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Supporting information for article:

Chiral bis(mandelato)borate salts for resolution *via* metathesis crystallization

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Table S1 Selected geometric parameters (Å, º) for **1** Li[B(R-Man)$_2$].H$_2$O

Li1—O1W	1.945 (4)	C14—C15	1.392 (4)
Li1—O10^{i}	1.963 (4)	C15—C16	1.384 (5)
Li1—O12	1.976 (4)	C16—C17	1.376 (4)
Li1—O20^{ii}	1.963 (4)	C17—C18	1.387 (3)
B1—O11	1.501 (2)	O20—C21	1.212 (3)
B1—O12	1.447 (3)	O21—C21	1.313 (2)
B1—O21	1.494 (3)	C21—C22	1.523 (3)
B1—O22	1.437 (3)	O22—C22	1.419 (2)
O10—C11	1.212 (2)	C22—C23	1.521 (3)
O11—C11	1.311 (2)	C23—C24	1.391 (4)
C11—C12	1.537 (2)	C23—C28	1.376 (4)
O12—C12	1.424 (2)	C24—C25	1.387 (4)
C12—C13	1.510 (3)	C25—C26	1.375 (6)
C13—C14	1.389 (3)	C26—C27	1.368 (5)
C13—C18	1.388 (3)	C27—C28	1.398 (4)
O10^{i}—Li1—O1W	105.57 (18)	O12—B1—O11	104.45 (15)
O12—Li1—O1W	126.2 (2)	O21—B1—O11	107.79 (15)
O12—Li1—O10^{i}	104.00 (17)	O21—B1—O12	110.95 (16)
O20^{ii}—Li1—O1W	105.10 (18)	O22—B1—O11	113.46 (16)
O20^{ii}—Li1—O10^{i}	122.2 (2)	O22—B1—O12	114.96 (17)
O20^{ii}—Li1—O12	95.56 (17)	O22—B1—O21	105.15 (15)

Table S2 Selected geometric parameters (Å, º) for **2** $NH_4[B(R\text{-}Man)_2]$

B1—O11	1.484 (2)	C13—C18	1.390 (3)
B1—O12	1.448 (2)	C14—C15	1.387 (3)
B1—O21	1.504 (2)	C15—C16	1.391 (3)
B1—O22	1.446 (2)	C16—C17	1.378 (4)
O10—C11	1.208 (2)	C17—C18	1.392 (3)
O11—C11	1.323 (2)	C21—C22	1.526 (3)
O12—C12	1.420 (2)	C22—C23	1.513 (2)
O20—C21	1.218 (2)	C23—C24	1.394 (3)
O21—C21	1.307 (2)	C23—C28	1.388 (3)
O22—C22	1.420 (2)	C24—C25	1.389 (3)
C11—C12	1.529 (3)	C25—C26	1.389 (3)
C12—C13	1.514 (3)	C26—C27	1.384 (3)
C13—C14	1.391 (3)	C27—C28	1.391 (3)
O12—B1—O11	104.96 (14)	O22—B1—O12	114.68 (15)
O21—B1—O11	108.15 (15)	O22—B1—O21	103.97 (15)
O21—B1—O12	112.29 (15)	O22—B1—O11	112.80 (15)

Table S3 Selected geometric parameters (Å, º) for **3** $NBu_4[B(R\text{-}Man)_2]$

N1—C51	1.522 (2)	B1—O11	1.519 (3)
N1—C55	1.520 (3)	B1—O12	1.442 (3)
N1—C61	1.529 (2)	B1—O21	1.494 (3)
N1—C65	1.519 (3)	B1—O22	1.437 (3)
N2—C71	1.520 (2)	B2—O31	1.516 (3)
N2—C75	1.528 (2)	B2—O32	1.438 (3)
N2—C81	1.523 (2)	B2—O41	1.499 (3)
N2—C85	1.523 (2)	B2—O42	1.431 (3)
C55—N1—C51	108.22 (15)	C66—C65—N1	114.75 (17)
C61—N1—C51	110.99 (15)	O12—B1—O11	104.22 (17)
C61—N1—C55	108.16 (16)	O21—B1—O11	108.22 (18)
C65—N1—C51	108.12 (15)	O21—B1—O12	112.87 (17)

