Electronic Supporting Information

The 1:1 and 1:2 salts of 1,4-diazabicyclo[2.2.2]octane with bis(trifluoromethylsulfonyl)amine: thermal behaviour and polymorphism

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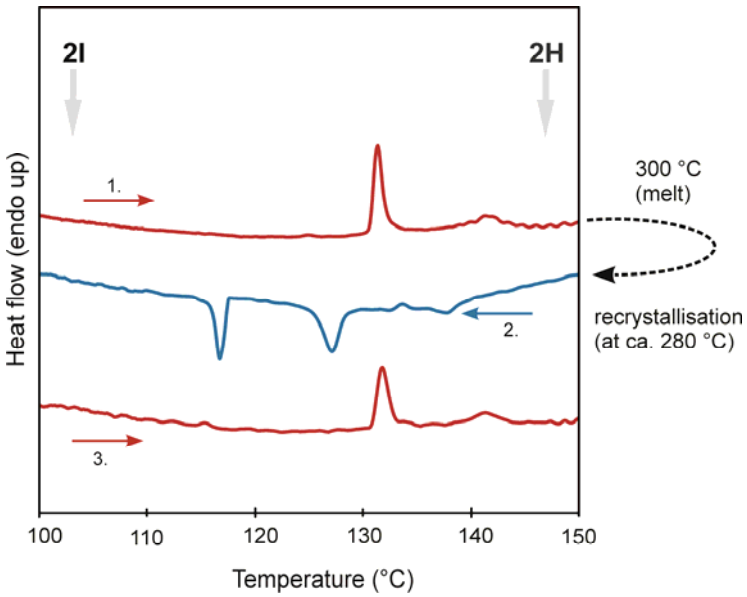

Fig. S1 DSC curves of **2** showing the temperature range of the second reversible phase transition between **2I** (intermediate temperature form) and the **2H** (high temperature form). The numbers in circles indicate the order of the heating/cooling cycles. The end temperature of the first heating run was 300 °C (higher than the melting point of **2H)**. On cooling, **2H** crystallizes from the melt at about 280 °C. Heating/cooling rate: 10 K min^{-1}.

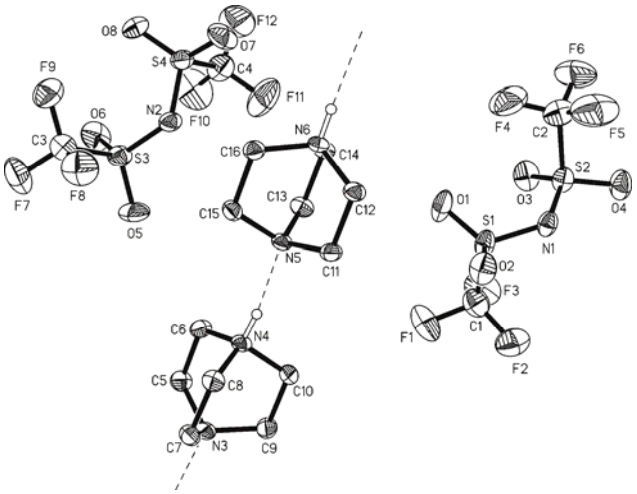

Fig. S2 The asymmetric unit of **1L** with atoms depicted as thermal ellipsoids drawn at the 50% level.

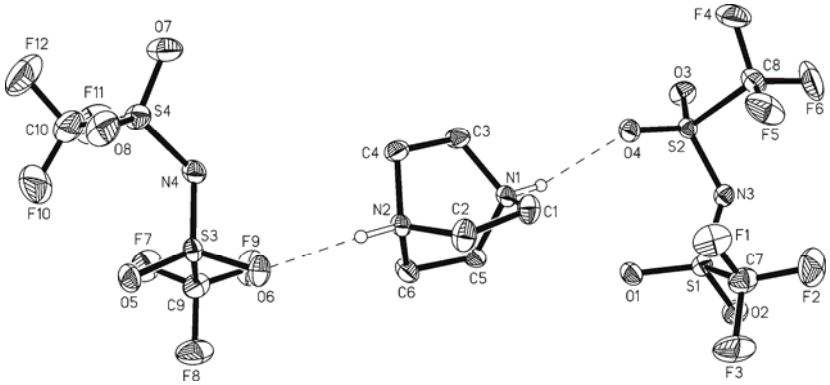

Fig. S3 The asymmetric unit of **2L** with atoms depicted as thermal ellipsoids drawn at the 50% level.

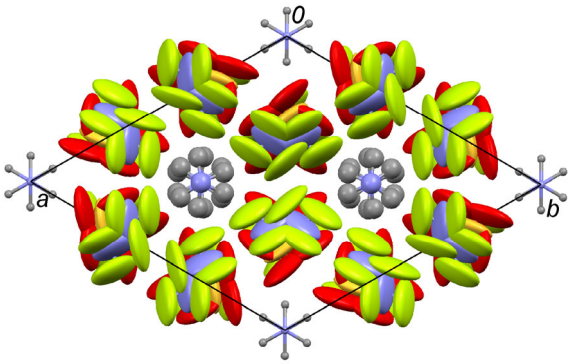

Fig. S3 Packing diagram of the hexagonal phase of **1H** at 333 K viewed along the chains of DABCO cations in the direction of the *c* axis. Displacement ellipsoids are drawn at the 50 % level.

