Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

(i) Solution grown p-MHB crystal

Atomic displacement parameters (Å²)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O2	0.0474(10)	0.0507(10)	0.0336(8)	-0.0020(8)	0.0158(7)	-0.0086(8)
O3	0.0552(11)	0.0605(11)	0.0327(10)	-0.0010(8)	0.0071(9)	-0.0048(9)
O8	0.0496(11)	0.0484(10)	0.0368(9)	0.0011(8)	0.0178(8)	0.0115(9)
O5	0.0555(11)	0.0491(10)	0.0427(9)	-0.0002(8)	0.0224(8)	0.0079(9)
O6	0.0597(12)	0.0518(11)	0.0409(11)	0.0004(8)	0.0087(9)	0.0051(9)
O9	0.0508(11)	0.0511(11)	0.0377(11)	0.0017(8)	0.0080(9)	0.0068(9)
O7	0.0604(15)	0.0572(13)	0.0504(14)	-0.0015(10)	0.0223(12)	0.0193(11)
O1	0.0604(13)	0.0562(12)	0.0434(11)	0.0008(9)	0.0207(10)	-0.0129(10)
O4	0.0597(13)	0.0659(14)	0.0480(12)	0.0003(10)	0.0197(11)	0.0198(11)
C18	0.0438(15)	0.0433(14)	0.0332(14)	-0.0031(11)	0.0191(12)	-0.0001(12)
C1	0.0377(13)	0.0414(12)	0.0275(12)	0.0000(9)	0.0151(11)	0.0072(10)
C9	0.0386(13)	0.0392(12)	0.0355(14)	-0.0013(10)	0.0160(11)	-0.0067(11)
C23	0.0357(14)	0.0383(13)	0.0351(14)	0.0011(10)	0.0155(12)	-0.0058(10)
C22	0.0396(15)	0.0505(15)	0.0293(13)	-0.0009(11)	0.0083(12)	0.0022(12)
C20	0.0386(14)	0.0405(14)	0.0422(16)	-0.0003(11)	0.0193(12)	0.0010(11)
C7	0.0393(13)	0.0415(13)	0.0293(12)	-0.0015(9)	0.0140(11)	0.0057(10)
C3	0.0396(14)	0.0491(15)	0.0262(12)	-0.0021(10)	0.0112(11)	0.0011(12)
C15	0.0439(14)	0.0357(12)	0.0386(14)	-0.0013(10)	0.0171(12)	-0.0073(10)
C19	0.0419(15)	0.0477(15)	0.0333(14)	0.0023(11)	0.0163(13)	0.0013(12)
C17	0.0347(13)	0.0369(13)	0.0339(14)	0.0001(10)	0.0155(12)	-0.0036(10)
C6	0.0435(13)	0.0525(15)	0.0251(11)	0.0003(10)	0.0131(10)	0.0029(11)
C5	0.0488(16)	0.0523(15)	0.0303(13)	0.0074(11)	0.0175(13)	0.0027(12)
C13	0.0438(14)	0.0561(16)	0.0325(14)	0.0032(11)	0.0139(12)	0.0016(12)
C11	0.0499(18)	0.0612(17)	0.0360(15)	-0.0110(13)	0.0162(14)	0.0025(14)
C21	0.0527(18)	0.0542(16)	0.0339(15)	-0.0094(12)	0.0165(14)	0.0027(13)
C10	0.0496(15)	0.0521(15)	0.0311(12)	-0.0032(11)	0.0143(12)	-0.0022(12)
C4	0.0410(13)	0.0420(13)	0.0363(14)	0.0009(10)	0.0193(12)	0.0035(10)
C8	0.0515(16)	0.0523(13)	0.0476(14)	-0.0056(11)	0.0237(13)	-0.0107(12)
C12	0.0396(14)	0.0475(14)	0.0419(16)	-0.0018(11)	0.0173(12)	-0.0010(11)
C24	0.0483(17)	0.0416(15)	0.0560(19)	0.0007(14)	0.0253(15)	0.0066(13)
C16	0.0576(19)	0.0439(14)	0.0591(18)	0.0004(13)	0.0302(16)	0.0019(13)
C2	0.0426(14)	0.0471(14)	0.0248(12)	0.0033(9)	0.0146(11)	0.0024(11)

Bond length (Å)

