Electronic Supplementary Material (ESI) for CrystEngComm
This journal is © The Royal Society of Chemistry 2012

Surprisingly Complex Supramolecular Behaviour in the Crystal Structures ofa Family of Mono-substituted Salicylic Acids.

Riccardo Montis*[a] and Michael B. Hursthouse [a,b].

[a] School of Chemistry, University of Southampton, Southampton, SO17 1BJ, [b]Department of Chemistry, Faculty of Science, King Abdulaziz University, Jeddah 21588, Saudi Arabia.

Electronic Supplementary Information

1. Crystallographic Data

	3-MeO h	3-MeO	4-MeO	5-MeO	6-MeO	3-NO_2h	5-NO_2
Formula	$C_8H_{10}O_5$	$C_8H_8O_4$	$C_8H_8O_4$	$C_8H_8O_4$	$C_8H_8O_4$	$C_7H_7NO_6$	$C_7H_5NO_5$
M.w.	186.16	168.14	168.14	168.14	168.14	201.14	183.12
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/c$	$P2_1/c$	$P2_1/n$	$P2_1/c$	P-1
a /Å	17.9971(3)	3.7935(2)	4.9629(2)	3.97840(10)	6.6697(2)	3.5943(2)	5.1246(5)
b /Å	14.3789(2)	27.8954(16)	11.0915(8)	16.1049(4)	9.3476(4)	21.115(2)	8.7762(8)
c /Å	6.73370(10)	7.0172(4)	13.6559(9)	11.5198(3)	12.2016(5)	10.7227(10)	9.2674(9)
α / º	90.00	90.00	90.00	90.00	90.00	90.00	62.252(6)
β / º	91.1210(10)	94.891(3)	98.788(4)	90.261(2)	104.305(2)	98.950(6)	75.292(6)
γ / º	90.00	90.00	90.00	90.00	90.00	90.00	82.654(7)
V /Å^3	1742.20(5)	739.86(7)	742.88(8)	738.09(3)	737.13(5)	803.87(12)	356.76(6)
T / K	120(2)	120(2)	120(2)	120(2)	120(2)	120(2)	120(2)
Crystal shape	block	block	block	needle	block	prism	plate
Colour	colourless	colourless	colourless	colourless	colourless	colourless	colourless
Z	8	4	4	4	4	4	2
All reflns	25551	8164	10375	11278	7885	9655	6568
Un. reflns	3981	1678	1704	1685	1678	1833	1634
R_{int}	0.0317	0.0470	0.0532	0.0337	0.0404	0.0826	0.0477
$R1_{obs}[I>2\sigma(I)]$	0.0368	0.0470	1704	0.0375	0.0514	0.0654	0.0474
$R1_{all}$	0.0435	0.0532	0.0640	0.0405	0.0599	0.1150	0.0734
wR2(obs)	0.0912	0.1122	0.1178	0.0985	0.1418	0.1271	0.1115
wR2 (all)	0.0959	0.1187	0.1274	0.1017	0.1491	0.1441	0.1278

