Electronic Supporting Information

Heterogeneous Microwave-assisted Ullmann type Methodology for Synthesis of Rigid-core Ionic Liquid Crystals.

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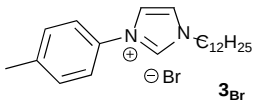
CCDC 1830443-1830446



$\mathbf{3_{Br}}$

Summary of Data CCDC 1830443

Compound Name:
Formula: C22 H35 N2 1+,Br1 1-
Unit Cell Parameters: a 20.4743(10) b 14.5386(6) c 7.5277(4) P21/c
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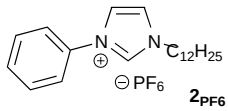
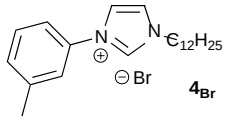


$\mathbf{2_{PF6}}$

Summary of Data CCDC 1830444

Compound Name:
Formula: C21 H33 N2 1+,F6 P1 1-
Unit Cell Parameters: a 8.3458(8) b 10.7404(11) c 26.252(3) P-1



$\mathbf{4_{Br}}$

Summary of Data CCDC 1830445

Compound Name:
Formula: C22 H35 N2 1+,Br1 1-
Unit Cell Parameters: a 19.1863(15) b 14.2196(12) c 8.1410(6) P21/c

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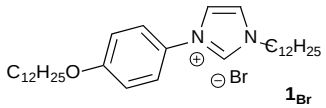

$\mathbf{1_{Br}}$

Summary of Data CCDC 1830446

Compound Name:
Formula: C33 H57 N2 O1 1+,Br1 1-
Unit Cell Parameters: a 28.2048(7) b 14.7269(4) c 7.9430(2) P21/c

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X-ray crystallography

The crystals were placed in oil, and a single crystal was selected, mounted on a glass fibre and placed in a low-temperature N_2 stream.

For compounds **1Br** and **3Br**, X-ray diffraction data collection was carried out on a Nonius Kappa-CCD diffractometer equipped with an Oxford Cryosystem liquid N_2 device, using Mo-K⍺ radiation (⅄ = 0.71073 Å). The crystal-detector distance was 36mm. The cell parameters were determined (Denzo software) [1] from reflections taken from one set of 10 frames (1.0° steps in phi angle), each at 20s exposure. The structures were solved by Direct methods using the program SHELXS-97 [2]. The refinement and all further calculations were carried out using SHELXL-2014 [3]. The H-atoms were included in calculated positions and treated as riding atoms using SHELXL default parameters. The non-H atoms were refined anisotropically, using weighted full-matrix least-squares on F2. For **3Br**, a semi-empirical absorption correction was applied using the MULscanABS routine in PLATON [4]; transmission factors: T_{min}/T_{max} = 0.58705/0.75162.

For salts **2PF6** and **4Br**, X-ray diffraction data collection was carried out on a Bruker APEX II DUO Kappa-CCD diffractometer equipped with an Oxford Cryosystem liquid N_2 device, using Mo-Kα radiation (ʎ = 0.71073 Å). The crystal-detector distance was 38mm. The cell parameters were determined (APEX2 software) [5] from reflections taken from tree sets of 12 frames, each at 10s exposure. The structure was solved by Direct methods using the program SHELXS-97 [2]. The refinement and all further calculations were carried out using SHELXL-2014 [3]. The H-atoms were included in calculated positions and treated as riding atoms using SHELXL default parameters. The non-H atoms were refined anisotropically, using weighted full-matrix least-squares on F2. A semi-empirical absorption correction was applied using SADABS in APEX2 [5]; transmission factors for **2PF6**: T_{min}/T_{max} = 0.6861/0.7458; for **4Br**: T_{min}/T_{max} = 0.4853/0.9119.

[1] "Kappa CCD Operation Manual", Nonius B. V., Ed. ; Delft: The Netherlands, 1997.

[2] G. M. Sheldrick, *Acta Cryst.* **1990**, A46, 467-473.

[3] G. M. Sheldrick, *Acta Cryst.* **2015**, C71, 3-8.

[4] Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13.

[5] "M86-E01078 APEX2 User Manual", Bruker AXS Inc., Madison, USA, 2006.

