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Supporting information for article:

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

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

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

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

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

14K					120K				
D-HA	d(D-	d(H	d(D	<(DH	D-HA	d(D-	d(H	d(D	<(DH
	H)	A)	A)	A)>		H)	A)	A)	A)>
O(4)-H(4)	1.248(2.4463	3.162(114.79	O(4)-	1.229(2.4427	3.161(114.7
O(3)#2	5)	(11)	1)	((3)	H(4)O(3	3)5)	(11)	2)	7(3)
)#2				
O(4)-H(4)	1.248(1.248(2.456(180.0	O(4)-	1.229(1.229(2.458(180.0
O(4)#2	3)	3)	1)		H(4)O(4	3)	3)	1)	
)#2	,			
C(2)-H(22)	0.985(8	2.468(9)	3.349(1)	148.7(7)	C(2)-	0.976(6)	2.524(6)	3.383(1)	146.8(5
0(3)#4)				H(22)O(3))
					#4				
N(1A1)-	0.963(7	1.712(8)	2.6739(1	176.0(9)	N(1A1)-	0.954(6)	1.724(6)	2.6764(1	176.7(7
H(1A1))		2)		H(1A1)O(2))
O(1)					1)				
C(1A)-	0.944(9	2.389(9)	3.3232(1	170.5(7)	C(1A)-	0.957(7)	2.393(7)	3.3416(1	171.3(5
H(1A))		2)		H(1A)O(4)			2))
O(4)5					#5				
N(1A2)-	0.926(1	1.737(10	2.6594(1	174.1(1	N(1A2)-	0.925(6)	1.742(6)	2.6637(1	174.1(7
H(1A2)O(2)	0))	2)	0)	H(1A2)			2))
#6					O(2)6				
C(2A)-	0.964(8	2.201(7)	3.1521(1	168.9(8)	C(2A)-	0.946(6)	2.231(6)	3.1611(1	167.5(6
H(2A))		4)		H(2A)O(3)			4))
O(3)7					#7				
C(3A)-	0.959(8	2.513(8)	3.2999(1	139.3(6)	C(3A)-	0.932	2.566(5)	3.3242(1	138.8(4
Н(ЗА))		3)		H(3A)O(3)	(6)		4))
O(3)									
C(3B)-H(3B)	0.986(1	2.520(18	3.0872(1	116.4(1	C(3B)-H(3B)	0.971	2.550(13	3.0950(1	115.5(8
O(1)#8	5))	6)	1)	O(1)#8	(11))	5))
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

