

Supporting Information for:

Observation of strong halogen bonds in the solid state structures of bis-haloimidazolium macrocycles

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Lists of CSD reference codes for data in tables 2 and 3

Table 2

Chloroimidazolium and Cl⁻: NUXPOL, XOMMER

Chloroimidazolium and Br⁻: this work (CSD no.: 963237)

Bromoimidazolium and Br⁻: AHEVIS, ALOKOC, ALOKUI, AWENOF, AWENUL, HABNAB, ICIKEM, VIBPAY

Iodoimidazolium and Cl⁻: KAQSOM, VIBPEC, VIBPEC01

Iodoimidazolium and Br⁻: KAQSIG, NEDPAP, WEBFEQ, this work (CSD: 963238)

Iodoimidazolium and I⁻: AWEPEX, HARXAZ, HEJLIR, ICIKOW, ICIKUC, KAQSEC, WEBFIU

Iodotriazolium and Cl⁻: DAMNOW, TACPIY

Iodotriazolium and Br⁻: DAMPAK, TACPEU, TACPUK

Iodotriazolium and I⁻: DAMNUC, TACPOE

Perfluoroiodoarene and Cl⁻: DATCOS, DATCUY, DATDAF, DATDEJ, GIXFOI, GIXGAV, LOFDEQ, LOFDOA, OHOVUD, RUWVUB, RUWWIQ

Perfluoroiodoarene and Br⁻: GIXFUO, GIXGEZ, GIXGID, LOFDAM, LOFDIU, MAHCEF, MAHCOP, OHOWAK, XERZID, XERZOJ, XERZUP

Perfluoroiodoarene and I⁻: CIZROT, CIZRUZ, CIZSAG, CIZSEK, CIZSIO, CIZSOU, CIZSUA, CODCEE, CODCEE01, CODCIL, DAXGIT, GIXGOJ, GIXGUP, HINXEH, MAHBUE, MAHCAB, MAHCUJ, OHOUAJ, OHOUAJ01, OHOUOX

Table 3

Chloroimidazolium and oxoanions: EHENIO, POMBEY

Bromoimidazolium and oxoanions: AKOJEQ, AYEHOB, FALCIF, VIBNUQ, this work (CSD: 936239)

Iodoimidazolium and oxoanions: ITUPAP, KAQSUS

Iodotriazolium and oxoanions: MEPHOW

Perfluoroarene and oxoanions: UZUQOW, UZUQUC, UZURAJ, UZUREN, UZURIR