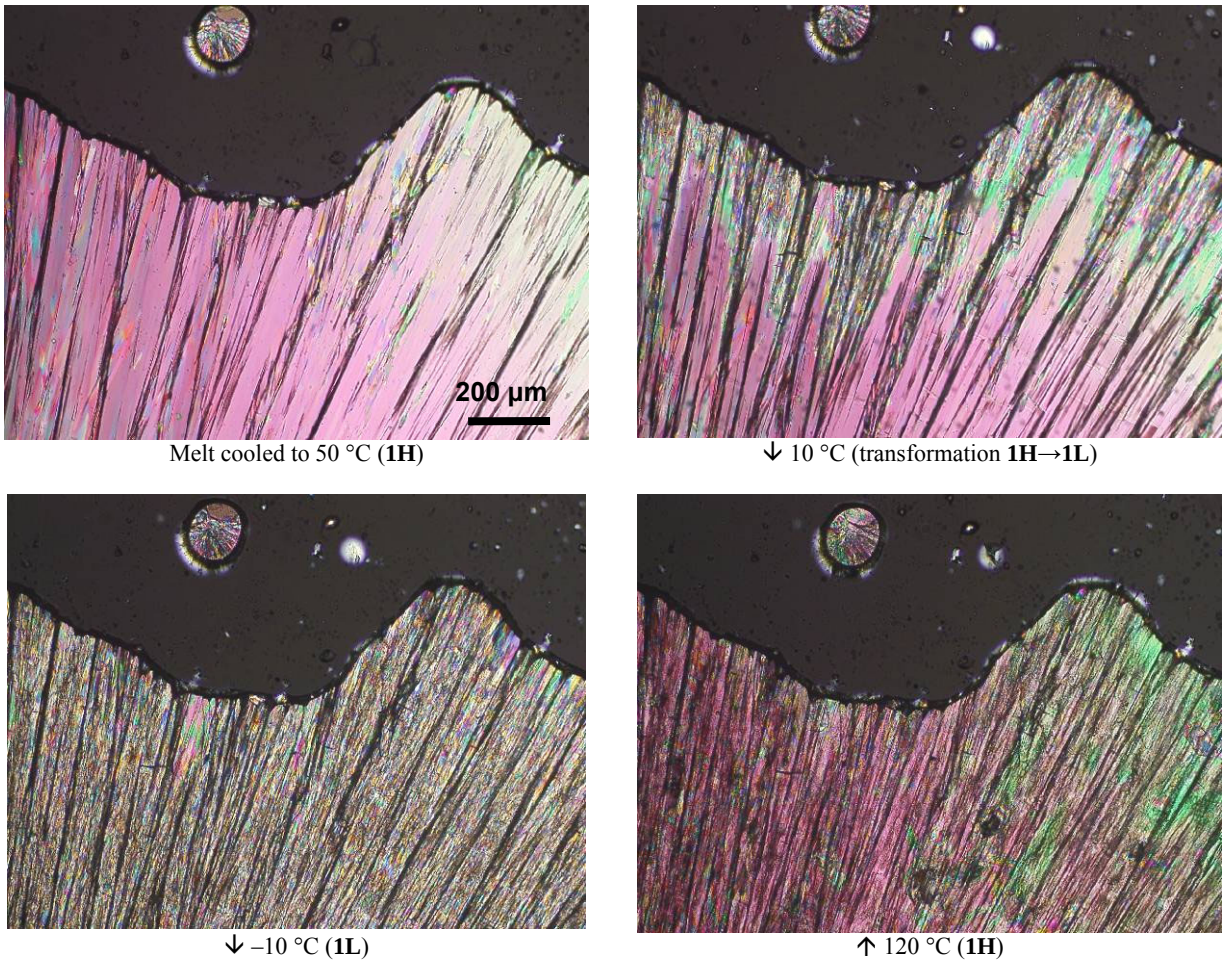

Fig. S4 Polarized light hot-stage microscopy of a recrystallized melt film of **1**, demonstrating the optical appearance of the phase transition. **1L**: low temperature form, **1H**: high temperature form; ↑: heating, ↓: cooling.

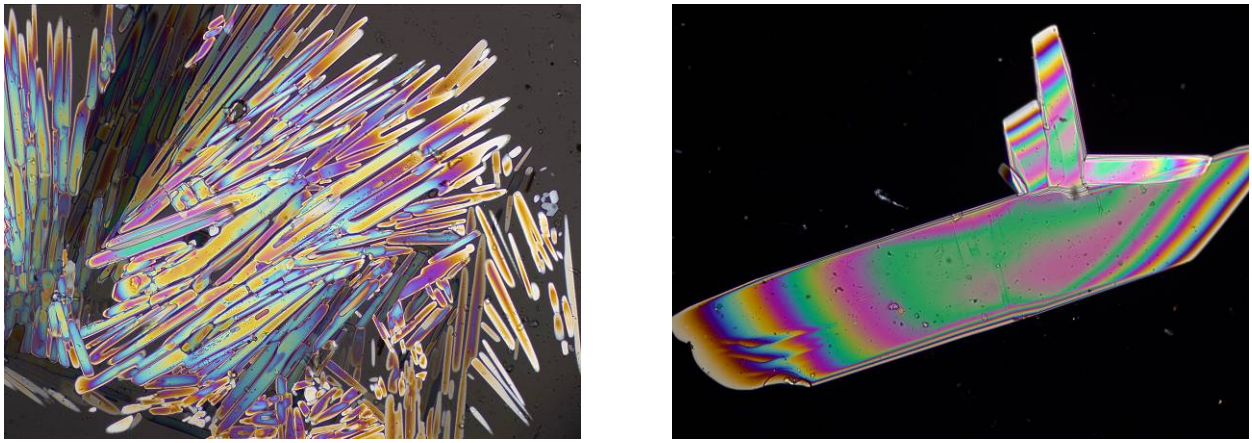

Fig. S5 Polarized light hot-stage microscopy of **1**. Left: photomicrograph showing the crystals of **1H** during the melting process. Right: single crystals of **1H** growing slowly in the melt just below the melting point.