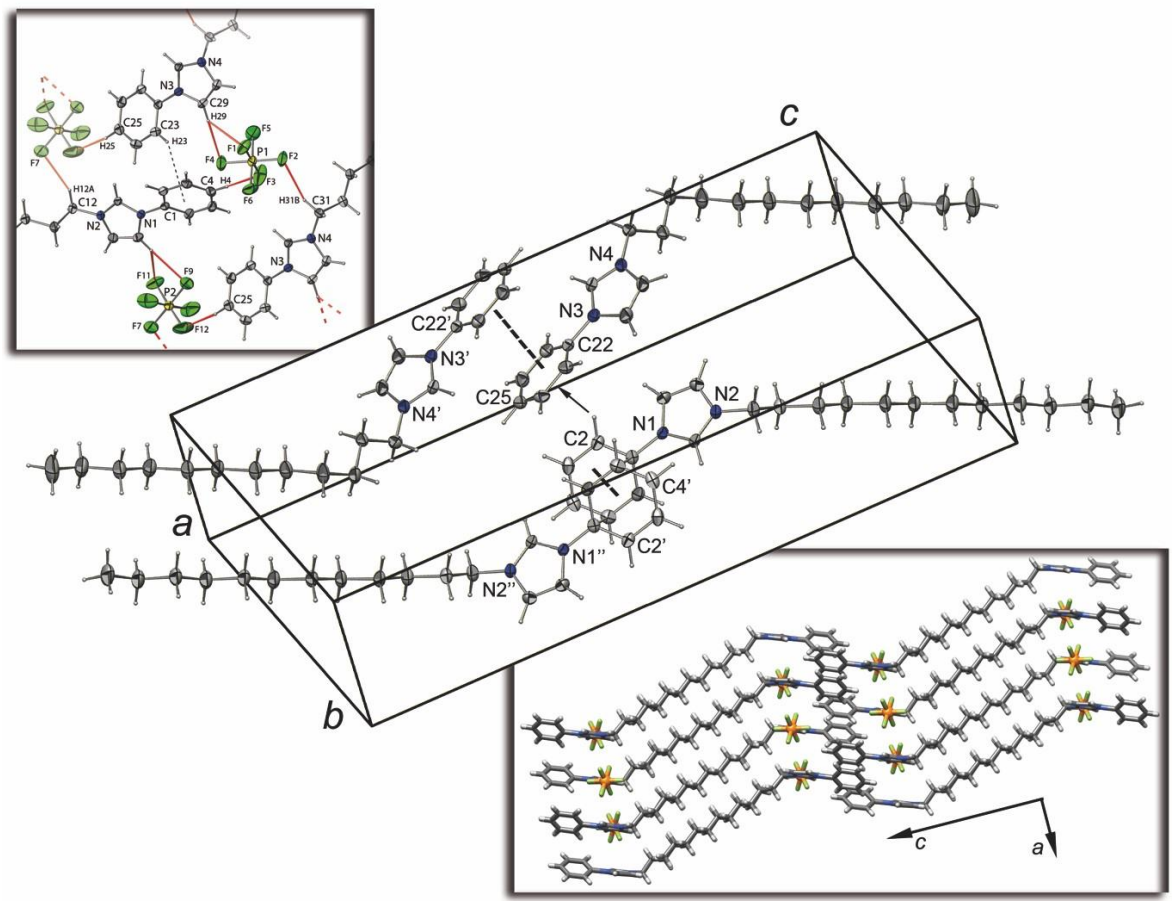

Fig X1 : ORTEP views and a packing view of compound 2_PF_6. The ellipsoids enclose 90% of the electronic density. Selected weak interactions are represented with arrow (CH-π), dashed lines (π - π) or red lines (hydrogen bonds).