	4-ACM	5-ACM h	4-NH_2	5-NH_2	4-Cl	5-Cl h	5-Cl
Formula	$C_9H_9NO_4$	$C_9H_{11}NO_5$	$C_7H_7NO_3$	$C_7H_7NO_3$	$C_7H_5ClO_3$	$C_7H_7ClO_4$	$C_7H_5ClO_3$
M.w.	195.17	213.19	153.14	153.14	172.56	190.58	172.56
Crystal system	orthorhombic	orthorhombic	monoclinic	monoclinic	monoclinic	triclinic	monoclinic
Space group	$Pna2_1$	$P2_12_12_1$	$P2_1/n$	$P2_1/n$	$P2_1/c$	P-1	$P2_1/c$
a /Å	13.5482(8)	3.7472(4)	7.1371(3)	3.7239(2)	3.7241(2)	3.7289(1)	23.3708(10)
b /Å	5.0245(3)	11.5109(17)	3.7278(2)	7.3696(4)	14.4178(8)	8.2430(4)	3.7089(1)
c /Å	12.9394(6)	21.979(3)	24.4465(12)	23.3107(11)	12.9156(6)	13.0565(7)	16.5722(7)
α / º	90.00	90.00	90.00	90.00	90.00	80.768(2)	90.00
β / º	90.00	90.00	94.386(2)	91.806(3)	97.933(3)	87.719(3)	104.853(2)
γ / º	90.00	90.00	90.00	90.00	90.00	83.755(3)	90.00
V /Å^3	880.82(8)	948.0(2)	648.51(5)	639.41(6)	686.84(6)	393.67(3)	1388.48(9)
T / K	120(2)	120(2)	120(2)	120(2)	120(2)	120(2)	120(2)
Crystal shape	plate	lath	plate	plate	block	block	lath
Colour	colourless	colourless	colourless	colourless	colourless	colourless	colourless
Z	4	4	4	4	4	2	8
All reflns	5835	4592	6128	5940	5857	7078	9922
Un. reflns	1894	1959	1475	1460	1556	1796	3153
R_{int}	0.0428	0.0725	0.0400	0.0443	0.0457	0.0313	0.0617
$R1_{obs}[I>2\sigma(I)]$	0.0390	0.0796	0.0458	0.0460	0.0488	0.0304	0.0489
$R1_{all}$	0.0461	0.1184	0.0560	0.0460	0.0638	0.0342	0.0829
wR2(obs)	0.0933	0.1559	0.1123	0.1159	0.0944	0.0750	0.1034
wR2 (all)	0.0980	0.1795	0.1221	0.1270	0.1033	0.0750	0.1206

This journal is © The Royal Society of Chemistry 2012

	5-I α	5-I β	SA	6-F	5-Br α	5-Br β	4-Me	5-Me
Formula	$C_7H_5IO_3$	$C_7H_5IO_3$	$C_7H_6O_3$	$C_7H_5FO_3$	$C_7H_5BrO_3$	$C_7H_5BrO_3$	$C_8H_8O_3$	$C_8H_8O_3$
M.w.	264.01	264.01	138.12	156.11	217.02	217.02	152.14	152.14
Crystal system	monoclinic	triclinic	monoclinic	monoclinic	triclinic	triclinic	triclinic	monoclinic
Space group	C2/c	P-1	$P2_1/c$	$P2_1/n$	P-1	P-1	P-1	$P2_1/n$
a /Å	38.4671(15)	4.8289(1)	4.8894(3)	5.3146(2)	4.85140(10)	6.9625(2)	3.8685(3)	7.2810(3)
b /Å	4.5765(2)	12.1776(3)	11.2411(13)	5.2118(2)	11.6936(3)	7.1714(3)	7.2380(9)	5.0146(2)
c /Å	19.9300(7)	14.6529(4)	11.3347(13)	22.5378(10)	14.4341(3)	8.0160(3)	13.2142(15)	20.2789(7)
α / º	90.00	109.752(1)	90.00	90.00	109.991 (1)	82.112(2)	100.756(5)	90.00
β / º	118.789(2)	97.974(2)	91.919(7)	91.907(3)	98.066(2)	73.835(2)	93.271(7)	95.498(2)
γ / º	90.00	100.626(2)	90.00	90.00	101.168 (1)	71.272(2)	90.788(7)	90.00
V /Å^3	3074.9(2)	777.99(3)	622.63(11)	623.92(4)	735.75(3)	363.56(2)	362.80(7)	737.00(5)
T / K	120(2)	120(2)	120(2)	120(2)	120(2)	120(2)	120(2)	120(2)
Crystal shape	block	block	needle	plate	block	plate	block	lath
Colour	colourless	colourless	colourless	colourless	colourless	colourless	colourless	colourless
Z	16	4	4	4	4	2	2	4
All reflns	11602	18951	5347	8172	10539	7522	6688	8182
Un. reflns	3442	3566	1413	1420	3325	1677	1630	1695
R_{int}	0.0356	0.0378	0.0462	0.0418	0.0231	0.0340	0.0619	0.0466
$R1_{obs}[I>2\sigma(I)]$	0.0340	3566	0.0656	0.0484	0.0212	0.0250	0.0653	0.0516
$R1_{all}$	0.0493	0.0308	0.1041	0.0581	0.0247	0.0298	0.1054	0.0654
wR2(obs)	0.0695	0.0578	0.1080	0.1213	0.0490	0.0532	0.1704	0.1164
wR2 (all)	0.0812	0.0602	0.1251	0.1276	0.0509	0.0584	0.1947	0.1267

