STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 76 (2020)

Supporting information for article:

Effect of disordered imidazole substructure on proton dynamics in imidazolium malonic acid salt

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Table S1. The crystal data of Im-MAL obtained at 14 K, 120 K, 295 K and 330 K

Temperature	14(2) K	120(2) K	295(2) K	330(2) K
Wavelength	0. 71073 Å			
Crystal system, space group	Triclinic, P -1	Triclinic, P -1	Triclinic, P -1	Triclinic, P -1
Unit cell dimensions	a = 6.9050(14)Å α = 116.20(3) deg.	a = 6.9990(10) Å α = 116.22(3) deg.	a = 6.9800(10)Å α=116.40(3)deg.	a = 7.2950(10) Å α= 115.79(3) deg.
	b = 8.3940(17)Å β = 101.65(3) deg.	b = 8.378(2)Å β= 101.88(3) deg.	b = 8.400(2) Å β = 101.57(3) deg.	b = 8.280(2) Å β = 103.12(3) deg.
	c = 9.2270(18) Å γ = 90.61(3) deg.	c = 9.249(2) Å γ = 91.18(3) deg.	c = 9.230(2) Å γ = 91.09(3) deg.	c = 9.249(2) Å γ = 91.91(3) deg.
Volume	466.93(16) Å^3	472.25(17) Å^3	471.26(17) Å^3	484.30(17) Å^3
Z, Calculated density	2, 1.467 Mg/m^3	2, 1.450 Mg/m^3	2, 1.693 Mg/m^3	2, 1.414 Mg/m^3
Absorption coeff.	0.120 mm^-1	0.119 mm^-1	0.117 mm^-1	0.116 mm^-1
F(000)	216			
Crystal size	0.34x0.32x0.21 mm	0.34x0.32x0.21 mm	0.34x0.32x0.21 mm	0.34x0.32x0.21 mm
Theta range for data collection	3.03 to 30.63 deg.	2.75 to 28.03 deg.	3.45 to 28.52 deg.	2.90 to 28.09 deg.
Limiting indices	-9<=h<=7, -12<=k<=8, -10<=l<=12	-9<=h<=8, -11<=k<=11, -11<=l<=11	-8<=h<=9, -11<=k<=11, -12<=l<=9	-9<=h<=8, -10<=k<=10, -11<=l<=11
Reflections collected / unique	3204 / 2245 [R(int) = 0.0387]	4533 / 2104 [R(int) = 0.0231]	3296 / 2075 [R(int) = 0.0243]	4534 / 2174 [R(int) = 0.0929]
Completeness to theta	30.63 78.1 %	28.03 92.0 %	28.52 86.6 %	28.09 92.2 %
Absorption correction	ANALYTICAL			
Max. and min. transmission	1.342 and 0.8954	1.3210 and 0.8324	1.223 and 0.8753	1.127 and 0.945
Refinement method	Full-matrix least-squares on F^2			
Data / restraints / parameters	2245 / 4 / 204	2104 / 6 / 204	2075 / 6 / 204	2174 / 6 / 204
Goodness-of-fit on F^2	1.172	1.271	0.954	1.088

Final R indices [I>2sigma(I)]	R1 = 0.0520, wR2 = 0.1176	R1 = 0.0314, wR2 = 0.0721	R1 = 0.0376, wR2 = 0.0664	R1 = 0.0498, wR2 = 0.1048
R indices (all data)	R1 = 0.0625, wR2 = 0.1231	R1 = 0.0408, wR2 = 0.0752	R1 = 0.0730, wR2 = 0.0767	R1 = 0.0849, wR2 = 0.1162
Extinction coefficient	0.0389(15)	0.038(3)	0.040(2)	0.115(3)
Largest diff. peak and hole	0.413 and -0.338 e.Å^-3	0.280 and -0.222 e. Å^-3	0.209 and -0.213 e.Å ^-3	0.171 and -0.197 e. Å^-3
Nonharmonic ADP				
R indices (all data)	wR2-7.69 wR2all-7.79	wR2-3.56 wR2all- 3.71	wR2- 3.07 wR2all- 3.91	wR2- 5.57 wR2all- 5.80
Data / parameters	2253/323	2104/323	2075/323	2178/303

Table S2. Lengths of hydrogen bonds (Å) in Im-MAL crystal at 14 K, 120 K, 295 K and 330 K.

14K					120K				
D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)>	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)>
O(4)-H(4)…O(3)#2	1.248(5)	2.4463(11)	3.162(1)	114.79((3)	O(4)-H(4)...O(3)#2	1.229(3)5)	2.4427(11)	3.161(2)	114.77(3)
O(4)-H(4)…O(4)#2	1.248(3)	1.248(3)	2.456(1)	180.0	O(4)-H(4)...O(4)#2	1.229(3)	1.229(3)	2.458(1)	180.0
C(2)-H(22)…O(3)#4	0.985(8)	2.468(9)	3.349(1)	148.7(7)	C(2)-H(22)...O(3)#4	0.976(6)	2.524(6)	3.383(1)	146.8(5)
N(1A1)-H(1A1)…O(1)	0.963(7)	1.712(8)	2.6739(12)	176.0(9)	N(1A1)-H(1A1)...O(1)	0.954(6)	1.724(6)	2.6764(12)	176.7(7)
C(1A)-H(1A)…O(4)5	0.944(9)	2.389(9)	3.3232(12)	170.5(7)	C(1A)-H(1A)...O(4)#5	0.957(7)	2.393(7)	3.3416(12)	171.3(5)
N(1A2)-H(1A2)O(2)#6	0.926(10)	1.737(10)	2.6594(12)	174.1(10)	N(1A2)-H(1A2)…O(2)6	0.925(6)	1.742(6)	2.6637(12)	174.1(7)
C(2A)-H(2A)…O(3)7	0.964(8)	2.201(7)	3.1521(14)	168.9(8)	C(2A)-H(2A)...O(3)#7	0.946(6)	2.231(6)	3.1611(14)	167.5(6)
C(3A)-H(3A)…O(3)	0.959(8)	2.513(8)	3.2999(13)	139.3(6)	C(3A)-H(3A)...O(3)	0.932(6)	2.566(5)	3.3242(14)	138.8(4)
C(3B)-H(3B)…O(1)#8	0.986(15)	2.520(18)	3.0872(16)	116.4(11)	C(3B)-H(3B)…O(1)#8	0.971(11)	2.550(13)	3.0950(15)	115.5(8)
C(2B)-H(2B)	0.974(1	2.404(17	3.0448(1	122.8(1	C(2B)-H(2B)	0.899(1	2.506(12	3.0596(1	120.3(8