O2-C7	1.329(3)	O2-C8	1.443(4)
O3-C7	1.211(3)	O8-C23	1.331(3)
O8-C24	1.440(3)	O5-C15	1.332(3)
O5-C16	1.445(4)	O6-C15	1.210(3)
O9-C23	1.213(3)	O7-C20	1.362(3)
O7-H7	0.82	O1-C4	1.353(3)
O1-H1	0.82	O4-C12	1.350(3)
O4-H4	0.82	C18-C19	1.384(4)
C18-C17	1.393(4)	C18-H18	0.93
C1-C6	1.396(3)	C1-C2	1.398(3)
C1-C7	1.470(4)	C9-C10	1.396(4)
C9-C14	1.397(3)	C9-C15	1.472(3)
C23-C17	1.479(4)	C22-C21	1.375(4)
C22-C17	1.384(4)	C22-H22	0.93
C20-C19	1.378(4)	C20-C21	1.393(4)
C3-C2	1.379(4)	C3-C4	1.392(4)
C3-H3	0.93	C19-H19	0.93
C6-C5	1.375(4)	C6-H6	0.93
C5-C4	1.385(4)	C5-H5	0.93
C13-C14	1.370(4)	C13-C12	1.388(4)
C13-H13	0.93	C11-C10	1.371(4)
C11-C12	1.390(4)	C11-H11	0.93
C21-H21	0.93	C10-H10	0.93
C8-H8A	0.96	C8-H8B	0.96
C8-H8C	0.96	C24-H24A	0.96
C24-H24B	0.96	C24-H24C	0.96
C16-H16A	0.96	C16-H16B	0.96
C16-H16C	0.96	C2-H2	0.93

Bond angles (°)

C7-O2-C8	116.8(3)	C23-O8-C24	117.5(2)
C15-O5-C16	116.7(2)	C20-O7-H7	109.5
C4-O1-H1	109.5	C12-O4-H4	109.5
C19-C18-C17	120.1(2)	C19-C18-H18	119.9
C17-C18-H18	119.9	C6-C1-C2	118.4(3)
C6-C1-C7	118.8(2)	C2-C1-C7	122.8(2)
C10-C9-C14	118.2(2)	C10-C9-C15	119.2(2)
C14-C9-C15	122.6(2)	O9-C23-O8	122.2(3)
O9-C23-C17	124.5(2)	O8-C23-C17	113.3(2)
C21-C22-C17	121.2(2)	C21-C22-H22	119.4
C17-C22-H22	119.4	O7-C20-C19	122.7(3)
O7-C20-C21	117.3(2)	C19-C20-C21	120.1(3)
O3-C7-O2	122.0(2)	O3-C7-C1	124.9(2)
O2-C7-C1	113.1(2)	C2-C3-C4	119.8(2)
C2-C3-H3	120.1	C4-C3-H3	120.1
O6-C15-O5	122.1(3)	O6-C15-C9	125.1(2)
O5-C15-C9	112.7(2)	C20-C19-C18	120.2(3)

C20-C19-H19	119.9	**C18-C19-H19**	119.9
C22-C17-C18	119.0(2)	**C22-C17-C23**	119.2(2)
C18-C17-C23	121.8(2)	**C5-C6-C1**	120.8(2)
C5-C6-H6	119.6	**C1-C6-H6**	119.6
C6-C5-C4	120.3(2)	**C6-C5-H5**	119.9
C4-C5-H5	119.9	**C14-C13-C12**	120.1(3)
C14-C13-H13	120.0	**C12-C13-H13**	120.0
C10-C11-C12	119.9(2)	**C10-C11-H11**	120.0
C12-C11-H11	120.0	**C22-C21-C20**	119.4(2)
C22-C21-H21	120.3	**C20-C21-H21**	120.3
C11-C10-C9	121.1(3)	**C11-C10-H10**	119.5
C9-C10-H10	119.5	**O1-C4-C5**	117.5(2)
O1-C4-C3	122.7(2)	**C5-C4-C3**	119.8(2)
O2-C8-H8A	109.5	**O2-C8-H8B**	109.5
H8A-C8-H8B	109.5	**O2-C8-H8C**	109.5
H8A-C8-H8C	109.5	**H8B-C8-H8C**	109.5
O4-C12-C13	122.9(3)	**O4-C12-C11**	117.4(2)
C13-C12-C11	119.7(3)	**O8-C24-H24A**	109.5
O8-C24-H24B	109.5	**H24A-C24-H24B**	109.5
O8-C24-H24C	109.5	**H24A-C24-H24C**	109.5
H24B-C24-H24C	109.5	**O5-C16-H16A**	109.5
O5-C16-H16B	109.5	**H16A-C16-H16B**	109.5
O5-C16-H16C	109.5	**H16A-C16-H16C**	109.5
H16B-C16-H16C	109.5	**C3-C2-C1**	120.9(2)
C3-C2-H2	119.6	**C1-C2-H2**	119.6
C13-C14-C9	121.0(2)	**C13-C14-H14**	119.5
C9-C14-H14	119.5		