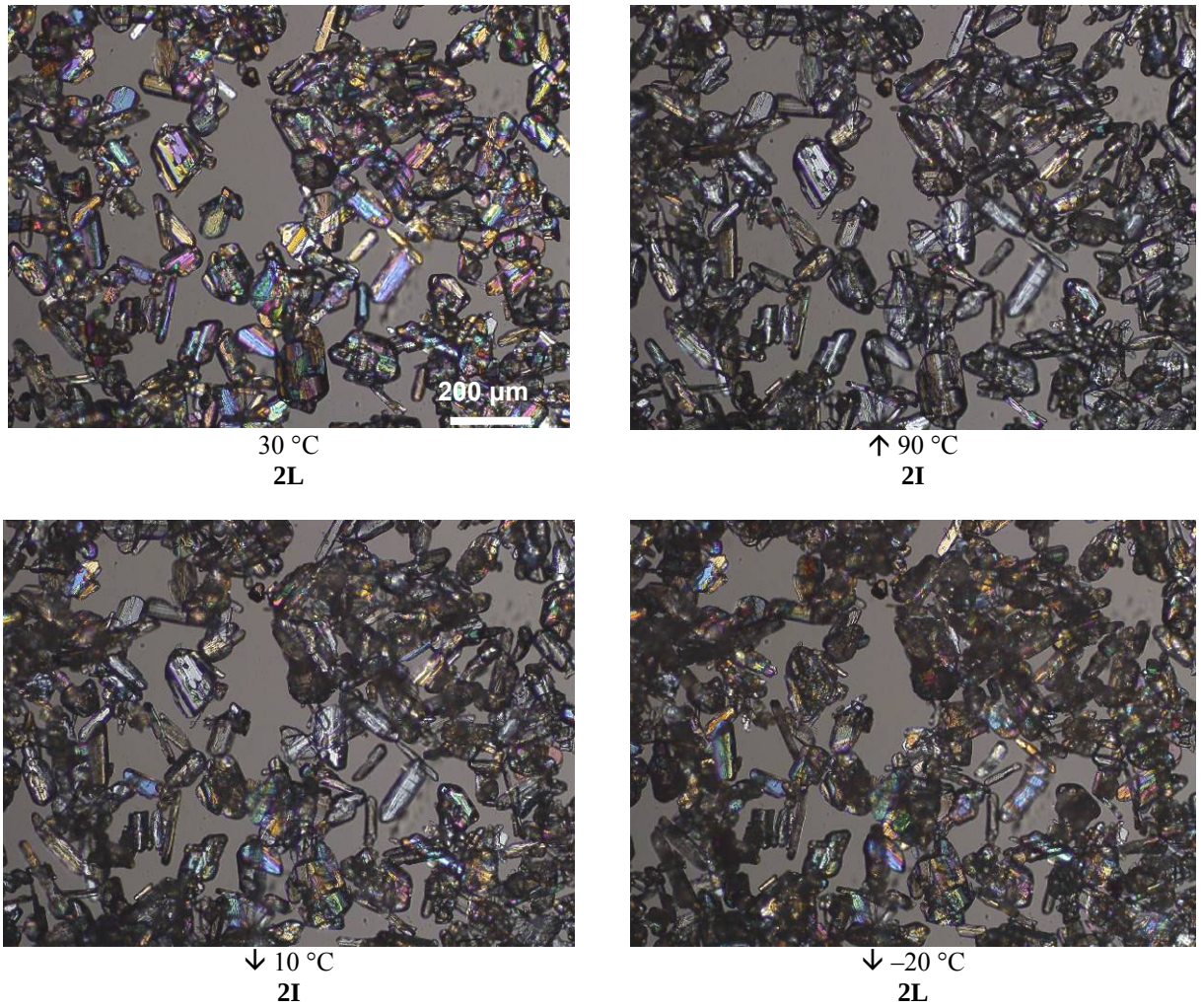

Fig. S6 Polarized light hot-stage microscopy of **2**, crystallized from an aqueous solution showing the transformation of the low temperature form (**2L**) to the intermediate temperature form (**2I**) and vice versa on heating (↑) and cooling (↓), respectively.

