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Supporting information for article:

A large anisotropic plasticity of l-leucinium hydrogen maleate preserved at cryogenic temperatures

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Table S1 Crystal data, data collection and structure refinement details of **(L-LeuH$^+$)·M$^-$** under all temperatures

	(l_leu_mal_100)	(l_leu_mal_125)	(l_leu_mal_150)	(l_leu_mal_175)
Crystal data				
Chemical formula	$C_6H_{14}NO_2^+ \cdot C_4H_3O_4^-$	$C_6H_{14}NO_2^+ \cdot C_4H_3O_4^-$	$C_6H_{14}NO_2^+ \cdot C_4H_3O_4^-$	$C_6H_{14}NO_2^+ \cdot C_4H_3O_4^-$
M_r	247.24	247.24	247.24	247.24
Crystal system, space group	Monoclinic, *C*2	Monoclinic, *C*2	Monoclinic, *C*2	Monoclinic, *C*2
Temperature (K)	100	125	150	175
a, *b*, *c* (Å)	21.2256 (7), 5.67647 (16), 32.0621 (7)	21.2633 (8), 5.67322 (19), 32.0530 (8)	21.3300 (7), 5.67423 (16), 32.0776 (7)	21.3889 (8), 5.67352 (19), 32.0754 (8)
β (°)	100.170 (3)	100.076 (3)	99.937 (3)	99.818 (3)
V (Å^3)	3802.35 (18)	3807.0 (2)	3824.14 (18)	3835.4 (2)
Z	12	12	12	12
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α
μ (mm^{-1})	0.11	0.11	0.11	0.11
Crystal size (mm)	4 × 0.12 × 0.06	4 × 0.12 × 0.06	4 × 0.12 × 0.06	4 × 0.12 × 0.06
Data collection				
Diffractometer	Stoe IPDS II	Stoe IPDS II	Stoe IPDS II	Stoe IPDS II
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan
T_{min}, T_{max}	0.899, 1.000	0.834, 1.000	0.915, 1.000	0.665, 1.000
No. of measured, independent and	22408, 7531, 5508	22550, 7553, 5218	22679, 7593, 5342	22830, 7614, 5110

observed [$I > 2\sigma(I)$] reflections				
R_{int}	0.064	0.074	0.066	0.065
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.625	0.625	0.625
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.099, 0.98	0.047, 0.107, 0.99	0.046, 0.112, 0.99	0.050, 0.133, 1.04
No. of reflections	7531	7553	7593	7614
No. of parameters	475	475	475	475
No. of restraints	1	1	1	1
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.26	0.21, −0.28	0.21, −0.30	0.21, −0.28
	(l_leu_mal_200)	(l_leu_mal_225)	(l_leu_mal_250)	(l_leu_mal_275)
Crystal data				
Chemical formula	$C_6H_{14}NO_2^+\cdot C_4H_3O_4^-$	$C_6H_{14}NO_2^+\cdot C_4H_3O_4^-$	$C_6H_{14}NO_2^+\cdot C_4H_3O_4^-$	$C_6H_{14}NO_2^+\cdot C_4H_3O_4^-$
M_r	247.24	247.24	247.24	247.24
Crystal system, space group	Monoclinic, *C*2	Monoclinic, *C*2	Monoclinic, *C*2	Monoclinic, *C*2
Temperature (K)	200	225	250	275
a, *b*, *c* (Å)	21.4563 (9), 5.67251 (19), 32.0779 (8)	21.5229 (9), 5.6692 (2), 32.0754 (9)	21.6021 (9), 5.6701 (2), 32.0856 (9)	21.6777 (9), 5.66500 (18), 32.0878 (8)
β (°)	99.653 (3)	99.486 (4)	99.299 (4)	99.115 (3)
V (Å^3)	3849.0 (2)	3860.3 (2)	3878.4 (2)	3890.8 (2)

Z	12	12	12	12
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α
μ (mm^{-1})	0.11	0.11	0.11	0.11
Crystal size (mm)	4 × 0.12 × 0.06	4 × 0.12 × 0.06	4 × 0.12 × 0.06	4 × 0.12 × 0.06
Data collection				
Diffractometer	Stoe IPDS II	Stoe IPDS II	Stoe IPDS II	Stoe IPDS II
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan
T_{min}, T_{max}	0.619, 1.000	0.874, 1.000	0.643, 1.000	0.674, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22918, 7634, 4962	22927, 7652, 4758	23037, 7684, 4651	23127, 7709, 4553
R_{int}	0.064	0.066	0.063	0.061
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.625	0.625	0.625
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.136, 1.04	0.051, 0.143, 1.07	0.053, 0.151, 1.05	0.051, 0.145, 1.05
No. of reflections	7634	7652	7684	7709
No. of parameters	475	475	475	475
No. of restraints	1	1	1	1
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.29	0.19, −0.24	0.17, −0.26	0.17, −0.20