(ii) Melt grown p-MHB crystal

Atomic displacement parameters (Å²)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O2	0.0466(10)	0.0496(9)	0.0319(8)	-0.0023(7)	0.0149(7)	-0.0084(8)
O3	0.0545(11)	0.0596(11)	0.0321(10)	-0.0007(8)	0.0069(9)	-0.0051(9)
O5	0.0540(11)	0.0475(9)	0.0418(9)	0.0001(8)	0.0215(8)	0.0078(9)
O8	0.0497(11)	0.0482(10)	0.0362(9)	0.0005(8)	0.0183(8)	0.0110(9)
O6	0.0588(12)	0.0511(11)	0.0401(11)	-0.0001(8)	0.0086(9)	0.0049(9)
O7	0.0604(15)	0.0557(12)	0.0489(13)	-0.0022(10)	0.0216(12)	0.0186(11)
O9	0.0499(11)	0.0507(11)	0.0370(11)	0.0021(8)	0.0080(9)	0.0077(9)
O1	0.0596(13)	0.0556(11)	0.0430(11)	0.0006(9)	0.0209(10)	-0.0133(10)
O4	0.0578(13)	0.0645(13)	0.0471(11)	0.0000(9)	0.0195(10)	0.0198(10)
C22	0.0434(15)	0.0434(14)	0.0316(14)	-0.0028(10)	0.0182(12)	-0.0005(12)
C1	0.0363(13)	0.0415(12)	0.0261(11)	-0.0001(9)	0.0136(10)	0.0075(10)
C9	0.0381(13)	0.0377(12)	0.0341(13)	-0.0021(9)	0.0157(11)	-0.0071(11)
C23	0.0358(14)	0.0379(13)	0.0333(13)	-0.0002(10)	0.0151(12)	-0.0064(10)
C20	0.0383(14)	0.0405(14)	0.0410(16)	-0.0014(11)	0.0188(12)	0.0005(11)
C7	0.0394(13)	0.0406(12)	0.0292(11)	-0.0023(9)	0.0144(11)	0.0053(10)
C18	0.0398(15)	0.0496(15)	0.0277(12)	-0.0011(10)	0.0081(11)	0.0016(12)
C19	0.0519(18)	0.0521(16)	0.0344(15)	-0.0099(12)	0.0168(14)	0.0021(13)
C3	0.0392(14)	0.0466(14)	0.0250(11)	-0.0019(9)	0.0107(10)	0.0014(11)
C24	0.0485(17)	0.0414(15)	0.0537(17)	0.0006(14)	0.0263(15)	0.0057(13)
C15	0.0427(14)	0.0354(12)	0.0387(13)	-0.0004(10)	0.0177(12)	-0.0069(10)
C17	0.0346(13)	0.0361(12)	0.0344(13)	0.0003(10)	0.0169(12)	-0.0025(10)
C6	0.0435(13)	0.0506(14)	0.0251(11)	0.0006(10)	0.0136(10)	0.0029(11)
C21	0.0406(14)	0.0482(15)	0.0332(13)	0.0019(11)	0.0165(12)	0.0014(12)
C4	0.0394(13)	0.0423(13)	0.0350(13)	0.0004(10)	0.0186(11)	0.0038(10)
C11	0.0430(14)	0.0544(15)	0.0316(13)	0.0030(11)	0.0131(12)	0.0020(12)
C14	0.0474(15)	0.0518(15)	0.0310(12)	-0.0033(11)	0.0139(11)	-0.0024(12)
C5	0.0485(16)	0.0517(14)	0.0297(12)	0.0076(11)	0.0181(12)	0.0022(12)
C12	0.0395(14)	0.0467(14)	0.0415(15)	-0.0012(11)	0.0179(12)	-0.0007(11)
C2	0.0415(13)	0.0450(13)	0.0249(12)	0.0027(9)	0.0143(11)	0.0013(11)
C16	0.0555(18)	0.0424(14)	0.0577(18)	0.0018(13)	0.0283(15)	0.0031(13)
C8	0.0518(16)	0.0515(13)	0.0464(14)	-0.0054(11)	0.0228(12)	-0.0105(12)
C10	0.0455(15)	0.0507(15)	0.0307(13)	-0.0056(10)	0.0168(12)	-0.0028(12)
C13	0.0503(18)	0.0604(17)	0.0357(14)	-0.0108(12)	0.0171(14)	0.0021(13)

Bond length (Å)