N(HB2) 0.974(1) 1.302(1) 2.0078(1) 17.50(1) N(HB2) 0.956(1) 1.808(14) 2.814(1) 17.50(1) H(HB2) 0.974(1) 2.302(5) 2.9778(1) 11.81(9) N(HB2) 0.956(1) 2.493(13) 2.9924(1) 11.25(8) N(HB2) 0.974(1) 2.302(5) 2.9778(1) 11.81(9) N(HB2) 0.956(1) 2.493(13) 2.9924(1) 11.55(8) O(2)5 0 0 1 0 1 0 1.56(8)	O(2)#5	6))	7)	0)	O(2)#5	1))	6))
IHERD 60 7 60 7 60 7 60 7 7 7 CHDS 0.974 2.92012 2.97781 118.10 N(B2) 0.9561 2.93131 2.9241 112.58 R1B2) 0.940 2.92161 18.10 N(B2) 0.9561 2.93141 2.92141 115.61 R1B1) 0.942 2.47801 3.02801 17.51 N(B1) 0.9511 2.9104 3.0111 116.08 R1B1) 0.942 2.47801 3.02801 17.41 N(B1) 0.9511 2.9104 3.0111 116.08 R1B1) 0.942 1.902 2.73971 17.42 N(B1) 0.9511 2.9104 3.0111 116.08 R1B1) 0.942 1.902 2.73971 17.42 N(B1) 0.9511 2.9104 3.02 17.914 R1B1) 0.942 1.902 7.914 1.620 1.014 0.01 1.014 0.01 1.014 <td< td=""><td>N(1B2)-</td><td>0.974(1</td><td>1.836(17</td><td>2.8078(1</td><td>175.0(1</td><td>N(1B2)-</td><td>0.956(1</td><td>1.888(14</td><td>2.8348(1</td><td>170.1(1</td></td<>	N(1B2)-	0.974(1	1.836(17	2.8078(1	175.0(1	N(1B2)-	0.956(1	1.888(14	2.8348(1	170.1(1
introdeintrodeintrodeintrodeintrodeintrodeintrodeintrodeintrodeN(B2)03742.392(1)2.392(1)1.25(8)N(B2)0.95(6)2.493(1)3.12(8)N(B2)0.94(2)2.479(1)3.028(1)1.75(1)N(B1)0.51(1)2.50(1)4.01N(B1)0.94(2)2.478(1)3.028(1)1.75(1)N(B1)0.51(1)1.79(1)4.01N(B1)0.94(2)2.478(1)3.028(1)1.79(1)1.19(1)4.011.19(1)4.01.19(1)N(B1)0.94(2)1.80(2)2.738(1)1.74(2)N(B1)0.51(1)1.79(1)3.03.0N(B1)0.401.80(2)2.738(1)1.74(1)N(B1)0.51(1)1.79(1)3.03.01.71(1)N(B1)0.40M(D40A.A.A.A.A.A.A.A.A.D(-1)-fixM(D1.11(1)<	H(1B2)	6))	4)	4)	H(1B2)	3))	3)	1)
NH2D 0.9740 2.8201 2.9780 11.80 NH2D 0.950 2.4301 2.9241 1.258 HH2D 0 0 0 0 0 0 0 0 0 NUBJ 0.940 2.4780 30.2901 17.50 NUBJ 0.501 2.50144 3.0110 1.503 NUBJ 0.940 2.4780 30.2901 1.701 NUBJ 0.501 2.5014 3.011 1.503 NUBJ 0.940 1.802 2.78701 1.701 NUBJ 0.501 1.7015 2.75301 1.701 NUBJ 0.940 1.802 2.78701 1.701 NUBJ 0.501 1.7015 2.75301 1.701 Q129 1.802 2.8780 NUB 0.501 0.501 1.7015 2.75301 1.701 Q129 1.001 Q1 Q1 Q1 Q1 Q1 Q1 Q1 Q1 Q1 Q149-H4 1.227 2.484 A A A A Q1 Q1 Q1 Q1 Q149-H4 1.227 2.484 A A A A A A Q149-H4 1.227 2.4948 A	O(1)#5					O(1)#5				
H(H2) Q(H3)6)14)411	N(1B2)-	0.974(1	2.392(15	2.9778(1	118.1(9)	N(1B2)-	0.956(1	2.493(13	2.9924(1	112.5(8
QQBS N(B) 0.94(2) 2.478(3) 2.028(1) 17.0 N(B) 0.95(1) 2.01(1) 3.04(1) 1.06.08 N(B) 0.94(2) 1.80(2) 2.738(1) 12.0 N(B) 0.91(2) 3.04(1) 1.16.08 N(B) 0.94(2) 1.80(2) 2.738(1) 17.40 N(B) 0.91(2) 2.745(3) 3.149(1) N(B) 0.94(2) 1.80(2) 2.738(1) 17.40 N(B) 0.95(1) 2.745(3) 3.149(1) N(B) 0.94(2) 1.80(2) 2.738(1) 17.40 N(B) 0.95(1) 2.745(3) 3.169(1) O(2)A	H(1B2)	6))	4)		H(1B2)	3))	3))
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	O(2)#5					O(2)5				
H(1B1)0(1))BB PA	N(1B1)-	0.94(2)	2.478(19	3.0289(1	117.5(1	N(1B1)-	0.951(1	2.501(14	3.0411(1	116.0(8
Intersection Image in the section in the	H(1B1)O(1			4)	2)	H(1B1)	5)		4)	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$)#8		,	.,		O(1)8		, ,		,