	(l_leu_mal_293)
Crystal data	
Chemical formula	$C_6H_{14}NO_2^+ \cdot C_4H_3O_4^-$
M_r	247.24
Crystal system, space group	Monoclinic, *C*2
Temperature (K)	293
a, *b*, *c* (Å)	21.7528 (11), 5.6663 (2), 32.0956 (10)
β (°)	98.955 (4)
V (Å^3)	3907.8 (3)
Z	12
Radiation type	Mo *K*α
μ (mm^{-1})	0.10
Crystal size (mm)	4 × 0.12 × 0.06
Data collection	
Diffractometer	Stoe IPDS II
Absorption correction	Multi-scan
T_{min}, T_{max}	0.553, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23451, 7754, 4814
R_{int}	0.060
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.052, 0.141, 1.03
No. of reflections	7754
No. of parameters	475
No. of restraints	1

H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.21

Computer programs: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018), olex2.solve (Bourhis *et al.*, 2015), *SHELXL* (Sheldrick, 2015), Olex2 (Dolomanov *et al.*, 2009).

Table S2 Hydrogen-bond geometry (Å, º) for **(L-LeuH$^+$)·M$^-$** structure at 100 K

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O61—H61···O41	0.84	1.59	2.425 (3)	176
N2—H2*A*···O61^{i}	0.91	2.02	2.890 (3)	160
N2—H2*B*···O23^{ii}	0.91	2.02	2.852 (4)	152
N2—H2*C*···O51^{iii}	0.91	1.88	2.763 (4)	162
O12—H12···O33^{iv}	0.84	1.78	2.598 (4)	164
O62—H62···O42	0.84	1.61	2.442 (3)	174
O63—H63···O43	0.84	1.59	2.427 (3)	179
N3—H3*A*···O22^{v}	0.91	1.93	2.788 (4)	156
N3—H3*B*···O53^{vi}	0.91	1.91	2.814 (4)	171
N3—H3*C*···O63^{vii}	0.91	1.99	2.856 (4)	158
O13—H13···O52^{viii}	0.84	1.77	2.602 (4)	172
O11—H11···O31	0.84	1.76	2.596 (3)	171
N1—H1*A*···O21^{ix}	0.91	2.14	2.870 (4)	137
N1—H1*A*···O31^{ix}	0.91	2.40	2.974 (4)	121
N1—H1*B*···O42^{v}	0.91	1.95	2.859 (3)	176
N1—H1*C*···O32^{viii}	0.91	1.97	2.863 (4)	165

Symmetry codes: (i) −*x*+1, *y*, −*z*+1; (ii) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1, −*z*+1; (iv) −*x*+1, *y*+1, −*z*+1; (v) *x*+1/2, *y*−1/2, *z*; (vi) *x*+1/2, *y*−1/2, *z*+1; (vii) *x*+1/2, *y*+1/2, *z*+1; (viii) *x*+1/2, *y*+1/2, *z*; (ix) −*x*+3/2, *y*−1/2, −*z*+1.

Table S3 Hydrogen-bond geometry (Å, º) for **(L-LeuH$^+$)·M$^-$** structure at 125 K

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O61—H61···O41	0.84	1.59	2.426 (3)	178
N2—H2*A*···O61^{i}	0.91	2.02	2.893 (4)	161

N2—H2*B*···O23^{ii}	0.91	2.02	2.851 (4)	151
N2—H2*C*···O51^{iii}	0.91	1.88	2.762 (4)	163
O12—H12···O33^{iv}	0.84	1.77	2.595 (4)	168
O62—H62···O42	0.84	1.60	2.442 (3)	176
O63—H63···O43	0.84	1.58	2.421 (4)	179
N3—H3*A*···O22^{v}	0.91	1.94	2.792 (4)	155
N3—H3*B*···O53^{vi}	0.91	1.91	2.809 (4)	171
N3—H3*C*···O63^{vii}	0.91	1.99	2.860 (4)	159
O13—H13···O52^{viii}	0.84	1.76	2.598 (4)	173
O11—H11···O31	0.84	1.76	2.594 (4)	172
N1—H1*A*···O21^{ix}	0.91	2.14	2.872 (4)	137
N1—H1*A*···O31^{ix}	0.91	2.39	2.979 (4)	122
N1—H1*B*···O42^{v}	0.91	1.95	2.858 (4)	177
N1—H1*C*···O32^{viii}	0.91	1.98	2.866 (4)	165

Symmetry codes: (i) −*x*+1, *y*, −*z*+1; (ii) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1, −*z*+1; (iv) −*x*+1, *y*+1, −*z*+1; (v) *x*+1/2, *y*−1/2, *z*; (vi) *x*+1/2, *y*−1/2, *z*+1; (vii) *x*+1/2, *y*+1/2, *z*+1; (viii) *x*+1/2, *y*+1/2, *z*; (ix) −*x*+3/2, *y*−1/2, −*z*+1.