C65—N1—C55	111.93 (15)	O22—B1—O11	111.84 (16)
C65—N1—C61	109.43 (16)	O22—B1—O12	114.35 (18)
C52—C51—N1	115.18 (16)	O22—B1—O21	105.34 (18)
C53—C52—C51	109.40 (17)	O32—B2—O31	104.29 (17)
C54—C53—C52	112.7 (2)	O41—B2—O31	107.73 (17)
C56—C55—N1	116.26 (17)	O41—B2—O32	112.81 (17)
C57—C56—C55	109.63 (18)	O42—B2—O31	113.08 (17)
C58—C57—C56	111.81 (19)	O42—B2—O32	113.84 (18)
C62—C61—N1	115.53 (17)	O42—B2—O41	105.13 (17)
C63—C62—C61	111.59 (19)		

Symmetry code(s): (i) *x*−1, *y*, *z*; (ii) −*x*, *y*−1/2, −*z*+1.

Table S4 Selected Torsion Angles (º) *(anomalous & gauche values highlighted)*

showing twist of Ph substituent from Chelate Ring in **1-3**:

Li Salt **1**

O(12) – C(12) –C(13) – C(18) -49.0(2) O(22) – C(22) –C(23) – C(28) -13.6(3)

NH_4 Salt **2**

O(12) – C(12) –C(13) – C(18) -67.6(2) O(22) – C(22) –C(23) – C(28) -43.2(2)

NBu_4 Salt **3**

O(12) – C(12) –C(13) – C(18) -11.4(3) O(22) – C(22) –C(23) – C(28) -4.0(3)

O(32) – C(32) –C(33) – C(38) -19.8(3) O(42) – C(42) –C(43) – C(48) 4.1(3)

Chain torsions for NBu_4 Ions in **3 :**

N(1) – C(51) – C(52) – C(53)	-169.5(2)	C(51) – C(52) – C(53) – C(54)	77.0(2)
N(1) - C(55) – C(56) – C(57)	-178.5(2)	C(55) – C(56) – C(57)-C(58)	171.8(2)
N(1) – C(61) – C(62) – C(63)	-162.6(2)	C(61) – C(62) – C(63) – C(64)	-72.0(2)
N(1) - C(65) – C(66) – C(67A)	-155.6(3)	C(65) – C(66) – C(67A)-C(68A)	-63.1(5)
N(2) – C(71) – C(72) – C(73)	179.9(2)	C(71) – C(72) – C(73) – C(74)	176.4(2)
N(2) - C(75) – C(76) – C(77)	-167.7(2)	C(75) – C(76) – C(77)-C(78)	-176.0(2)
N(2) – C(81) – C(82) – C(83)	173.9(2)	C(81) – C(82) – C(83) – C(84)	-64.2(3)
N(2) - C(85) – C(86) – C(87)	-176.5(2)	C(85) – C(86) – C(87)-C(88)	- 179.8(2)

Table S5 Hydrogen-bond parameters for **1** $Li[B(R\text{-}Man)_2].H_2O$ and **2** $NH_4[B(R\text{-}Man)_2]$

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
O1W-H1Wa-O22^{i}	0.88(5)	2.03(5)	2.856(2)	156(4)
N1—H1a···O22^{ii}	0.92(3)	1.95(3)	2.857 (2)	173(3)
N1—H1b···O20^{iii}	0.96(3)	1.82(3)	2.767 (2)	167(3)
N1—H1c···O10^{iv}	0.91(3)	2.13(3)	2.926 (2)	145(3)
N1—H1d···O12	0.89(3)	1.96(3)	2.823 (2)	163(3)

Symmetry code(s): (i) −*x*, *y*+1/2, 1−*z*;

(ii) −*x*+1, *y*−1/2, −*z*+1; (iii) −*x*, *y*−1/2, −*z*+1; (iv) *x*, *y*−1, *z*.

Figure S1 a) Packing diagram for **1** along [001] showing rectangular 2D grid for coordination polymer with b) Six-membered ring 'honeycomb' topological connectivity.