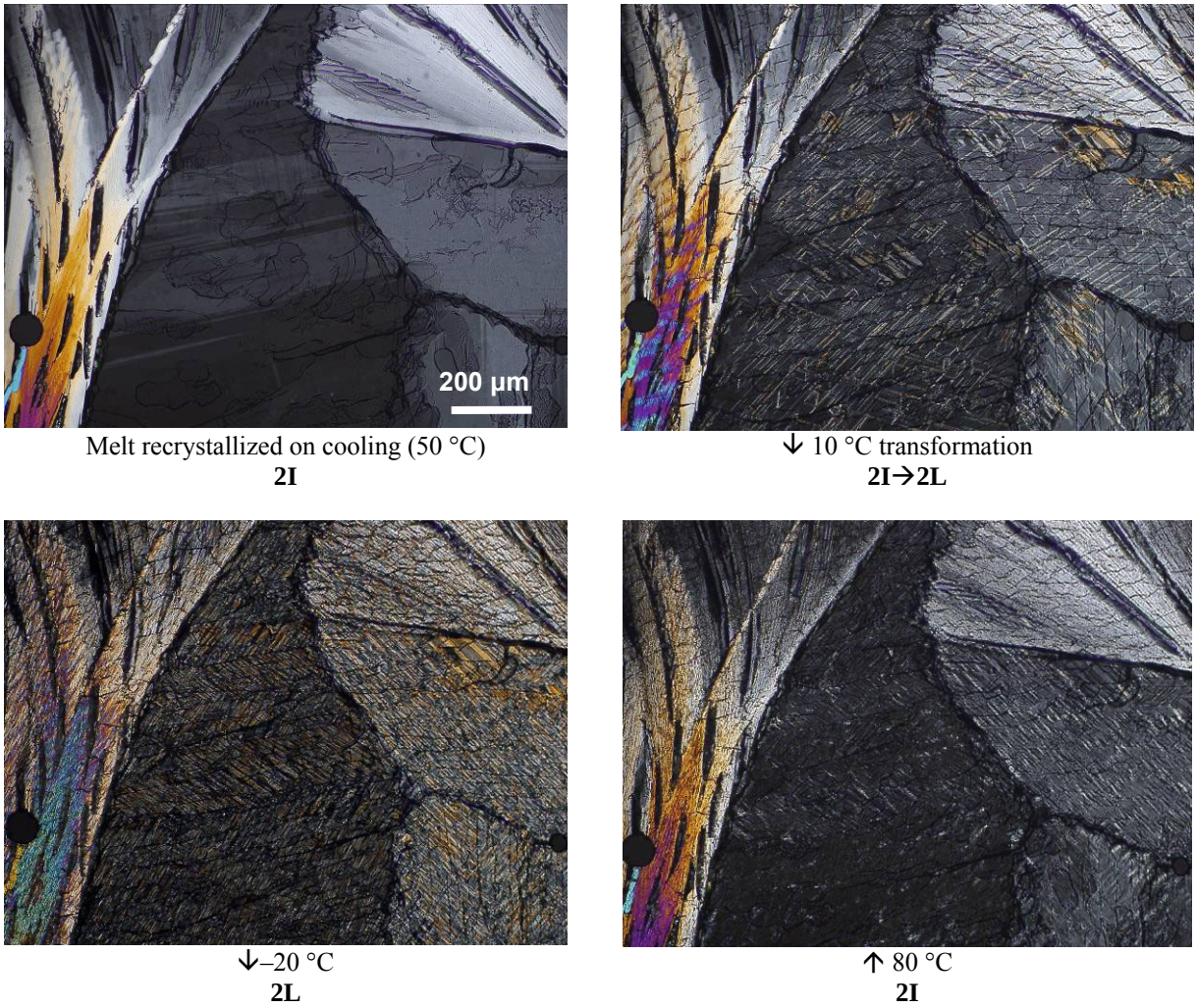

Fig. S7 Polarised light hot-stage microscopy of **2**, crystallized from the melt, showing the transformation of the intermediate temperature form (**2I**) to the low temperature form (**2L**) and vice versa on heating (↑) and cooling (↓).

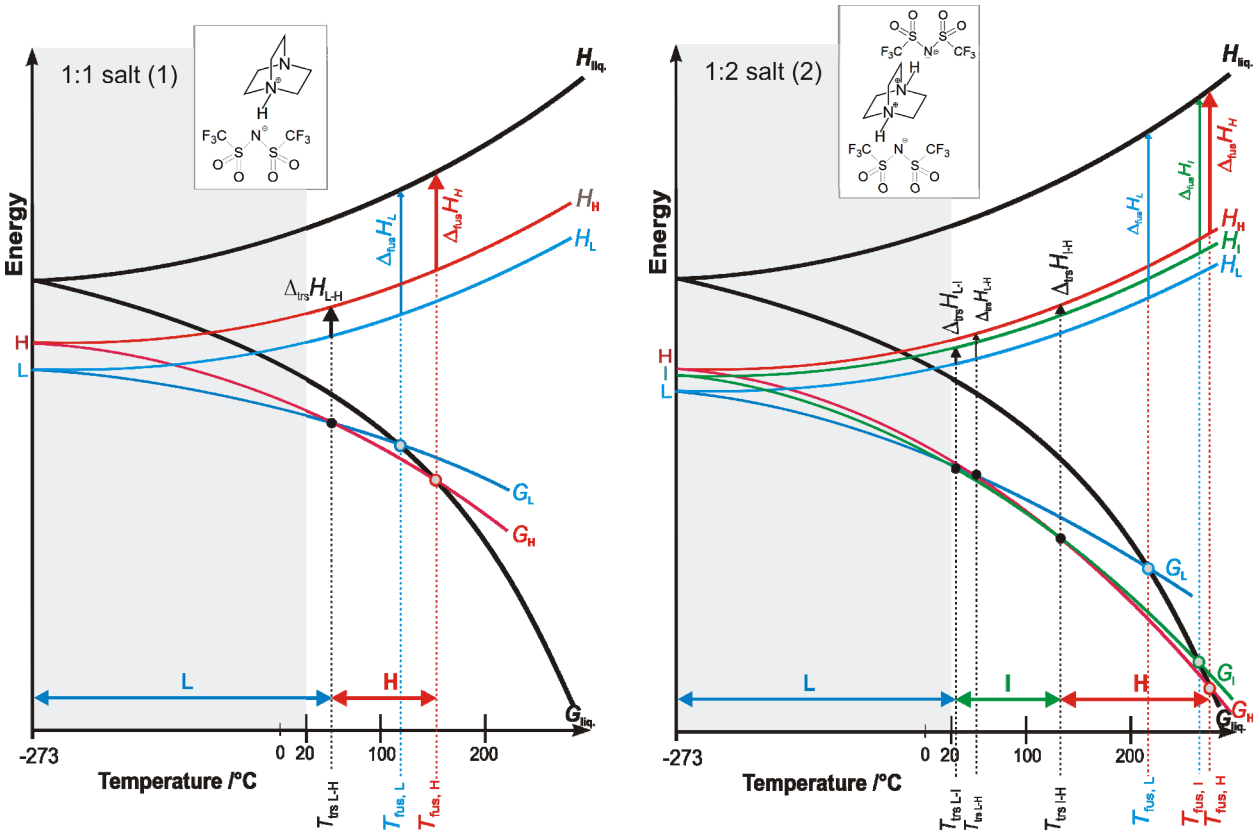

Fig. S8 Semi-schematic energy/temperature diagram of the polymorphic forms of the 1:1 and 1:2 salts. The letters **L**, **H** and **I** denote the low-, high- and intermediate temperature forms, respectively. The bold vertical arrows signify experimentally measured enthalpies and the horizontal arrows the temperature range where individual forms are thermodynamically stable. T_{fus}: melting point, G: Gibbs free energy, H: enthalpy, $\Delta_{fus}H$: enthalpy of fusion, T_{trs}: transition point, $\Delta_{trs}H$: transition enthalpy, *liq*: liquid phase (melt).