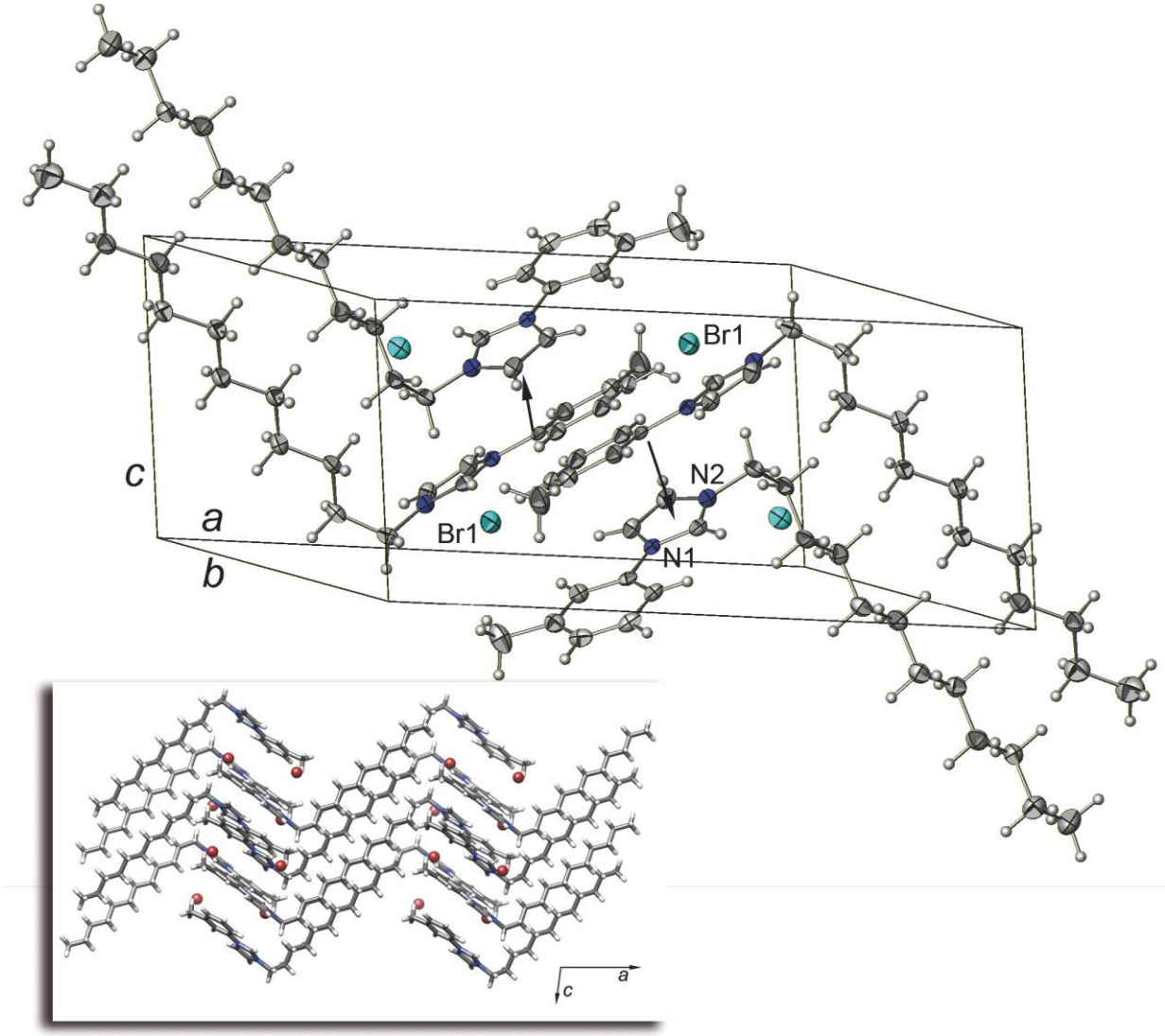

Fig X2 : ORTEP view and a packing view of compound 4_Br. The ellipsoids enclose 90% of the electronic density. Selected weak interactions (CH-π) are represented with arrows.