…O(2)#5	6)	)	7)	0)	…O(2)#5	1)	)	6)	)
N(1B2)-H(1B2)…O(1)#5	0.974(16)	1.836(17)	2.8078(14)	175.0(14)	N(1B2)-H(1B2)…O(1)#5	0.956(13)	1.888(14)	2.8348(13)	170.1(11)
N(1B2)-H(1B2)…O(2)#5	0.974(16)	2.392(15)	2.9778(14)	118.1(9)	N(1B2)-H(1B2)…O(2)5	0.956(13)	2.493(13)	2.9924(13)	112.5(8)
N(1B1)-H(1B1)...O(1)#8	0.94(2)	2.478(19)	3.0289(14)	117.5(12)	N(1B1)-H(1B1)…O(1)8	0.951(15)	2.501(14)	3.0411(14)	116.0(8)
N(1B1)-H(1B1)…O(2)#8	0.94(2)	1.80(2)	2.7387(14)	174(2)	N(1B1)-H(1B1)…O(2)8	0.951(15)	1.796(15)	2.7453(13)	174.9(13)
295K					330K				
D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)>	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)>
O(4)-H(4)…O(3)#2	1.227(3)	2.4481(12)	3.1641(13)	114.73(3)	O(4)-H(4)…O(3)#2	1.226(3)	2.4333(12)	3.1676(14)	115.94(4)
O(4)-H(4)…O(4)#2	1.227(3)3	1.227(3)	2.4538(14)	180.0	O(4)-H(4)…O(4)#2	1.226(3)3	1.226(3)	2.4516(17)	180.0
C(2)-H(22)…O(3)#4	1.000(7)	2.496(8)	3.3796(15)	147.0(6)	C(2)-H(22)…O(3)#4	0.959(9)	2.638(10)	3.4690(17)	145.1(7)
N(1A1)-H(1A1)…O(1)	0.937(8)	1.735(8)	2.6714(13)	176.6(10)	N(1A1)-H(1A1)…O(1)	0.933(9)	1.751(9)	2.6832(14)	177.0(10)
C(1A)-H(1A)…O(4)5	1.003(8)	2.352(8)	3.3408(14)	168.3(6)	C(1A)-H(1A)…O(4)5	0.951(12)	2.418(11)	3.3578(16)	169.4(8)
N(1A2)-H(1A2)…O(2)#6	0.964(8)	1.702(8)	2.6583(13)	171.0(9)	N(1A2)-H(1A2)…O(2)#6	0.912(9)	1.767(9)	2.6698(14)	170.4(10)
C(2A)-H(2A)…O(3)7	0.944(7)	2.232(7)	3.1613(16)	167.8(7)	C(2A)-H(2A)…O(3)#7	0.938(9)	2.268(9)	3.1796(17)	163.7(9)
C(3A)-H(3A)…O(3)	0.923(8)	2.586(7)	3.3199(15)	136.9(6)	C(3A)-H(3A)…O(3)	0.865(12)	2.713(11)	3.3882(18)	135.9(8)
C(3B)-H(3B)…O(1)#8	1.018(13)	2.473(16)	3.095(2)	118.8(10)	C(3B)-H(3B)…O(1)#8	0.985(16)	2.534(19)	3.087(3)	115.4(12)
C(2B)-H(2B)…O(2)#5	0.823(17)	2.534(17)	3.065(2)	123.3(12)	C(2B)-H(2B)…O(2)#5	0.848(18)	2.570(19)	3.060(3)	117.9(13)
N(1B2)-H(1B2)…O(1)#5	0.986(17)	1.843(17)	2.8258(17)	174.1(14)	N(1B2)-H(1B2)…O(1)#5	1.006(19)	1.847(18)	2.842(2)	169.9(14)
N(1B2)-H(1B2)…O(2)#5	0.986(17)	2.448(18)	2.9899(17)	114.1(10)	N(1B2)-H(1B2)…O(2)#5	1.006(19)	2.297(19)	2.990(2)	125.1(12)
N(1B1)-	1.031(1	2.412(16	3.0331(1	117.8(1	N(1B1)-	1.04(2)	2.51(2)	3.0440(1	111.2(1

H(1B1)…O(1)#8	8)	)	7)	0)	H(1B1)…O(1)#8			9)	3)
N(1B1)-H(1B1)…O(2)#8	1.031(18)	1.718(18)	2.7492(17)	179.7(15)	N(1B1)-H(1B1)…O(2)#8	1.04(2)	1.73(2)	2.754(2)	169.9(17)

A.1.

A.2.