Table S1 Crystal data and refinement details of the high temperature forms of **1** and **2**

Compound	**1H**	**2H**
Empirical formula	$(C_6H_{13}N_2)^+ (C_2F_6NO_4S_2)^-$	$(C_6H_{14}N_2)^{2+} \cdot 2(C_2F_6NO_4S_2)^-$
Crystal system	Hexagonal	Orthorhombic
Space group	$P6_3cm$	$Cmc2_1$
Temperature/K	333(1)	413(1)
a/Å	16.2784(1)	10.5040(1)
b/Å	16.2784(1)	21.8333(2)
c/Å	10.5723(1)	10.6353(1)
Unit cell volume/Å^3	2426.19(3)	2439.06(3)
Z	6	4
D_x/g cm^{-3}	1.62	1.84
Geometry	Capillary, Ø = 0.5 mm	
2θ range, stepsize	3–70°, 0.009°	
Reflections collected	234	334
Independent reflections	187	245
Profile parameters, structural parameters, restraints	24, 57, 48	29, 90, 80
Goodness-of-fit (on y(obs))	1.47	2.05
Weighted pattern residual Rwp	0.068	0.063
Bragg R-factor	0.051	0.056
Bérar's e.s.d. correction factor[57]	2.4	2.7

Table S2 Selected torsion angles (º) in triflimide anions of **1L** and **2L**.

1L			
C1—S1—N1—S2	92.9(2)	C3—S3—N2—S4	–94.1(2)
S1—N1—S2—C2	87.0(2)	S3—N2—S4—C4	–87.3(2)
C1—S1—S2—C2	166.8(2)	C3—S3—S4—C4	–168.1(2)
2L			
C7—S1—N3—S2	–86.12(14)	C9—S3—N4—S4	125.25(13)
S1—N3—S2—C8	115.06(13)	S3—N4—S4—C10	–84.38(16)
C7—S1—S2—C8	28.5(1)	C9—S3—S4—C10	39.7(1)

Table S3. Torsion angles (°) for non–coordinating triflimide anions used to generate the diagram shown in Fig. 5 (top).

Refcode	φ_1	φ_2	C–S···S–C
ALAMEF	116.1	–90.1	25.1
ALAMEF	109.7	–89.2	19.3
ALANAC	90.6	92.9	171.2
BIFWAP	–93.5	–90.1	–170.9
DOCNIT	–91.3	–107.6	174.2
DOCNIT	90.8	93.5	172.1
DOCNOZ	122.1	–83.9	37.2
DOCNOZ	88.5	90.2	165.4
DOCNOZ	93.7	93.6	174.0
DOCNOZ	95.3	91.6	173.2
DOCNUF	99.2	96.5	–177.0
DOCNUF	–95.4	–95.0	–177.3
DOCNUF	–109.5	–88.3	174.4
DOCPAN	–90.2	–83.2	–160.4
DOCPAN	–95.0	–86.7	–169.6
DOCPAN	–94.8	–87.9	–170.2
DOCPAN	92.1	89.9	169.2
DOCPAN	89.2	100.4	177.5
DOCPER	–86.1	116.2	27.7
DOCPER	–93.4	–97.8	–177.4
DOCPER	93.9	86.8	168.3
DOQGOG	–93.6	–141.5	136.4
DOSBET	–86.3	120.9	34.1
GEDLIL	95.2	93.7	176.5
GEDLIL	86.8	89.1	163.1
GOMROQ	93.2	–122.5	–29.0
GOMROQ	90.7	88.6	167.1
GOMROQ	93.3	–140.5	–47.7
GOMROQ	–115.2	–92.1	165.3
GOMROQ	–95.5	–90.2	–171.3
GOMROQ	96.7	106.2	–169.7
IZUZAE	124.7	–90.9	33.7
JERDAM	98.4	92.5	178.1
JERFAO	–127.3	–98.3	146.9
JERFAO	–98.2	160.9	66.4
JERFAO	–86.7	151.2	64.8

JOSXIY	–90.9	–92.0	–169.8
KEKVEC	–97.6	–89.3	–173.9
KEKVEC	–89.6	–97.9	–174.8
LAZREK	89.3	85.5	161.7
LAZROU	–125.9	90.6	–34.5
LAZROU	–117.5	92.1	–24.7
LEVWEP	–91.2	–90.0	–168.6
LEVWEP	–94.5	–97.3	–178.9
LEWZIX	101.3	87.5	175.6
LONYUJ	–91.4	143.8	52.7
NAVCOD	–94.2	–88.3	–170.5
NAVCOD	–90.3	–93.0	–170.5
NAVCOD	88.9	93.7	170.6
NAVCOD	96.7	90.0	174.1
NEMMOI	–143.2	91.5	–50.1
PADDEE	–87.0	118.7	31.5
PADDEE	117.3	–84.0	32.9
PADDII	–92.8	–95.5	–175.7
RENSEJ	112.9	–84.4	26.9
RENSEJ	–92.5	118.6	27.0
SEFHER	89.6	91.0	168.2
SEFHER	91.5	93.7	173.2
SEJJAT	–94.4	–91.0	–172.7
SOFFUP	–94.9	143.5	50.4
TOJPOY	–117.2	–90.5	165.0
TOJPUE	–118.8	99.5	–18.6
TOJPUE	93.5	–114.5	–21.4
TOJQAL	–91.0	–97.0	–174.6
TOJQEP	–133.4	98.1	–35.7
TOJQEP	96.2	93.3	176.3
TOJQIT	96.8	99.7	–175.0
TOJQIT	94.0	85.7	167.1
TOJQOZ	–88.9	118.1	28.8
TOJQUF	84.9	99.6	171.7
TOJQUF	96.1	93.8	177.7
TOJRAM	99.5	88.2	175.8
TOJRAM	–91.5	–96.2	–175.4
TOJREQ	96.3	91.7	175.9
UCOPAE	88.6	100.8	176.3
VIBNUQ	90.4	99.8	176.6
VIBNUQ	–98.5	–97.1	178.5
WESZAW	88.2	–121.3	–32.1
WESZAW	85.9	–134.5	–49.2
WESZIE	–130.2	86.2	–43.7
WESZOK	92.2	96.1	174.6
WIJLAD	–85.6	131.3	45.2
WOLKOY	127.7	83.5	–160.4
WOLKOY	95.0	104.1	–173.1
WOLKUE	–91.4	–96.7	–175.8
WOLLEP	112.6	–98.9	13.3
WOLLIT	92.6	96.2	176.0
WOLLOZ	–92.0	–98.0	–176.4
WOLLOZ	91.3	93.4	171.7
XOMDAE	92.1	94.3	173.8
XOMDEI	97.5	90.1	174.5
XOMDIM	–95.8	–90.4	–173.4