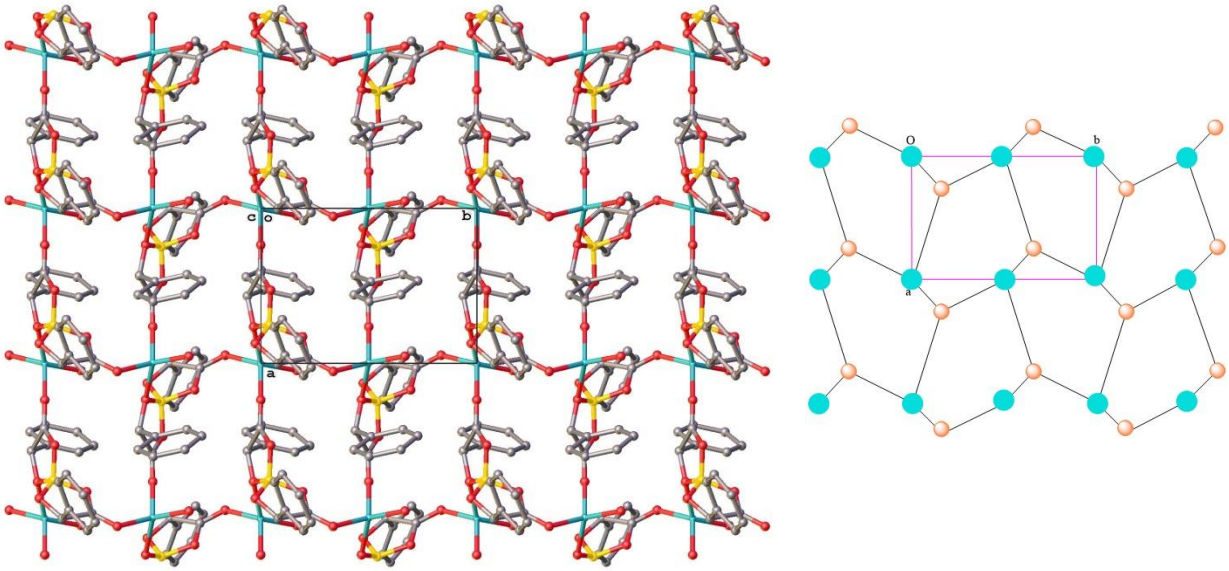

Figure S2 Packing diagram for **1** along [100] showing 2D coordination polymer slabs along c-axis.

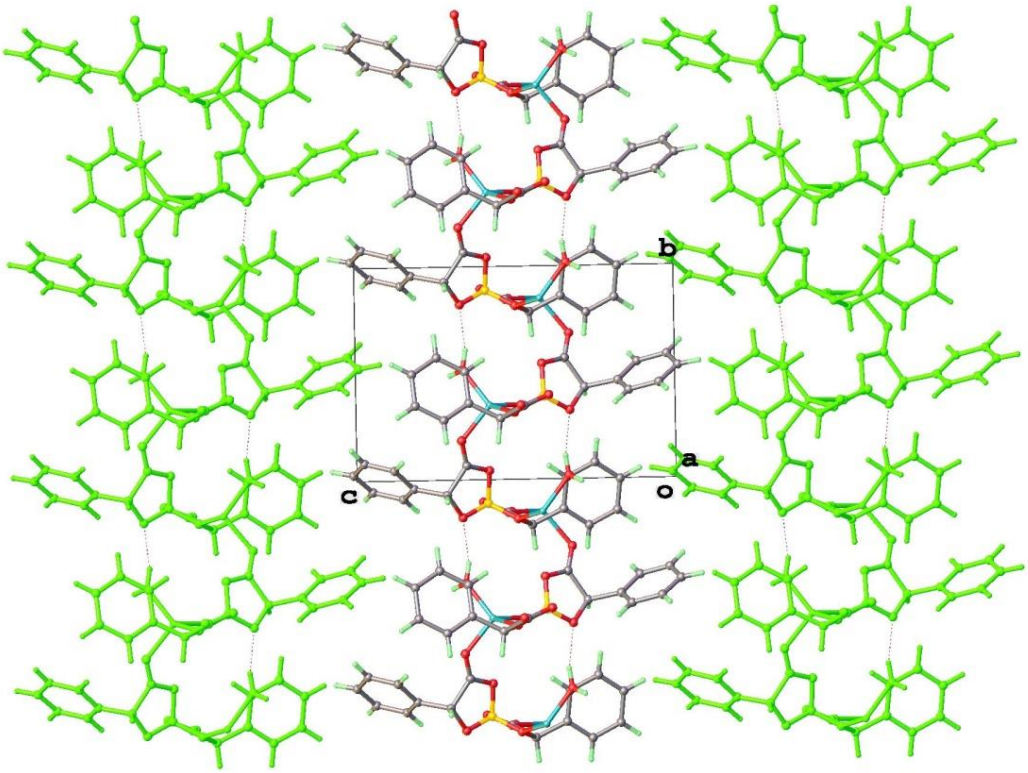

Figure S3 Powder diffractogram for Li[B(R-Man)$_2$].H_2O **1**.