Number of the sector	N(1B1)-	0.94(2)	1.80(2)	2.7387(1	174(2)	N(1B1)-	0.951(1	1.796(15	2.7453(1	174,9(1
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	H(1B1)					H(1B1)	5)		3)	3)
$ \begin{array}{ c c c c c c c } c c c c c } c c c c c$				()				,	5)	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	0(2)#8 205K					22012				
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		d(D	d(Н	d(D	<(DH		d(D	d(Н	d(D	<(DH
$ \begin{array}{ c c c c c c } \hline \begin bold in the image in the image. The image in the image. The image in the image. The image in the image in the image in $	D-11A	u(D-	u(11	u(D		D-11A	u(D-	u(11	u(D	
0(4)-H(4) 1.227 2.481 3.1641 14.73 0(4)-H(4) 1.226 2.4333 3.1676 115.91 0(3)#2 3) (12) (13) (3) 0(3)#2 3) (12) (14) 4(4) 0(4)-H(4) 1.227 (1.27) 2.4588 0(3)#2 3) (17) 1000 0(3)#2 100 2.4960 3.3961 0(3)#4 1 1.227 2.4516 1.80.0 0(3)#4 1 2.4960 3.3961 0(3)#4 1.217 2.6321 170.10 0(3)#4 1 0(3)#4 1.51(9) 2.68321 170.10 N(1A1) 0.393 2.352(8) 2.65831 168.3(6) H(1A) 1.51(9) 2.66941 1.70(1) N(1A2) 1.303(8 2.352(8) 1.663(8) H(1A) 1.51(9) 2.66981 1.70(1) N(1A2) 1.303(8 2.352(8) 1.663(8) H(1A) 1.51(9) 2.66981 1.70(1) N(1A2)		H)	A)	A)	A)>		H)	A)	A)	A)>
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	O(4)-H(4)	1.227(2.4481	3.1641	114.73	O(4)-H(4)	1.226(2.4333	3.1676	115.9
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	0(3)#2		(12)	(17)		0(3)#2	3)	(12)	(14)	4(4)
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		3)	(12)	(13)	(3)		,			
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	O(4)-H(4)	1.227(1.227(2.4538		O(4)-H(4)	1.226(1.226(2.4516	180.0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $					180.0		2)2			
C(2)-H(22) 1.000(7) 2.496(8) 3.379(1) 147.0(6) C(2)-H(22) 0.959(9) 2.638(1) 3.4690(1) 145.1(7) N(1A1)- 0.937(8) 1.735(8) 2.6714(1) 176.6(1) N(1A1)- 0.933(9) 1.751(9) 2.683(1) 177.0(1) H(1A) 0 0 0(1) - 40 0 C(1A)- 1.003(8) 2.352(8) 3.3408(1) 168.3(6) H(1A) 2.01(1) 3.3578(1) 169.4(8) H(1A) 1.003(8) 2.352(8) 3.3408(1) 168.3(6) H(1A) 2.01(1) 3.3578(1) 169.4(8) H(1A) 0.964(8) 1.702(8) 3.3408(1) 168.3(6) H(1A) 2.01(1) 3.3578(1) 169.4(8) M(1A2) 0.964(8) 1.702(8) 3.3408(1) 171.0(9) H(1A2) 0.912(9) 1.767(9) 2.6698(1) 170.4(1) M(1A2) 0.994(7) 3.1613(1) 167.8(7) H(2A) 0.913(9) 3.1796(1) 163.7(9) M(2A) <	0(4)#2	3)3	3)	(14)		0(4)#2	3)3	3)	(17)	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	C(2)-H(22)	1.000(7	2 496(8)	3.3796(1	147 0(6)	C(2)-H(22)	0.959(9)	2.638(10	3.4690(1	145.1(7
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	O(3)#4)	2.150(0)	5)	11/10(0)	O(3)#4)	7))
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N(1A1)-	0.937(8		2.6714(1	176.6(1	N(1A1)-	0.933(9)	1.751(9)	2.6832(1	177.0(1
$ \begin{array}{c c c c c c c } \hline (1) & (1) & (2) & (3) & (3) & (4) & ($	H(1A1)		1.735(8)	3)	0)	H(1A1)			4)	0)
C(1A)- 1.003(8	O(1)	,			0)	O(1)				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(1A)-	1.003(8		3 3/08/1		C(1A)-	0.951(1	2.418(11	3.3578(1	169.4(8