Table S4 Hydrogen-bond geometry (Å, º) for **(L-LeuH^{+})·M^{-}** structure at 150 K

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O61—H61···O41	0.84	1.59	2.428 (3)	179
N2—H2*A*···O61^{i}	0.91	2.02	2.895 (4)	162
N2—H2*B*···O23^{ii}	0.91	2.03	2.856 (4)	150
N2—H2*C*···O51^{iii}	0.91	1.88	2.764 (4)	163
O12—H12···O33^{iv}	0.84	1.79	2.598 (4)	162
O62—H62···O42	0.84	1.60	2.440 (3)	175
O63—H63···O43	0.84	1.58	2.423 (4)	179
N3—H3*A*···O22^{v}	0.91	1.93	2.791 (4)	157

N3—H3*B*···O53^{vi}	0.91	1.92	2.817 (4)	171
N3—H3*C*···O63^{vii}	0.91	2.00	2.861 (4)	157
O13—H13···O52^{viii}	0.84	1.77	2.601 (4)	171
O11—H11···O31	0.84	1.76	2.593 (4)	172
N1—H1*A*···O21^{ix}	0.91	2.13	2.870 (4)	138
N1—H1*A*···O31^{ix}	0.91	2.39	2.982 (4)	123
N1—H1*B*···O42^{v}	0.91	1.95	2.863 (4)	178
N1—H1*C*···O32^{viii}	0.91	1.98	2.868 (4)	163

Symmetry codes: (i) −*x*+1, *y*, −*z*+1; (ii) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1, −*z*+1; (iv) −*x*+1, *y*+1, −*z*+1; (v) *x*+1/2, *y*−1/2, *z*; (vi) *x*+1/2, *y*−1/2, *z*+1; (vii) *x*+1/2, *y*+1/2, *z*+1; (viii) *x*+1/2, *y*+1/2, *z*; (ix) −*x*+3/2, *y*−1/2, −*z*+1.

Table S5 Hydrogen-bond geometry (Å, º) for **(L-LeuH^{+})·M^{-}** structure at 175 K

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O61—H61···O41	0.84	1.59	2.425 (4)	176
N2—H2*A*···O61^{i}	0.91	2.02	2.895 (4)	162
N2—H2*B*···O23^{ii}	0.91	2.04	2.860 (5)	150
N2—H2*C*···O51^{iii}	0.91	1.88	2.766 (5)	164
O12—H12···O33^{iv}	0.84	1.78	2.598 (5)	163
O62—H62···O42	0.84	1.60	2.440 (4)	178
O63—H63···O43	0.84	1.58	2.421 (5)	177
N3—H3*A*···O22^{v}	0.91	1.93	2.788 (5)	157
N3—H3*B*···O53^{vi}	0.91	1.92	2.819 (5)	171
N3—H3*C*···O63^{vii}	0.91	2.00	2.860 (5)	157
O13—H13···O52^{viii}	0.84	1.77	2.596 (5)	168
O11—H11···O31	0.84	1.76	2.594 (4)	172
N1—H1*A*···O21^{ix}	0.91	2.14	2.877 (5)	138
N1—H1*A*···O31^{ix}	0.91	2.41	2.991 (5)	122

N1—H1*B*···O42^{v}	0.91	1.95	2.863 (4)	176
N1—H1*C*···O32^{viii}	0.91	1.98	2.868 (5)	166

Symmetry codes: (i) −*x*+1, *y*, −*z*+1; (ii) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1, −*z*+1; (iv) −*x*+1, *y*+1, −*z*+1; (v) *x*+1/2, *y*−1/2, *z*; (vi) *x*+1/2, *y*−1/2, *z*+1; (vii) *x*+1/2, *y*+1/2, *z*+1; (viii) *x*+1/2, *y*+1/2, *z*; (ix) −*x*+3/2, *y*−1/2, −*z*+1.

Table S6 Hydrogen-bond geometry (Å, º) for **(L-LeuH^{+})·M^{-}** structure at 200 K

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O61—H61···O41	0.84	1.59	2.425 (4)	174
N2—H2*A*···O61^{i}	0.91	2.02	2.901 (4)	161
N2—H2*B*···O23^{ii}	0.91	2.03	2.860 (5)	151
N2—H2*C*···O51^{iii}	0.91	1.88	2.766 (5)	163
O12—H12···O33^{iv}	0.84	1.79	2.598 (5)	161
O62—H62···O42	0.84	1.60	2.437 (4)	174
O63—H63···O43	0.84	1.58	2.421 (5)	179
N3—H3*A*···O22^{v}	0.91	1.93	2.787 (5)	156
N3—H3*B*···O53^{vi}	0.91	1.92	2.823 (5)	171
N3—H3*C*···O63^{vii}	0.91	2.01	2.867 (5)	157
O13—H13···O52^{viii}	0.84	1.77	2.598 (5)	170
O11—H11···O31	0.84	1.76	2.594 (4)	173
N1—H1*A*···O21^{ix}	0.91	2.14	2.881 (5)	138
N1—H1*A*···O31^{ix}	0.91	2.41	2.994 (5)	122
N1—H1*B*···O42^{v}	0.91	1.95	2.861 (4)	176
N1—H1*C*···O32^{viii}	0.91	1.97	2.865 (5)	166

Symmetry codes: (i) −*x*+1, *y*, −*z*+1; (ii) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1, −*z*+1; (iv) −*x*+1, *y*+1, −*z*+1; (v) *x*+1/2, *y*−1/2, *z*; (vi) *x*+1/2, *y*−1/2, *z*+1; (vii) *x*+1/2, *y*+1/2, *z*+1; (viii) *x*+1/2, *y*+1/2, *z*; (ix) −*x*+3/2, *y*−1/2, −*z*+1.