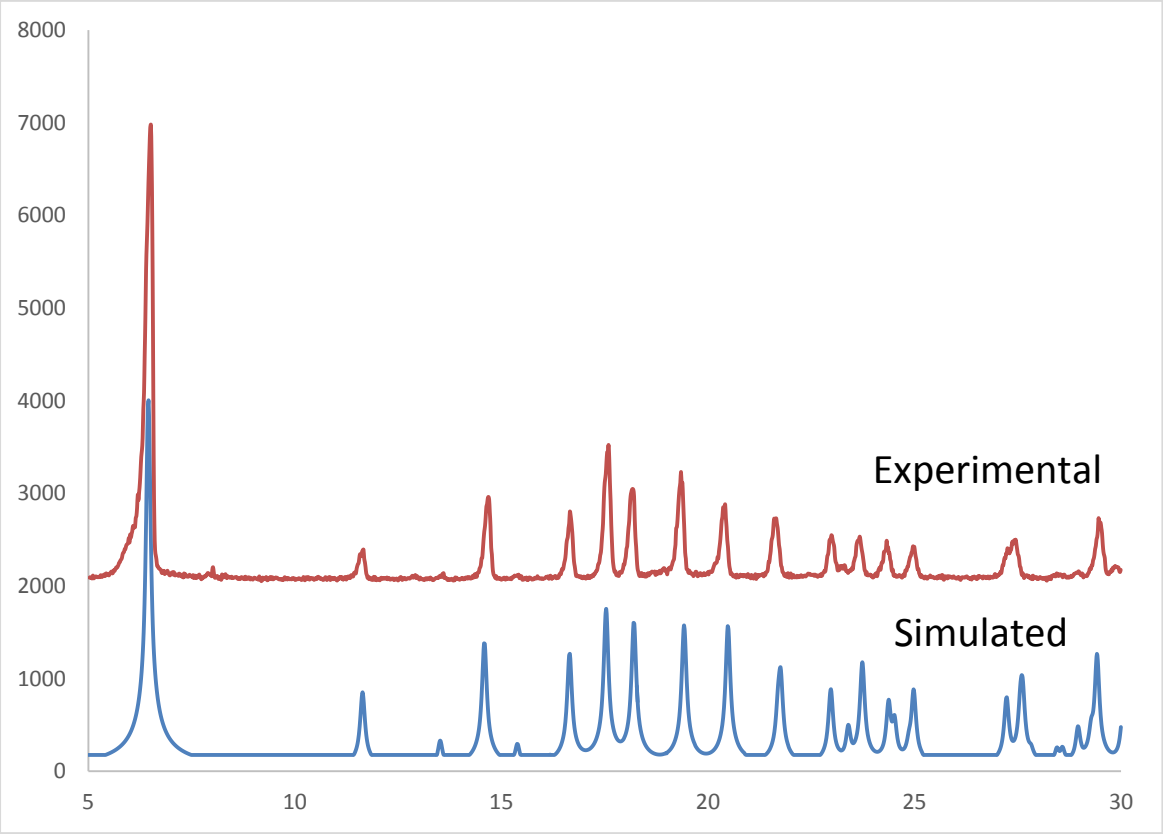

Figure S4 UV spectra of **1** in ethanol.