XOMDOS	86.1	93.2	166.2
YEDKAU	90.6	103.4	–178.8
YEDKAU	–94.2	–95.1	–176.6
YESSUL	–91.3	–100.7	–179.1
YESSUL	95.3	90.4	172.6
YESTAS	89.5	105.3	–177.9
YESTEW	–93.9	–92.9	–174.2
YESTEW	117.3	86.8	–168.7
YESTEW	105.3	92.7	–175.1
YESTIA	–93.5	–78.9	–159.1
YESTIA	134.4	–92.3	42.7
YESTIA	–84.3	124.1	39.0
YONKIW	131.0	–87.0	47.1
YONKIW	92.3	92.5	167.7
YONKIW	–111.8	122.8	13.9
YONKOC	–90.6	–105.9	176.3
YONKOC	–91.5	–95.2	–172.6
ZURWIS	90.7	95.1	171.9
Bentivoglio et al., 2009			
CCDC 686015	92.8	91.8	171.6
CCDC 686016	97.6	94.8	179.4
CCDC 686017	90.7	119.8	–162.2
Schwärzler et al., 2009			
CCDC 726935	–89.5	–94.6	–171.1
CCDC 726938	–96.4	–88.1	–171.6
CCDC 726940	–90.7	–90.4	–167.6
CCDC 726940	90.1	91.3	–167.6
CCDC 726940	93.4	92.3	172.5
CCDC 726941	92.6	94.7	174.1
This work			
(**1L**)	–87.3	–94.1	–168.1
(**1L**)	87.0	92.9	166.8
(**2L**)	–84.4	125.3	39.7
(**2L**)	115.0	–86.1	28.5

Bentivoglio, G., Schwärzler, A., Wurst, K., Kahlenberg, V., Nauer, G., Bonn, G., Schottenberger, H. & Laus, G. (2009). *J. Chem. Crystallogr.* **39**, 662–668.

Schwärzler, A., Laus, G., Kahlenberg, V., Wurst, K., Gelbrich, T., Kreutz, C., Kopacka, H., Bonn, G. & Schottenberger, H. (2009). *Z. Naturforsch. B* **64**, 603–616.

Table S4. Torsion angles (˚) for metal–coordinating triflimide anions (O–*M* or N–*M*) used to generate the diagram shown in Fig. 5 (bottom).

Refcode	φ_1	φ_2	C–S···S–C
ACOLOU	–105.2	112.0	7.1
ACOLOU	–109.5	119.1	9.7
ACOLOU	118.4	–107.9	10.3
ACOLOU	–109.4	116.7	7.9
ACOLUA	–111.2	109.1	5.7
ACOLUA	–115.8	115.6	0.4
ACOLUA	–112.9	110.2	–2.3
ACOLUA	–106.3	114.7	8.7
ACOMAH	–97.9	119.6	20.5
ACOMAH	–112.1	102.6	–10.4
ACOMAH	–93.1	123.5	29.3
ALAMIJ	111.8	–102.5	9.6
ALAMOP	120.0	92.8	–161.6
ALAMUV	–114.2	113.6	–0.8
DISHET	88.6	88.6	163.4
DISHET	–87.8	–87.8	–162.7
DIZXIU	106.2	104.1	–164.0
DIZXIU	–136.7	–102.7	135.3
DOCNIT	–86.7	–96.1	–170.1
DOCNIT	–112.2	102.4	–9.3
DOCNIT	107.7	–115.3	–7.4
DOCNIT	–91.8	–98.2	–177.3
DOCNOZ	82.0	–127.2	–44.2
DOCNOZ	–115.4	–102.3	155.6
DOCNOZ	82.9	105.3	176.5
DOCPAN	–91.4	–91.7	–171.4
ETODEW	–113.7	–110.9	–147.2
EZUNIW	–101.7	–139.0	133.3
FITYOX	100.8	–110.8	–10.2
FITYUD	–99.4	115.3	15.9
FITZAK	120.7	–89.0	30.9
FITZAK	–88.0	119.9	31.3
GELTOH	–104.4	116.0	11.6
GELTOH	114.9	110.0	–149.0
GELTOH	–100.0	116.3	15.6
GIYBOF	–94.6	112.5	17.1
GIYBOF	104.5	–90.1	13.8
GIYBOF01	–97.7	107.2	9.4
GIYBOF01	93.0	–107.0	–13.2
HOGGUG	88.8	121.0	–164.6
HOGGUG	123.2	–96.4	26.1
HOGGUG	–100.1	–87.5	–173.1
HOGHAN	–151.5	–96.8	125.2
HOGHAN	–149.8	–92.4	131.3
HOGHAN	–113.3	105.8	–8.0
HOGHAN	106.3	119.4	–149.0
JAFKEH	103.3	103.5	–166.7
JINGIX	94.6	85.0	166.8
JINGOD	–91.0	–92.0	–170.2
JINGUJ	–89.3	–88.6	–164.7
LEGJOX	–95.4	122.3	26.0
LEGJOX	–151.4	–91.8	129.7