Table S7 Hydrogen-bond geometry (Å, º) for **(L-LeuH^{+})·M^{-}** structure at 225 K

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O61—H61···O41	0.83	1.59	2.423 (4)	176

N2—H2*A*···O61^{i}	0.90	2.05	2.902 (5)	159
N2—H2*B*···O23^{ii}	0.90	2.03	2.855 (5)	152
N2—H2*C*···O51^{iii}	0.90	1.90	2.776 (5)	163
O12—H12···O33^{iv}	0.83	1.81	2.596 (5)	157
O62—H62···O42	0.83	1.61	2.435 (4)	176
O63—H63···O43	0.83	1.60	2.421 (5)	172
N3—H3*A*···O22^{v}	0.90	1.93	2.784 (5)	158
N3—H3*B*···O53^{vi}	0.90	1.93	2.822 (5)	170
N3—H3*C*···O63^{vii}	0.90	2.02	2.862 (5)	156
O13—H13···O52^{viii}	0.83	1.78	2.596 (5)	169
O11—H11···O31	0.83	1.77	2.596 (5)	172
N1—H1*A*···O21^{ix}	0.90	2.15	2.882 (5)	138
N1—H1*A*···O31^{ix}	0.90	2.42	3.001 (5)	123
N1—H1*B*···O42^{v}	0.90	1.97	2.870 (5)	177
N1—H1*C*···O32^{viii}	0.90	1.98	2.864 (5)	165

Symmetry codes: (i) −*x*+1, *y*, −*z*+1; (ii) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1, −*z*+1; (iv) −*x*+1, *y*+1, −*z*+1; (v) *x*+1/2, *y*−1/2, *z*; (vi) *x*+1/2, *y*−1/2, *z*+1; (vii) *x*+1/2, *y*+1/2, *z*+1; (viii) *x*+1/2, *y*+1/2, *z*; (ix) −*x*+3/2, *y*−1/2, −*z*+1.

Table S8 Hydrogen-bond geometry (Å, º) for **(L-LeuH^{+})·M^{-}** structure at 250 K

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O61—H61···O41	0.83	1.59	2.424 (5)	179
N2—H2*A*···O61^{i}	0.90	2.05	2.906 (5)	160
N2—H2*B*···O23^{ii}	0.90	2.04	2.863 (5)	151
N2—H2*C*···O51^{iii}	0.90	1.90	2.780 (6)	164
O12—H12···O33^{iv}	0.83	1.80	2.596 (6)	160
O62—H62···O42	0.83	1.61	2.439 (4)	174
O63—H63···O43	0.83	1.60	2.421 (5)	172

N3—H3*A*···O22^{v}	0.90	1.93	2.780 (5)	158
N3—H3*B*···O53^{vi}	0.90	1.94	2.834 (6)	171
N3—H3*C*···O63^{vii}	0.90	2.02	2.867 (5)	155
O13—H13···O52^{viii}	0.83	1.79	2.599 (6)	163
O11—H11···O31	0.83	1.77	2.599 (5)	172
N1—H1*A*···O21^{ix}	0.90	2.15	2.890 (5)	138
N1—H1*A*···O31^{ix}	0.90	2.42	3.005 (5)	123
N1—H1*B*···O42^{v}	0.90	1.97	2.867 (5)	177
N1—H1*C*···O32^{viii}	0.90	1.99	2.863 (6)	165

Symmetry codes: (i) −*x*+1, *y*, −*z*+1; (ii) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1, −*z*+1; (iv) −*x*+1, *y*+1, −*z*+1; (v) *x*+1/2, *y*−1/2, *z*; (vi) *x*+1/2, *y*−1/2, *z*+1; (vii) *x*+1/2, *y*+1/2, *z*+1; (viii) *x*+1/2, *y*+1/2, *z*; (ix) −*x*+3/2, *y*−1/2, −*z*+1.