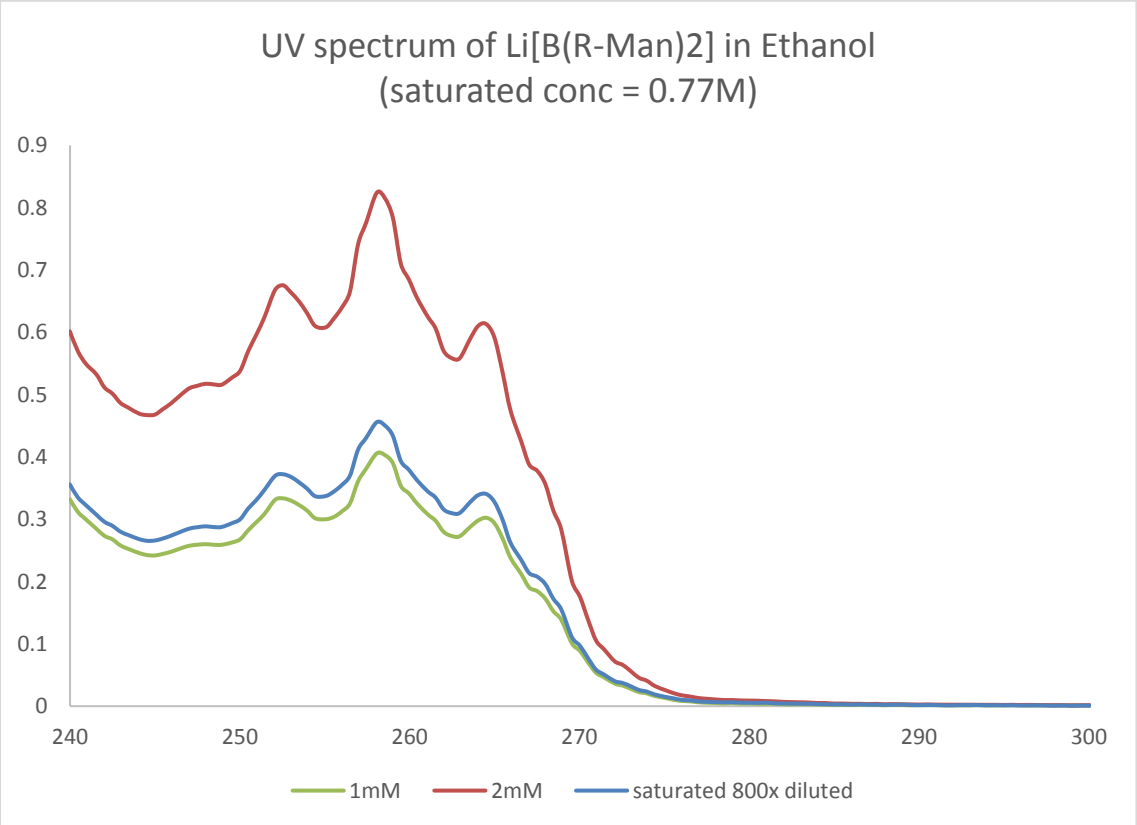

Figure S5 Packing diagram for **2** along [100] showing alternating regions along c-axis.

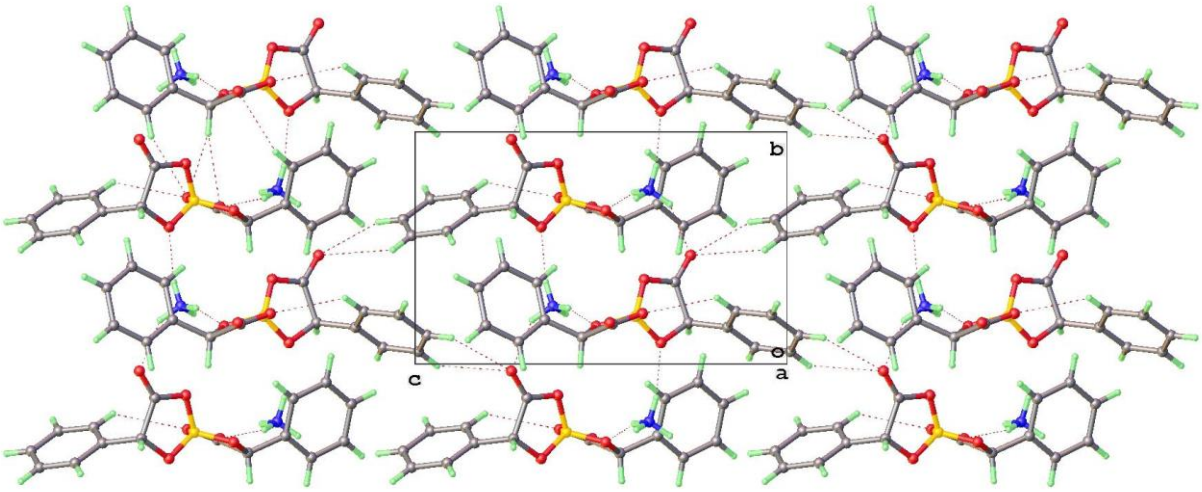

Figure S6 Powder diffractogram for $NH_4[B(R\text{-}Man)_2]$ **2**.