$ \begin{array}{ c c c c c c } \hline (4) & (4$	H(1A)	1.005(0	2.352(8)	1)00+00(1	168.3(6)	H(1A)	2))	6))
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	O(4)5)		(4)		O(4)5				
H(1A2) $0.994(6)$ $1.702(8)$ $2.6363(1)$ $171.0(9)$ H(1A2) $(1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$ $(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$ $(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1$	N(1A2)-	0.004/0		2.6502(1		N(1A2)-	0.912(9)	1.767(9)	2.6698(1	170.4(1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	H(1A2)	0.964(8	1.702(8)	2.6583(1	171.0(9)	H(1A2)			4)	0)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(2)#6)		3)		O(2)#6				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(2A)-					C(2A)-	0.938(9)	2.268(9)	3.1796(1	163.7(9
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	H(2A)	0.944(7	2.232(7)	3.1613(1	167.8(7)	H(2A)			7))
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	0(3)7)		6)		0(3)#7				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(3A)-					C(3A)-	0.865(1	2.713(11	3.3882(1	135.9(8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H(3A)	0.923(8	2.586(7)	3.3199(1	136.9(6)	H(3A)	2)		8)	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	0(3))		5)		0(3)		, ,		,
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(3B)-					C(3B)-	0.985(2 534(3.087(115.4(
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C(SD)	1.018(2.473(3.095(118.8(0.505(2.00-1	5.007(110.4(
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	H(3B)	12)	16)	2)	10)	H(3B)	16)	19)	3)	12)
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	O(1)#8	15)	10)	2)	10)	O(1)#8				
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C(2B)-H(2B)	0.823(1	2.534(17		123.3(1	C(2B)-H(2B)	0.848(1	2.570(19	3.060(3)	117.9(1
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	O(2)#5	7))	3.065(2)	2)	O(2)#5	8)			3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	N(1B2)-	0.000(1	1.040/17	2.0250/4	1741/1	N(1B2)-	1.006(1	1.847(18	2.842(2)	169.9(1
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	H(1B2)	0.986(1	1.843(1/	2.8258(1	1/4.1(1	H(1B2)	9))		4)
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	O(1)#5	7))	7)	4)	O(1)#5				
0.986(1) 2.448(18) 2.9899(1) 114.1(1) H(1B2) 9)) 2) M(1B2) 7)) 7) 0) 0(2)#5 0(2)#5 0 2) 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)	N(1B2)-	0.00011		D.0000044		N(1B2)-	1.006(1	2.297(19	2.990(2)	125.1(1
T T O	H(1B2)	0.986(1	2.448(18	2.9899(1	114.1(1	H(1B2)	9)			2)
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	0(2)#5	7))	7)	0)	0(2)#5		Í		
	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

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H(1B1)	0)		7)	0)	H(1B1)			9)	3)
O(1)#8	0))	/)	0)	O(1)#8				
N(1B1)-	1.001/1	1 710/10	2 7402(1	170 7/1	N(1B1)-	1.04(2)	1.73(2)	2.754(2)	169.9(1
H(1B1)	1.031(1	1./18(18	2./492(1	1/9./(1	H(1B1)				7)
O(2)#8	8))	7)	5)	O(2)#8				

A.1.

A.2.