Table S 1. Summary of crystallographic data

2. XPac: Supramolecular Constructs and Translational Vectors.

SC	D	Description	Figs	#	Base	Dependencies
A0	0	Centrosymm. carboxylic acid dimer	-	18	-	-
A11	1	Stack of A0 dimers > translation	9	8	t1	A0 → A11
A12	1	Tape of A0 dimers > translation	11	2	t2	A0 → A12
A13	1	Steps row A0 dimers > translation	13,14	3	t3	A0 → A13
A14	1	Stack of A0 dimers > translation	9	5	t4	A0 → A14
A15	1	Stack of pairs of A0 dimers > inversion, translation	9,10	2	t5	A0 → A15
A16	1	Row of A0 dimers > inversion, translation	18	6	t6	A0→ A16
A17	1	Chain of A0 dimers > inversion, translation	22	4	t7	A0→ A17
X11	1	Stack of single molecules > translation	9	12	t1	X0→X11
X12	1	Stack of pairs of X11 > inversion	9	7	t1	X0→X11→ X12
X13	1	Row of single molecules > translation	12	6	t8	X0→X13
X14	1	Stack of single molecules > translation	9	6	t4	X0→X14
A21	2	Row of A11 stacks > translation	16	5	t1, t9	A0·A11·A16 → A21
A22	2	Row of Zig-zag chains of A0 dimers > translation	17	2	t1, t10	A0·A11→ A22
Isostructural:			**5-Br α, 5-I β**			

Table S 2. Supramolecular Construct descriptions. SC = Supramolecular Construct; D = dimensionality; Description, '>' = is related by; # = Number of structures in which construct occurs; Base = base vector of SC (see Table S3); Dependencies show lower dimensionality SCs present in given SC.

This journal is © The Royal Society of Chemistry 2012

	t1	***d1***	***t2***	***d2***	***t3***	***d3***	***t4***	***d4***	***t5***	***d5***	***t6***	***d6***	***t7***	***d7***	***t8***	***d8***	***t9***	***d9***	***t10***	***d10***	***δ t1, t7***	***δ t1, t8***
3-MeO h															*001*	6.734						
3-MeO	*100*	3.793									*-101*	*8.326*			*10-1*	8.257	*001*	7.017			94.89	
4-MeO							*100*	4.963														
5-MeO	*100*	3.978																				
6-MeO																						
3-NO_2h	*100*	3.594																				
5-NO_2			*001*	9.267	*-111*	15.142																
4-ACM																						
5-ACMh	*100*	3.747																				
4-NH_2	*0-10*	3.728													*-100*	7.137	*100*	7.137			90	
5-NH_2	*-100*	3.724									*-1-10*	*8.143*										
4-Cl	*100*	3.724			*110*	14.891																
5-Clh	*100*	3.729																				
5-Cl	*010*	3.709																	*101*	24.945		90
5-I α									*010*	4.576												
5-I β													*2-10*	*16.881*								
SA					*-2-10*	14.899	*-100*	4.889														
5-F	*-100*	3.818									*001*	*8.211*			*-10-1*	8.357	*001*	8.211			78.83	
6-F							*0-10*	5.212	*-100*	5.315												
5-Br α							*100*	4.805					*2-10*	*16.805*								
5-Br β											*10-1*	*9.036*	*01-2*	*16.640*								
4-Me	*-100*	3.868									*110*	*8.160*			*0-10*	7.238	*010*	7.238			89.21	
5-Me			*110*	8.841			*010*	5.015														
5-NO	*00-1*	3.667									*011*	*8.826*			*0-10*	8.028	*010*	8.028	*1-11*	24.412	90	97.63

Table S 3. Translation vectors ***tn*** with lengths ***dn*** (Å) and angles ***δ*** (°).