O2-C7	1.326(3)	**O2-C8**	1.447(4)
O3-C7	1.212(3)	**O5-C15**	1.331(3)
O5-C16	1.445(3)	**O8-C23**	1.337(3)
O8-C24	1.439(3)	**O6-C15**	1.209(3)
O7-C20	1.363(3)	**O7-H7**	0.82
O9-C23	1.214(3)	**O1-C4**	1.349(3)
O1-H1	0.82	**O4-C12**	1.350(3)
O4-H4	0.82	**C22-C21**	1.382(4)
C22-C17	1.390(4)	**C22-H22**	0.93
C1-C6	1.398(3)	**C1-C2**	1.400(3)
C1-C7	1.466(4)	**C9-C14**	1.396(4)
C9-C10	1.397(3)	**C9-C15**	1.474(3)
C23-C17	1.479(4)	**C20-C21**	1.381(4)
C20-C19	1.389(4)	**C18-C19**	1.375(4)
C18-C17	1.387(4)	**C18-H18**	0.93
C19-H19	0.93	**C3-C2**	1.379(4)
C3-C4	1.394(3)	**C3-H3**	0.93
C24-H24A	0.96	**C24-H24B**	0.96
C24-H24C	0.96	**C6-C5**	1.375(4)
C6-H6	0.93	**C21-H21**	0.93
C4-C5	1.388(4)	**C11-C10**	1.372(4)
C11-C12	1.385(4)	**C11-H11**	0.93
C14-C13	1.369(4)	**C14-H14**	0.93
C5-H5	0.93	**C12-C13**	1.392(4)
C2-H2	0.93	**C16-H16A**	0.96
C16-H16B	0.96	**C16-H16C**	0.96
C8-H8A	0.96	**C8-H8B**	0.96
C8-H8C	0.96	**C10-H10**	0.93
C13-H13	0.93		

Bond angles (°)

C7-O2-C8	116.8(2)	**C15-O5-C16**	116.7(2)
C23-O8-C24	117.4(2)	**C20-O7-H7**	109.5
C4-O1-H1	109.5	**C12-O4-H4**	109.5

C21-C22-C17	120.2(2)	**C21-C22-H22**	119.9
C17-C22-H22	119.9	**C6-C1-C2**	118.2(2)
C6-C1-C7	119.0(2)	**C2-C1-C7**	122.8(2)
C14-C9-C10	118.2(2)	**C14-C9-C15**	119.2(2)
C10-C9-C15	122.6(2)	**O9-C23-O8**	122.0(3)
O9-C23-C17	124.9(2)	**O8-C23-C17**	113.2(2)
O7-C20-C21	122.6(3)	**O7-C20-C19**	117.4(2)
C21-C20-C19	120.0(2)	**O3-C7-O2**	122.1(2)
O3-C7-C1	124.8(2)	**O2-C7-C1**	113.16(19)
C19-C18-C17	120.8(2)	**C19-C18-H18**	119.6
C17-C18-H18	119.6	**C18-C19-C20**	119.8(2)
C18-C19-H19	120.1	**C20-C19-H19**	120.1
C2-C3-C4	119.9(2)	**C2-C3-H3**	120.1
C4-C3-H3	120.1	**O8-C24-H24A**	109.5
O8-C24-H24B	109.5	**H24A-C24-H24B**	109.5
O8-C24-H24C	109.5	**H24A-C24-H24C**	109.5
H24B-C24-H24C	109.5	**O6-C15-O5**	122.3(2)
O6-C15-C9	125.0(2)	**O5-C15-C9**	112.6(2)
C18-C17-C22	119.2(2)	**C18-C17-C23**	118.9(2)
C22-C17-C23	121.9(2)	**C5-C6-C1**	121.0(2)
C5-C6-H6	119.5	**C1-C6-H6**	119.5
C20-C21-C22	120.1(3)	**C20-C21-H21**	120.0
C22-C21-H21	120.0	**O1-C4-C5**	117.5(2)
O1-C4-C3	122.9(2)	**C5-C4-C3**	119.6(2)
C10-C11-C12	120.1(2)	**C10-C11-H11**	119.9
C12-C11-H11	119.9	**C13-C14-C9**	121.2(2)
C13-C14-H14	119.4	**C9-C14-H14**	119.4
C6-C5-C4	120.3(2)	**C6-C5-H5**	119.8
C4-C5-H5	119.8	**O4-C12-C11**	122.7(3)
O4-C12-C13	117.5(2)	**C11-C12-C13**	119.8(2)
C3-C2-C1	121.0(2)	**C3-C2-H2**	119.5
C1-C2-H2	119.5	**O5-C16-H16A**	109.5
O5-C16-H16B	109.5	**H16A-C16-H16B**	109.5
O5-C16-H16C	109.5	**H16A-C16-H16C**	109.5
H16B-C16-H16C	109.5	**O2-C8-H8A**	109.5
O2-C8-H8B	109.5	**H8A-C8-H8B**	109.5
O2-C8-H8C	109.5	**H8A-C8-H8C**	109.5
H8B-C8-H8C	109.5	**C11-C10-C9**	120.9(2)
C11-C10-H10	119.6	**C9-C10-H10**	119.6
C14-C13-C12	119.8(2)	**C14-C13-H13**	120.1
C12-C13-H13	120.1		