXS SMART Vers. 5.054 1997/98	
Diffractometer measurement device	Siemens SMART CCD area detector system	
Diffractometer measurement method	Full sphere data collection	
	in omega at 0.3° scan width	
	two runs with 720 frames, phi = 0°, 270°	
	and two runs with 436 frames, phi = 88°, 180°	
Theta range for data collection	1.94° to 28.59°	
Completeness to theta = 28.59°	97.1 %	
Index ranges	-9<=h<=9, -13<=k<=16, -26<=l<=17	
Computing data reduction	Bruker AXS SAINT program Vers. 6.02A	
Absorption coefficient	0.088 mm^{-1}	
Computing absorption correction	Bruker AXS SADABS program multiscan V2.03	
Absorption correction details	R.H. Blessing, Acta Cryst. (1995) A51 33-38	
Max. / min. transmission	1.00 / 0.65	
R(merg) before/after correction	0.1191 / 0.0508	
Computing structure solution	Bruker AXS SHELXTL Vers. 6.12 DOS/WIN95/NT/2000/ME	

Computing structure refinement	Bruker AXS SHELXTL Vers. 6.12 DOS/WIN95/NT/2000/ME
Refinement method	Full-matrix least-squares on F^2
Reflections collected	10514
Independent reflections	4129 [*R*(int) = 0.0377]
Data / restraints / parameters	3193 / 0 / 217
Goodness-of-fit on F^2	1.069
Weighting details	$w = 1/[\sigma^2 (Fo^2)+ (0.1162*P)^2]$
	where $P = (Fo^2+2Fc^2)/3$
Final R indices [I>2sigma(I)]	*R*1 = 0.0709, *wR*2 = 0.1635
R indices (all data)	*R*1 = 0.0872, *wR*2 = 0.1772
Absolute structure parameter	0.7(15)
Largest diff. peak and hole	0.761 and -0.289 eÅ^{-3}
Disorder	The hydrogen atoms of hydroxy groups
	disordered over two sites with occupancies 0.5

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

	x	y	z	U(eq)
O(11)	10520(2)	2042(1)	686(1)	44(1)
O(12)	10689(2)	2220(1)	1818(1)	51(1)
C(11)	9881(3)	2374(2)	1243(1)	35(1)
C(12)	8056(3)	2964(2)	1252(1)	38(1)
C(13)	6558(3)	3467(2)	1269(1)	36(1)
C(14)	4788(3)	4074(2)	1296(1)	31(1)
C(15)	3549(3)	4121(2)	734(1)	39(1)
C(16)	1826(3)	4708(2)	768(1)	40(1)
C(17)	1294(3)	5265(2)	1350(1)	36(1)
C(18)	2542(3)	5216(2)	1910(1)	37(1)
C(19)	4277(3)	4625(2)	1889(1)	35(1)
C(110)	-568(3)	5902(2)	1385(1)	50(1)
O(21)	-15997(3)	11132(1)	641(1)	51(1)
O(22)	-15990(3)	11153(1)	1782(1)	50(1)
C(21)	-15258(3)	10905(2)	1224(1)	36(1)
C(22)	-13451(3)	10309(2)	1212(1)	40(1)
C(23)	-11949(3)	9811(2)	1210(1)	38(1)
C(24)	-10158(3)	9213(2)	1214(1)	36(1)
C(25)	-9173(4)	9011(2)	608(1)	53(1)
C(26)	-7432(4)	8433(2)	611(1)	59(1)
C(27)	-6643(3)	8054(2)	1215(1)	43(1)
C(28)	-7644(3)	8242(2)	1815(1)	41(1)
C(29)	-9381(3)	8820(2)	1820(1)	41(1)
C(210)	-4751(3)	7422(2)	1210(2)	59(1)

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

O(11)-C(11)	1.248(2)
O(12)-C(11)	1.272(2)
C(11)-C(12)	1.452(3)
C(12)-C(13)	1.203(3)
C(13)-C(14)	1.431(3)
C(14)-C(15)	1.393(3)
C(14)-C(19)	1.395(3)
C(15)-C(16)	1.391(3)
C(16)-C(17)	1.386(3)
C(17)-C(18)	1.394(3)
C(17)-C(110)	1.505(3)
C(18)-C(19)	1.400(3)
O(21)-C(21)	1.282(3)
O(22)-C(21)	1.243(2)
C(21)-C(22)	1.445(3)
C(22)-C(23)	1.202(3)
C(23)-C(24)	1.437(3)
C(24)-C(25)	1.391(3)
C(24)-C(29)	1.392(3)
C(25)-C(26)	1.394(3)
C(26)-C(27)	1.385(4)
C(27)-C(28)	1.382(3)
C(27)-C(210)	1.518(3)
C(28)-C(29)	1.392(3)
O(11)-C(11)-O(12)	125.05(17)
O(11)-C(11)-C(12)	118.81(19)
O(12)-C(11)-C(12)	116.13(19)
C(13)-C(12)-C(11)	178.8(2)
C(12)-C(13)-C(14)	179.2(2)
C(15)-C(14)-C(19)	119.06(17)
C(15)-C(14)-C(13)	120.71(18)
C(19)-C(14)-C(13)	120.23(18)
C(16)-C(15)-C(14)	120.18(18)