Table S9 Hydrogen-bond geometry (Å, º) for **(L-LeuH^{+})·M^{-}** structure at 275 K

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O61—H61···O41	0.82	1.60	2.422 (4)	176
N2—H2*A*···O61^{i}	0.89	2.07	2.914 (5)	158
N2—H2*B*···O23^{ii}	0.89	2.05	2.863 (5)	152
N2—H2*C*···O51^{iii}	0.89	1.91	2.777 (5)	164
O12—H12···O33^{iv}	0.82	1.82	2.599 (5)	158
O62—H62···O42	0.82	1.61	2.434 (4)	178
O63—H63···O43	0.82	1.60	2.422 (5)	179
N3—H3*A*···O22^{v}	0.89	1.94	2.778 (5)	156
N3—H3*B*···O53^{vi}	0.89	1.96	2.838 (5)	171
N3—H3*C*···O63^{vii}	0.89	2.03	2.870 (5)	157
O13—H13···O52^{viii}	0.82	1.80	2.597 (5)	165
O11—H11···O31	0.82	1.78	2.599 (5)	173
N1—H1*A*···O21^{ix}	0.89	2.16	2.891 (5)	139

N1—H1*A*···O31^{ix}	0.89	2.44	3.014 (5)	123
N1—H1*B*···O42^{v}	0.89	1.99	2.875 (5)	175
N1—H1*C*···O32^{viii}	0.89	2.00	2.867 (5)	166

Symmetry codes: (i) −*x*+1, *y*, −*z*+1; (ii) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1, −*z*+1; (iv) −*x*+1, *y*+1, −*z*+1; (v) *x*+1/2, *y*−1/2, *z*; (vi) *x*+1/2, *y*−1/2, *z*+1; (vii) *x*+1/2, *y*+1/2, *z*+1; (viii) *x*+1/2, *y*+1/2, *z*; (ix) −*x*+3/2, *y*−1/2, −*z*+1.

Table S10 Hydrogen-bond geometry (Å, º) for **(L-LeuH^{+})·M^{-}** structure at 293 K

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O61—H61···O41	0.82	1.60	2.415 (4)	176
N2—H2*A*···O61^{i}	0.89	2.07	2.918 (4)	159
N2—H2*B*···O23^{ii}	0.89	2.06	2.875 (5)	152
N2—H2*C*···O51^{iii}	0.89	1.91	2.776 (5)	164
O12—H12···O33^{iv}	0.82	1.80	2.596 (5)	163
O62—H62···O42	0.82	1.61	2.430 (4)	177
O63—H63···O43	0.82	1.60	2.424 (5)	178
N3—H3*A*···O22^{v}	0.89	1.92	2.782 (5)	162
N3—H3*B*···O53^{vi}	0.89	1.96	2.843 (5)	169
N3—H3*C*···O63^{vii}	0.89	2.06	2.875 (5)	152
O13—H13···O52^{viii}	0.82	1.80	2.592 (5)	163
O11—H11···O31	0.82	1.79	2.602 (5)	173
N1—H1*A*···O21^{ix}	0.89	2.16	2.894 (5)	139
N1—H1*A*···O31^{ix}	0.89	2.43	3.018 (5)	124
N1—H1*B*···O42^{v}	0.89	1.99	2.879 (4)	177
N1—H1*C*···O32^{viii}	0.89	2.01	2.873 (5)	164

Symmetry codes: (i) −*x*+1, *y*, −*z*+1; (ii) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1, −*z*+1; (iv) −*x*+1, *y*+1, −*z*+1; (v) *x*+1/2, *y*−1/2, *z*; (vi) *x*+1/2, *y*−1/2, *z*+1; (vii) *x*+1/2, *y*+1/2, *z*+1; (viii) *x*+1/2, *y*+1/2, *z*; (ix) −*x*+3/2, *y*−1/2, −*z*+1.

Table S11 Parameters of the Salje thermal equations of state for **(L-LeuH^{+})·M^{-}** structure

Data collection	*cooling from 293 K to 100 K*
V_0 (Å^3)	3792.8(8)
$p_1 \cdot 10^5$ (Å/K)	97(1)
θ_{sat} (K)	169(2)
$\alpha_{(295\ K,\ 1\ atm)} \cdot 10^5$ (K^{-1})	16.7(8)

Table S12 Change in atom positions of asymmetric unit cell of **(L-LeuH$^+$)·M$^-$** structure with in temperature range from 100 K to 293 K. Results obtained using "Structure Overlay" tool which built-into Mercury programme V. 3.10.

The temperature at which the position of the atom was refined	root-mean-square deviation (RMSD), Å
100	0
125	0.020
150	0.035
175	0.052
200	0.072
225	0.096
250	0.119
275	0.141
293	0.162

Table S13 RMSD of atom positions of every maleate anion and every L-leucinium cation with in temperature range from 100 K to 293 K. Results obtained using "Molecule Overlay" tool which built-in to Mercury programme V. 3.10. Numeration of molecules according to .cif file (last digital of atoms corresponds to molecule number, e.g. atom O5**1** belongs to molecule #**1**)

	maleate anion 1		maleate anion 2		maleate anion 3		L-leucinium cation 1		L-leucinium cation 2		L-leucinium cation 3	
T,K	RMSD, Å	Max.D, Å	RMSD, Å	Max.D, Å	RMSD, Å	Max.D, Å	RMSD, Å	Max.D, Å	RMSD, Å	Max.D, Å	RMSD, Å	Max.D, Å
100	0	0	0	0	0	0	0	0	0	0	0	0
125	0.0046	0.0073	0.0045	0.0086	0.0049	0.0076	0.0053	0.007	0.0069	0.0111	0.0042	0.0062
150	0.0034	0.0046	0.0032	0.0044	0.0065	0.0119	0.0071	0.011	0.0096	0.0179	0.0092	0.0174