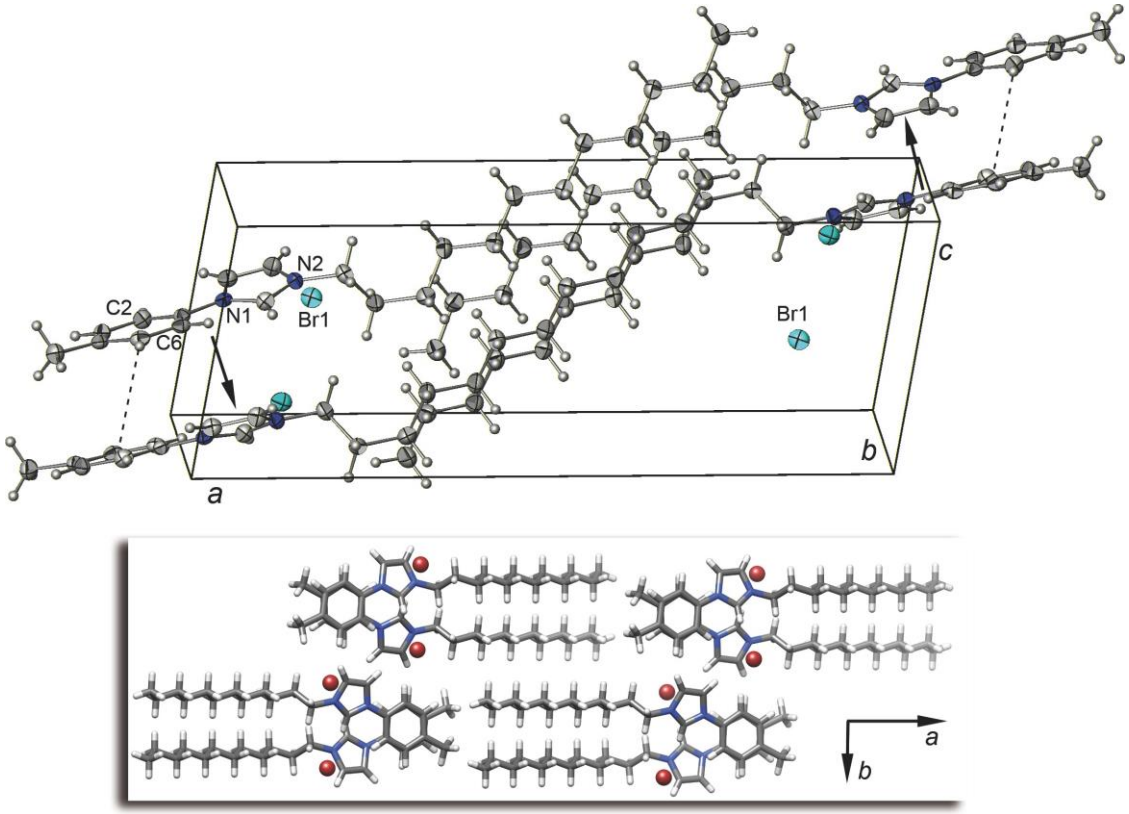

Fig X3 : ORTEP view and a packing view of compound 3_Br. The ellipsoids enclose 90% of the electronic density. Selected weak interactions (CH-π) are represented with arrows.

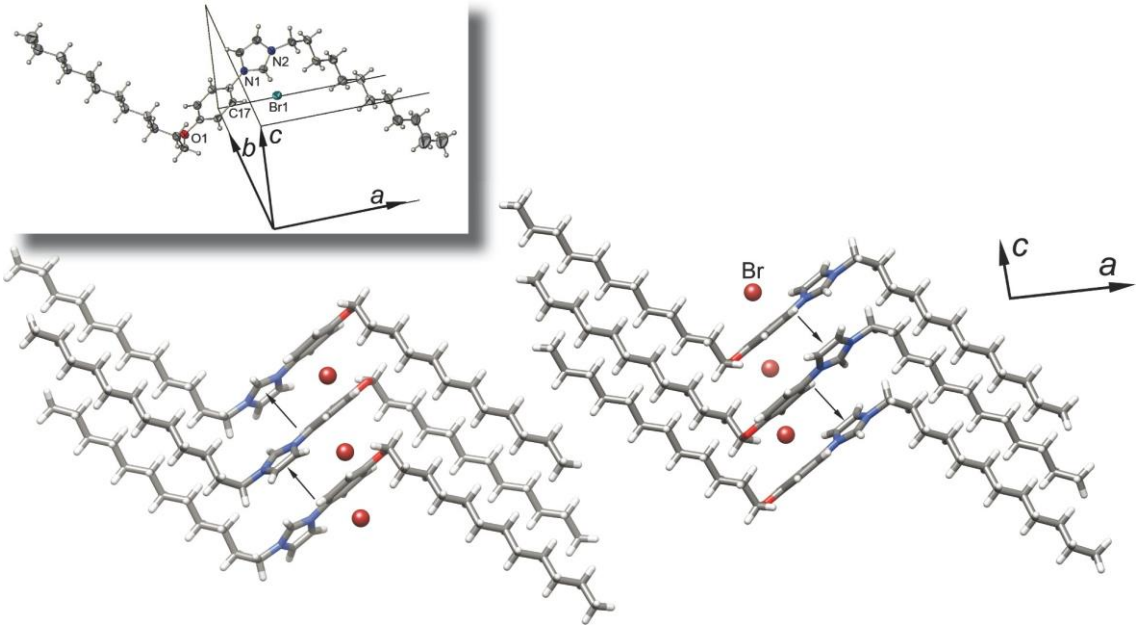

Fig X4 : ORTEP view and a packing view of compound 1_Br. The ellipsoids enclose 90% of the electronic density. Selected weak interactions (CH-π) are represented with arrows.

References for crystal structure views:

ORTEP views : E. Dowty, *ATOMS, Shapesoftware,* Kingsport, TN 37663 USA

Packing views : CHIMERA, J Comput Chem. 2004 Oct;25(13):1605-12