C(17)-C(16)-C(15)	121.73(19)
C(16)-C(17)-C(18)	117.77(18)
C(16)-C(17)-C(110)	121.67(19)
C(18)-C(17)-C(110)	120.6(2)
C(17)-C(18)-C(19)	121.46(18)
C(14)-C(19)-C(18)	119.80(18)
O(22)-C(21)-O(21)	124.82(18)
O(22)-C(21)-C(22)	119.20(19)
O(21)-C(21)-C(22)	115.98(19)
C(23)-C(22)-C(21)	179.3(3)
C(22)-C(23)-C(24)	179.5(3)
C(25)-C(24)-C(29)	118.71(18)
C(25)-C(24)-C(23)	120.4(2)
C(29)-C(24)-C(23)	120.9(2)
C(24)-C(25)-C(26)	120.4(2)
C(27)-C(26)-C(25)	120.9(2)
C(28)-C(27)-C(26)	118.48(19)
C(28)-C(27)-C(210)	121.2(2)
C(26)-C(27)-C(210)	120.3(2)
C(27)-C(28)-C(29)	121.2(2)
C(24)-C(29)-C(28)	120.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2f**. 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(11)	34(1)	49(1)	49(1)	-12(1)	-4(1)	12(1)
O(12)	38(1)	68(1)	45(1)	-5(1)	-4(1)	22(1)
C(11)	26(1)	31(1)	47(1)	-2(1)	1(1)	5(1)
C(12)	29(1)	35(1)	49(1)	-2(1)	0(1)	6(1)
C(13)	30(1)	32(1)	45(1)	-3(1)	1(1)	3(1)
C(14)	24(1)	29(1)	41(1)	1(1)	1(1)	3(1)
C(15)	40(1)	41(1)	36(1)	-6(1)	2(1)	5(1)
C(16)	30(1)	44(1)	45(1)	0(1)	-7(1)	2(1)
C(17)	27(1)	30(1)	51(1)	2(1)	1(1)	1(1)
C(18)	34(1)	34(1)	41(1)	-2(1)	6(1)	8(1)
C(19)	28(1)	38(1)	39(1)	1(1)	-4(1)	4(1)
C(110)	28(1)	45(1)	78(2)	-2(1)	-2(1)	8(1)
O(21)	39(1)	63(1)	50(1)	-2(1)	-3(1)	18(1)
O(22)	39(1)	61(1)	49(1)	5(1)	5(1)	20(1)
C(21)	29(1)	34(1)	45(1)	2(1)	0(1)	7(1)
C(22)	32(1)	42(1)	47(1)	2(1)	-3(1)	6(1)
C(23)	31(1)	36(1)	47(1)	2(1)	2(1)	8(1)
C(24)	25(1)	32(1)	50(1)	3(1)	-2(1)	8(1)
C(25)	49(1)	60(2)	51(1)	9(1)	6(1)	25(1)
C(26)	52(2)	67(2)	58(1)	11(1)	19(1)	24(1)
C(27)	27(1)	31(1)	72(2)	3(1)	3(1)	7(1)
C(28)	33(1)	35(1)	53(1)	0(1)	-10(1)	7(1)
C(29)	36(1)	40(1)	45(1)	-4(1)	0(1)	11(1)
C(210)	27(1)	48(1)	103(2)	11(1)	9(1)	14(1)

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

	x	y	z	U(eq)
H(11)	11852	1802	694	66
H(12)	11875	1867	1805	76
H(15)	3879	3757	330	47
H(16)	1003	4726	385	48
H(18)	2214	5588	2311	44
H(19)	5092	4598	2273	42
H(11A)	-1251	5846	954	75
H(11B)	-273	6651	1478	75
H(11C)	-1382	5618	1747	75
H(21)	-17191	11558	688	76
H(22)	-17348	11409	1810	75
H(25)	-9669	9278	194	64
H(26)	-6797	8291	196	70
H(28)	-7154	7968	2227	49
H(29)	-10023	8953	2234	49
H(21A)	-4407	7226	1673	89
H(21B)	-3722	7860	1015	89
H(21C)	-4914	6776	939	89