175	0.004	0.0065	0.0049	0.0095	0.0103	0.0187	0.0108	0.018	0.0138	0.0252	0.0166	0.0314
200	0.067	0.09	0.0053	0.0091	0.0132	0.0251	0.014	0.024	0.0177	0.0311	0.0221	0.04
225	0.0075	0.0125	0.0083	0.0135	0.0171	0.0293	0.0181	0.032	0.0248	0.0453	0.0318	0.0583
250	0.0097	0.0167	0.0107	0.0153	0.0191	0.0319	0.0205	0.038	0.0292	0.0553	0.0419	0.0825
275	0.0111	0.0168	0.0149	0.0219	0.024	0.0403	0.0246	0.045	0.0341	0.0599	0.0504	0.0964
293	0.0136	0.0222	0.0132	0.0173	0.0264	0.0403	0.0275	0.054	0.0399	0.0721	0.0574	0.1113

Table S14 "Slope" coefficients calculated from linearisation of the distances between pairs of the centroids against temperature. Positive value of the slope parameter indicates approach of the corresponding centroids, whereas negative value means separation of centroids (highlighted in orange). Numeration according to Fig.7.

Centroid 1 – centroid 2	11-12	21-22	31-32	41-42	51-52	61-62
Slope	-5.337E-5	-15.43E-5	46.58E-5	62.35E-5	-19.49E-5	51E-5
Standard error	1.475E-5	1.419E-5	1.564E-5	1.327E-5	1.845E-5	2.463E-5
Relative movement	separate	separate	approach	approach	separate	approach
Centroid 1 – centroid 2	12-13	22-23	32-33	42-43	52-53	62-63
Slope	155E-5	99E-5	65.98E-5	99E-5	155E-5	97.60E-5
Standard error	5.668E-5	5.062E-5	3.439E-5	5.062E-5	5.668E-5	6.452E-5
Relative movement	approach	approach	approach	approach	approach	approach

Figure S1 Absolute changes in the unit cell parameters a, b, c and β (a, b, c, d) and relative changes of a, b, c parameters (e) of **(L-LeuH$^+$)·M$^-$** on cooling from 293 K to 100 K.