LEGJOX	90.0	117.6	–166.5
LEGJOX	105.7	140.9	–123.9
LEGJOX	–99.6	–88.2	–173.3
LONYUJ	–158.7	–95.5	116.6
NATPOO	–115.8	108.8	–7.2
NATPOO	107.3	–116.9	–9.6
NATPOO	–118.1	107.5	–10.6
NATPOO	105.4	–112.9	–7.9
NAVCUJ	117.8	–93.1	24.6
NAVCUJ	100.5	102.1	–171.9
NEZNUC	–138.4	–87.2	148.0
NEZNUC	–126.3	–126.8	122.2
NEZPAK	78.0	141.4	–152.7
NEZPAK	99.0	96.7	–178.6
NEZPAK	–81.9	–116.4	174.4
QAPHOE	86.8	90.1	163.2
RARCAP	–86.3	–139.0	148.0
RARCAP	–150.7	–102.1	122.9
TECXUV	120.8	90.2	–163.3
TECXUV	–95.5	122.3	25.8
TECXUV	–99.3	–88.0	–173.0
TECYAC	100.9	102.7	–170.4
TECYAC	–127.3	129.3	1.6
TECYAC	–115.9	115.0	–1.8
TECYEG	100.8	103.3	–170.2
TECYEG	–129.4	128.6	–1.0
TECYEG	116.3	–118.3	–2.7
TECYIK	118.3	90.0	–165.9
TECYIK	–95.6	122.7	26.2
TECYIK	–100.3	–89.2	–174.8
TOJQAL	–102.9	–85.5	–174.6
TURZEL	109.5	–109.5	0.0
TURZOV	98.3	86.8	172.6
TURZUB	100.7	–112.3	–11.9
VAVNEM	–83.1	–96.4	–167.5
XAKDAP	–78.3	–88.6	–152.9
XAKDET	105.7	82.6	176
XAKDIX	112.0	–110.8	0.4
XAKDOD	78.9	96.0	161.5
XAKDOD	95.4	96.9	178.0

Preliminary crystal data for 1H

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6. POWDER SPECIMEN AND CRYSTAL DATA

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; ?
;
# The next three fields give the specimen dimensions in mm.  The equatorial
# plane contains the incident and diffracted beam.

_pd_spec_size_axial             ?       # perpendicular to
                                # equatorial plane
_pd_spec_size_equat             ?       # parallel to
                                # scattering vector
                                # in transmission
_pd_spec_size_thick             ?       # parallel to
                                # scattering vector
                                # in reflection

# The next five fields are character fields that describe the specimen.

_pd_spec_mounting                       # This field should be
                                # used to give details of the
                                # container.
; ?
;
_pd_spec_mount_mode             ?       # options are 'reflection'
                                # or 'transmission'
_pd_spec_shape                  ?       # options are 'cylinder'
                                # 'flat_sheet' or 'irregular'
_pd_char_particle_morphology    ?
_pd_char_colour                 ?       # use ICDD colour descriptions

# The following three fields describe the preparation of the specimen.
# The cooling rate is in K/min.  The pressure at which the sample was
# prepared is in kPa.  The temperature of preparation is in K.

_pd_prep_cool_rate              ?
_pd_prep_pressure               ?
_pd_prep_temperature            ?

# The next four fields are normally only needed for transmission experiments.

_exptl_absorpt_coefficient_mu       ?
_exptl_absorpt_correction_type      ?
_exptl_absorpt_process_details      ?
_exptl_absorpt_correction_T_min     ?
_exptl_absorpt_correction_T_max     ?

#============================================================================

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;

# The following item is used to identify the equipment used to record
# the powder pattern when the diffractogram was measured at a laboratory
# other than the authors' home institution, e.g. when neutron or synchrotron
# radiation is used.

_pd_instr_location
; ?
;
_pd_calibration_special_details         # description of the method used
                                # to calibrate the instrument
; ?
;

_diffrn_ambient_temperature         ?
_diffrn_source                  ? # Put here: 'rotating-anode X-ray tube'
```

```
_diffrn_radiation_type          'X-ray'
_diffrn_source_target           ? # Put here the chemical symbol of the anode

_diffrn_radiation_monochromator      ?
_diffrn_measurement_device_type      ?
_diffrn_measurement_method           ?
_diffrn_detector_area_resol_mean     ?   # Not in version 2.0.1
_diffrn_detector                     ?
_diffrn_detector_type                ?   # make or model of detector
_pd_meas_scan_method                 ?   # options are 'step', 'cont',
                                 # 'tof', 'fixed' or
                                 # 'disp' (= dispersive)
_pd_meas_special_details
;  ?
;

#  The following four items give details of the measured (not processed)
#  powder pattern.  Angles are in degrees.

_pd_meas_number_of_points         7545
_pd_meas_2theta_range_min         3.05400
_pd_meas_2theta_range_max         70.95000
_pd_meas_2theta_range_inc         0.009001

#============================================================================

# 8. REFINEMENT DATA

_refine_special_details
; ?
;

# Use the next field to give any special details about the fitting of the
# powder pattern.

_pd_proc_ls_special_details
; ?
;

# The next three items are given as text.

_pd_proc_ls_profile_function      ?
_pd_proc_ls_background_function   ?
_pd_proc_ls_pref_orient_corr
; ?
;

#  The following profile R-factors are NOT CORRECTED for background
#  The sum is extended to all non-excluded points.
#  These are the current CIF standard

_pd_proc_ls_prof_R_factor              4.6263
_pd_proc_ls_prof_wR_factor             6.8005
_pd_proc_ls_prof_wR_expected           4.6273

#  The following profile R-factors are CORRECTED for background
#  The sum is extended to all non-excluded points.
#  These items are not in the current CIF standard, but are defined above

_pd_proc_ls_prof_cR_factor             16.4796
_pd_proc_ls_prof_cwR_factor            13.7520
_pd_proc_ls_prof_cwR_expected          9.3573

#  The following items are not in the CIF standard, but are defined above

_pd_proc_ls_prof_chi2                  2.1599
_pd_proc_ls_prof_echi2                 2.4048

#  Items related to LS refinement
```

```
_refine_ls_R_I_factor                 5.0572
_refine_ls_number_reflns                234
_refine_ls_number_parameters             81
_refine_ls_number_restraints             48

# The following four items apply to angular dispersive measurements.
# 2theta minimum, maximum and increment (in degrees) are for the
# intensities used in the refinement.