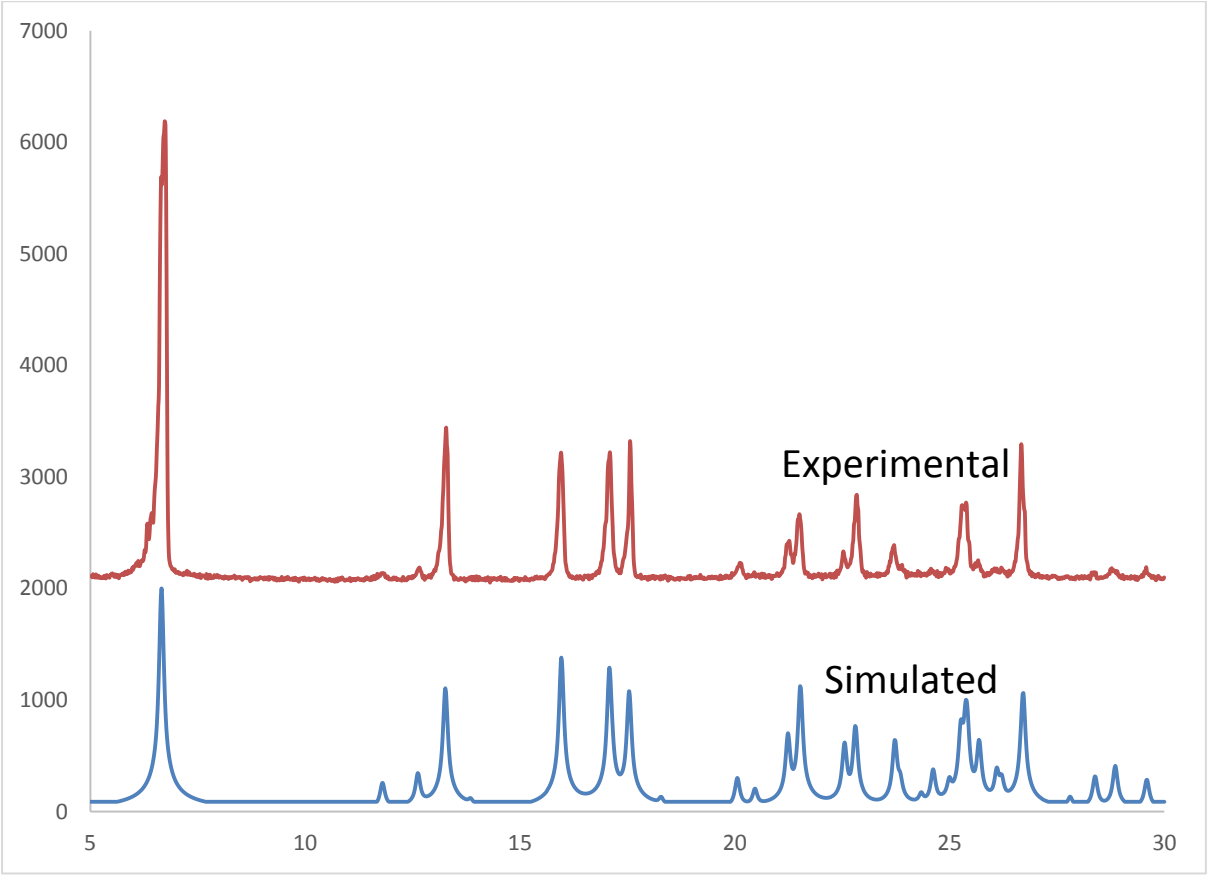

Figure S7 Packing diagram for **3** along [100] with colour coding of symmetry related [NBu_4] ions.