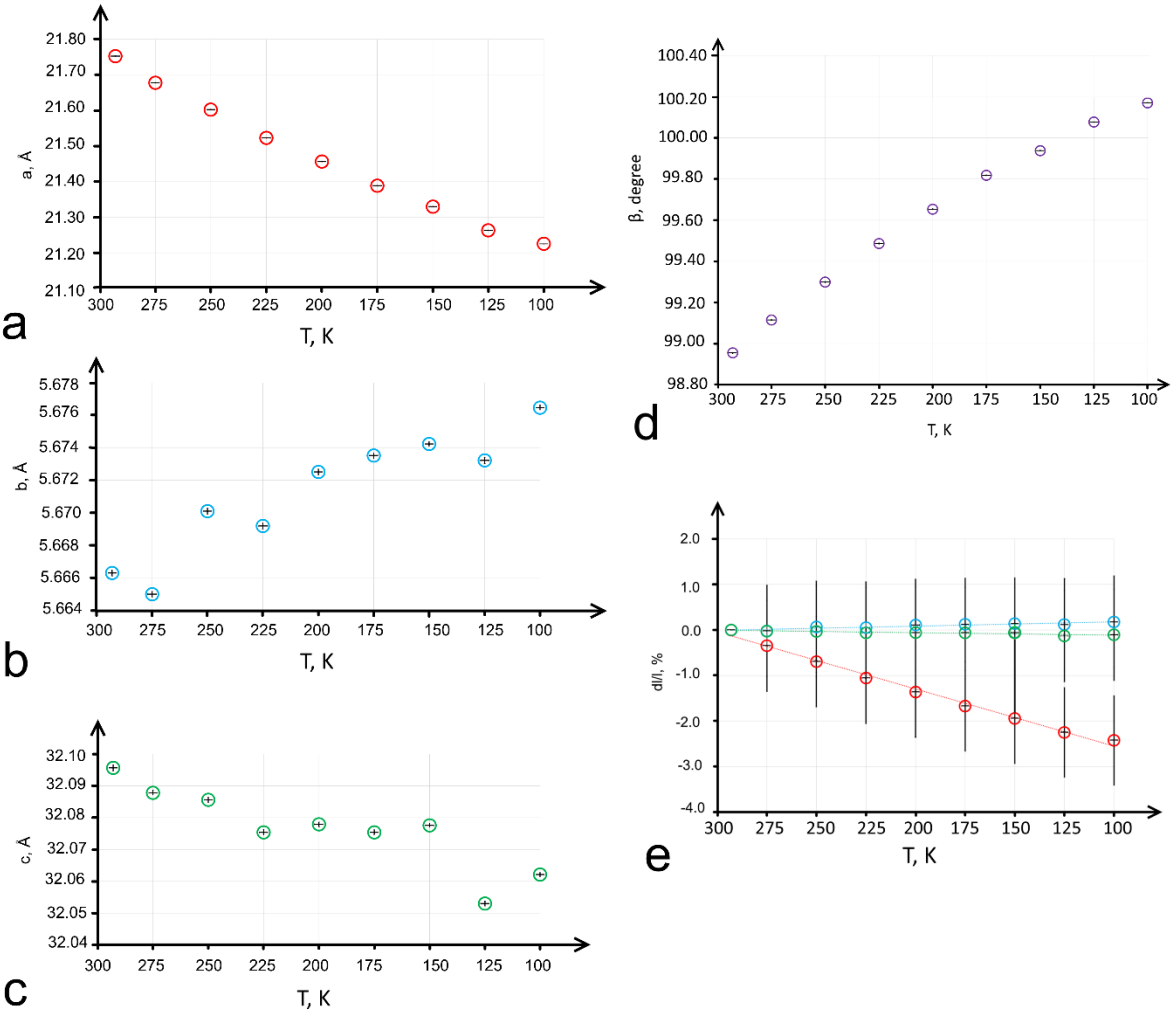

Figure S2 The change of Donor - Acceptor distances in the hydrogen bonds of **(L-LeuH$^+$)·M$^-$** on cooling process from 293 K to 100 K.

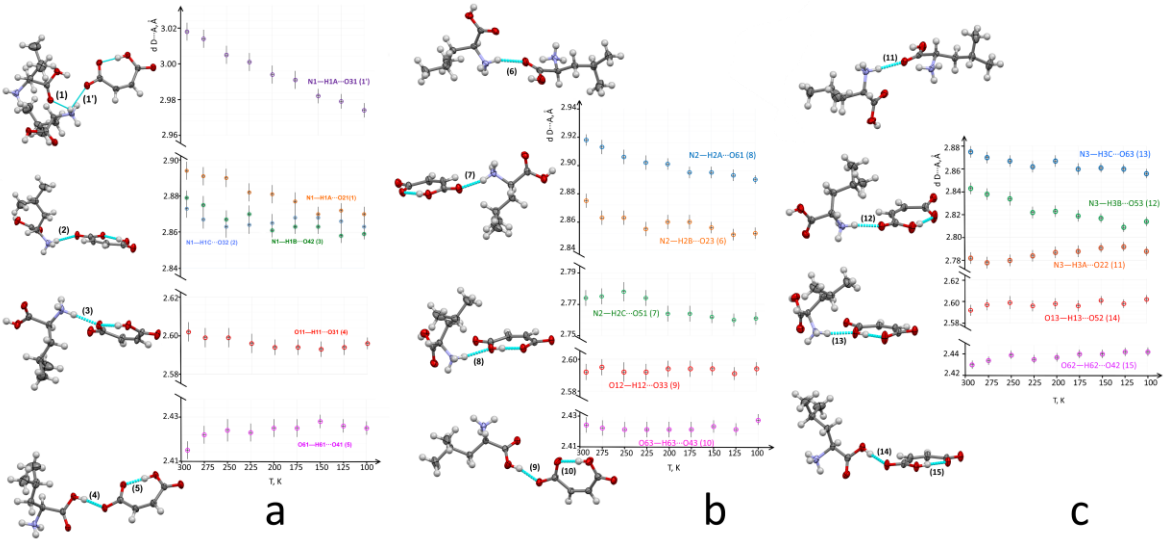

Figure S3 The length changing of $C^6_6(36)$ chain of **(L-LeuH$^+$)·M$^-$** on cooling from 293 K to 100 K.