_pd_proc_2theta_range_min              3.0540
_pd_proc_2theta_range_max             70.9500
_pd_proc_2theta_range_inc            0.009001
_pd_proc_wavelength                  1.540593

_pd_block_diffractogram_id       ?  # The id used for the block containing
                                    # the powder pattern profile (section 11)

# Give appropriate details in the next two text fields.

_pd_proc_info_excluded_regions    ?
_pd_proc_info_data_reduction      ?

# The following items are used to identify the programs used.

_computing_data_collection          ?
_computing_structure_solution       ?
_computing_structure_refinement     FULLPROF
_computing_molecular_graphics       ?
_computing_publication_material     ?

#=============================================================================

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
   _atom_site_label
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_U_iso_or_equiv
   _atom_site_occupancy
   _atom_site_adp_type             # Not in version 2.0.1
   _atom_site_type_symbol
 S2     0.2941(5)   0.00000     0.9788(8)   0.422(9)    1.00000    Uani S
 S9     0.3746(6)   0.00000     0.7426(8)   0.422(9)    1.00000    Uani S
 O7     0.2121(8)   0.00000     1.014(3)    0.422(9)    1.00000    Uani O
 C10    0.3244(3)   0.00000     0.5951(5)   0.422(9)    1.00000    Uani N
 F5     0.4258(4)   0.00000     1.116(3)    0.422(9)    1.00000    Uani F
 F12    0.2468(4)   0.00000     0.6227(11)  0.422(9)    1.00000    Uani F
 N1     0.332(2)    0.0418(18)  0.8422(15)  0.422(9)    0.50000    Uani N
 O8     0.2364(19) -0.1016(8)   0.990(4)    0.422(9)    0.50000    Uani O
 O15    0.3778(9)  -0.0769(8)   0.794(3)    0.422(9)    1.00000    Uani O
 C3     0.3862(3)   0.0534(3)   1.1062(6)   0.422(9)    0.50000    Uani N
 F4     0.4649(18)  0.1372(14)  1.115(3)    0.422(9)    0.50000    Uani F
 F6     0.3352(12)  0.058(2)    1.1989(16)  0.422(9)    0.50000    Uani F
 F11    0.2717(15) -0.0834(11)  0.637(3)    0.422(9)    0.50000    Uani F
 F13    0.3343(16) -0.040(2)    0.4934(18)  0.422(9)    0.50000    Uani F
 N1a    0.00000     0.00000     0.4197(4)   0.022(4)    1.00000    Uiso N
 N2a    0.00000     0.00000     0.1833(4)   0.022(4)    1.00000    Uiso N
 C3a    0.00000     0.0865(3)   0.3822(4)   0.022(4)    1.00000    Uiso C
 C4a    0.00000     0.0854(3)   0.2377(4)   0.022(4)    1.00000    Uiso C
 N1b    0.33333     0.66667     0.2664(7)   0.140(5)    1.00000    Uiso N
 N2b    0.33333     0.66667     0.4980(7)   0.140(5)    1.00000    Uiso N
 C3b    0.3238(12)  0.7482(8)   0.3048(5)   0.140(5)    1.00000    Uiso C
 C4b    0.3437(13)  0.7566(6)   0.4455(5)   0.140(5)    1.00000    Uiso C

loop_
   _atom_site_aniso_label
```

```
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_12
  _atom_site_aniso_U_13
  _atom_site_aniso_U_23
  _atom_site_aniso_type_symbol
S2   0.157(6)  0.608(11) 0.500(8)  -0.079(6) -0.140(5)  0.070(5)   S
S9   0.157(6)  0.608(11) 0.500(8)  -0.079(6) -0.140(5)  0.070(5)   S
O7   0.157(6)  0.608(11) 0.500(8)  -0.079(6) -0.140(5)  0.070(5)   O
C10  0.157(6)  0.608(11) 0.500(8)  -0.079(6) -0.140(5)  0.070(5)   N
F5   0.157(6)  0.608(11) 0.500(8)  -0.079(6) -0.140(5)  0.070(5)   F
F12  0.157(6)  0.608(11) 0.500(8)  -0.079(6) -0.140(5)  0.070(5)   F
N1   0.157(6)  0.608(11) 0.500(8)   0.052(10) -0.140(5)  0.030(17)  N
O8   0.157(6)  0.608(11) 0.500(8)   0.052(10) -0.140(5)  0.030(17)  O
O15  0.157(6)  0.608(11) 0.500(8)   0.052(10) -0.140(5)  0.030(17)  O
C3   0.157(6)  0.608(11) 0.500(8)   0.052(10) -0.140(5)  0.030(17)  N
F4   0.157(6)  0.608(11) 0.500(8)   0.052(10) -0.140(5)  0.030(17)  F
F6   0.157(6)  0.608(11) 0.500(8)   0.052(10) -0.140(5)  0.030(17)  F
F11  0.157(6)  0.608(11) 0.500(8)   0.052(10) -0.140(5)  0.030(17)  F
F13  0.157(6)  0.608(11) 0.500(8)   0.052(10) -0.140(5)  0.030(17)  F

# Note: if the displacement parameters were refined anisotropically
# the U matrices should be given as for single-crystal studies.

#===============================================================================
```