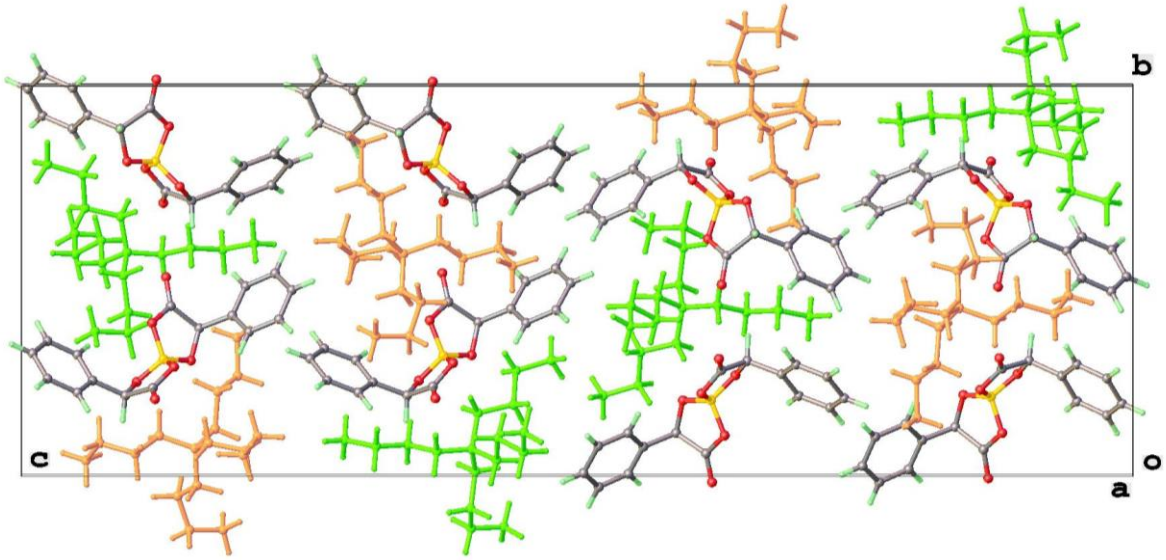

Figure S8 Overlay of the two independent NBu_4 cations in **3**.

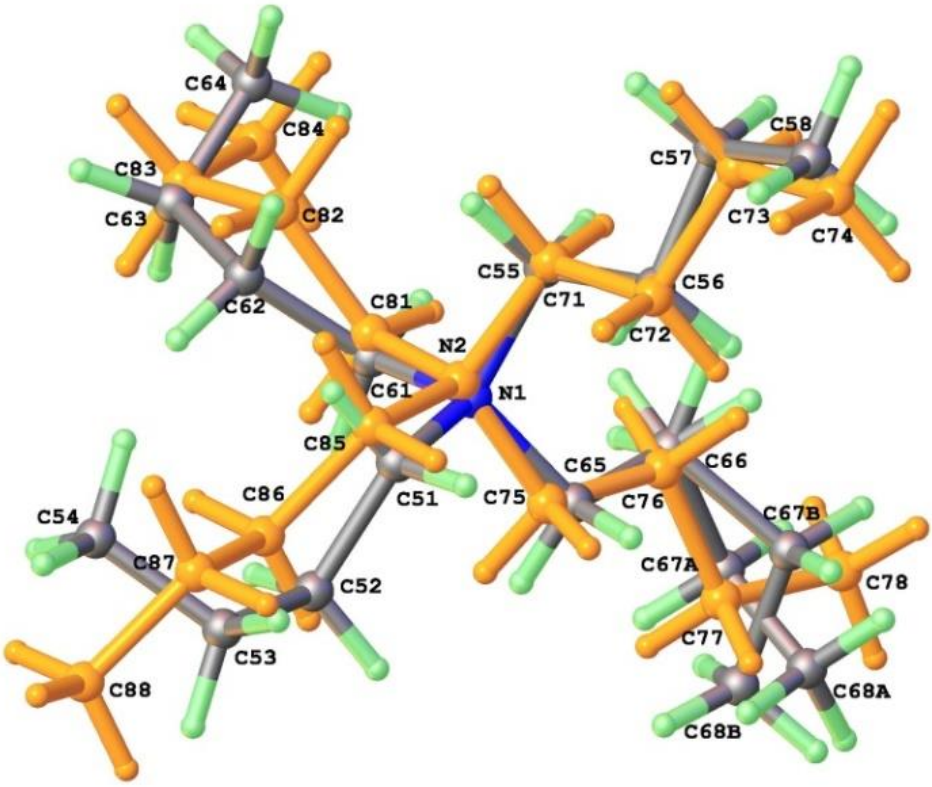

Figure S9 Differential scanning calorimetry plot for **3**, with melting to chiral ionic liquid at 41°C.