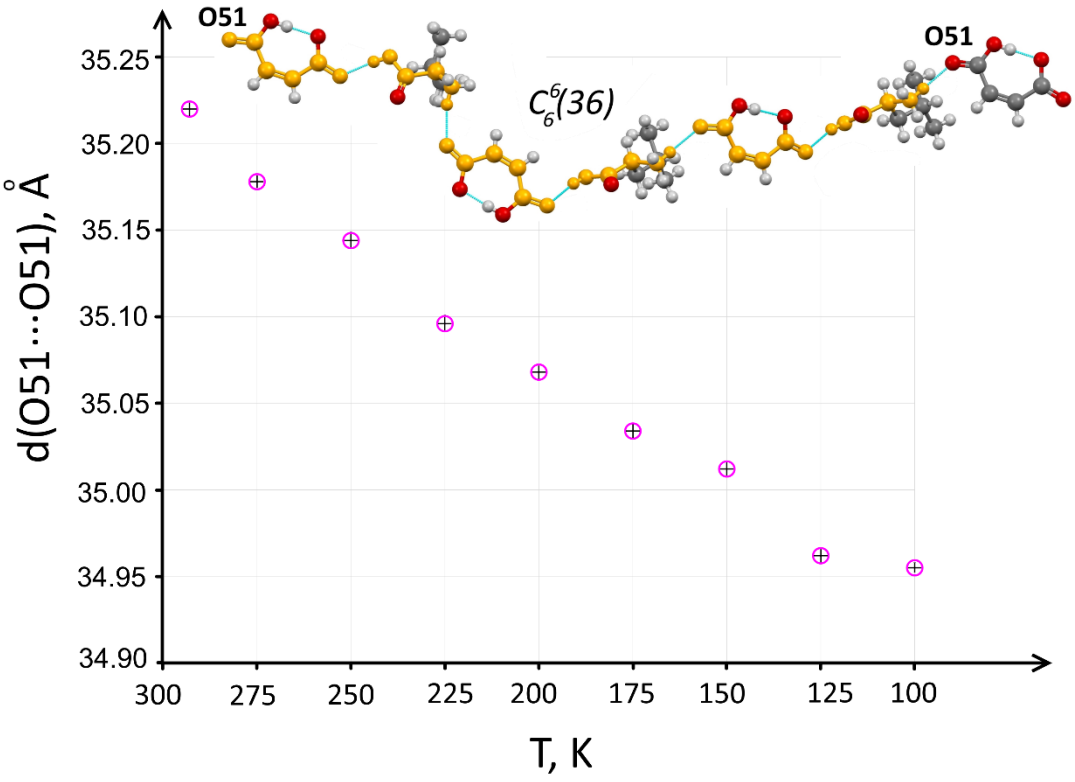

Figure S4 The change in the intramolecular distance between two external oxygen atoms of a maleate anion: a small stretching of the maleate anions on cooling from 293 K to 100 K in **(L-LeuH$^+$)·M$^-$**.

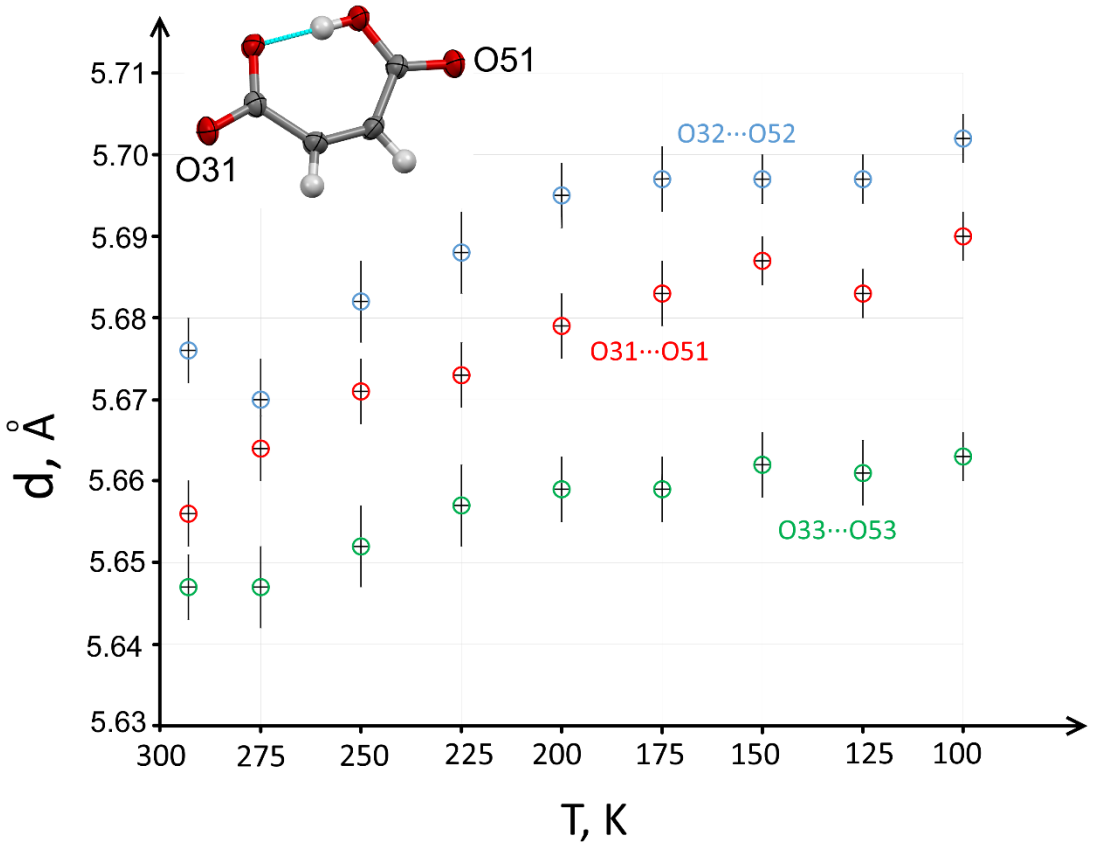

Figure S5 An example of the linearisation of the temperature dependences of the distances between centroids 11 and 12 (top line), and centroids 12 and 13 (bottom line). Coefficients *a* (intercept) and *b* (slope) are given in inserted tables. Full set of *a* coefficients for all pairs of the centroids is given in Table S14. Numeration according to Fig. 7.