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Halogen *vs.* ionic bonding: an unusual isomorphism between the neutral $(C_5Me_5)_2Fe/C_2I_2$ cocrystal and ionic $[(C_5Me_5)_2Fe]Br_3$ crystal

Yury V. Torubaev,*[a] Ivan V. Skabitsky,[a] Georgy A. Saratov[b,c] and Petr Yu. Barzilovich[c]

[a] *N. S. Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, 119991 Moscow, Russian Federation. E-mail: torubaev@igic.ras.ru*
[b] *Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Moscow Region, Russian Federation*
[c] *M. M. Shemyakin–Yu. A. Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, 117997 Moscow, Russian Federation*

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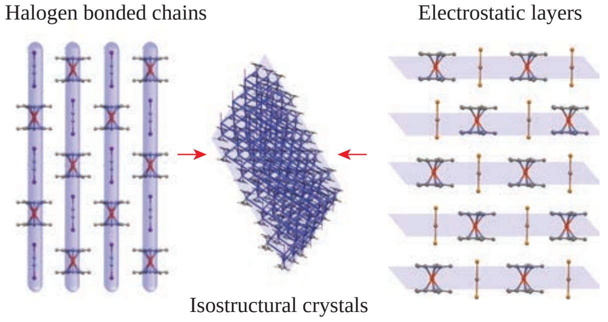
Almost equal molecular sizes of diiodoacetylene (C_2I_2) and the $[Br_3]^-$ anion result in isomorphic neutral cocrystal (DMFc–C_2I_2) and $[DMFc]^+Br_3^-$ salt. This isomorphic pair of neutral and ionic crystals provides a unique example for the analysis of different types of bonding resulting in isotypic solid-state structures. Their energy frameworks visualize the obvious difference between their energetic structures: the lattice of DMFc–C_2I_2 is built upon the chains stabilized by I···(η^5-C_5Me_5) halogen bonds; at the same time, $[DMFc]^+Br_3^-$ consists of electrostatically assembled layers associated by Br···π(Cp*) XBs interactions.



Keywords: self-assembly, charge-transfer complexes, ferrocene, ferrocenyl, halogen bonding, polybromides, polyiodides, ferrocenium, iodoacetylene, cocrystals, supramolecular, energy framework, intermolecular interactions.

In addition to the unique redox and magnetic activity of ferrocene derivatives,[1] these compounds are important building blocks in the crystal design. They are typical guests in Hg, Ag and Cu anti-crowns[2] and inclusion compounds of calixarenes, cyclodextrins, cucurbiturils, thiourea, COFs and MOFs.[3] Their charge-transfer (CT) complexes,[4] π···π associates with aromatic hydrocarbons and polyfluorinated aromatics,[5] fullerenes[6] are significant in the design of redox-active[7] and conducting materials.[8] Along with growing interest in halogen bonding (XB),[9] chalcogen bonding,[10] and other noncovalent interactions,[11] this also stimulates theoretical studies of bonding in CT ferrocene complexes and cocrystals.[12] Polyhalides attract significant attention[13,14] in the context of halogen bonding and other σ-hole interactions.[15]

Our crystal engineering exercises with the ferrocene co-former afforded conducting cocrystals with diiodoacetylene (C_2I_2)[16] and provided information on domain boundaries in the structural landscape of triptycene.[17] In continuation, we studied the crystal structure[†] of permethylated ferrocene (decamethylferrocene, DMFc) and the electric conductivity of its cocrystal with C_2I_2 (for details, see Online Supplementary Materials). The conductivity of DMFc–C_2I_2 appeared rather unremarkable, but its solid-state structure revealed a surprising parallel with the structure of ionic $[DMFc]Br_3$.

Molecules of C_2I_2 and Br_3^- anions of almost equal lengths (5.16 and 5.06 Å, respectively) produce isomorphic crystals with $(C_5Me_5)_2Fe$: neutral $(C_5Me_5)_2Fe/C_2I_2$ **1** and ionic $[(C_5Me_5)_2Fe]Br_3$ **2**.[18] At first glance, both crystals contain parallel polymeric 1-D chains self-assembled by weak halogen I···π(Cp*) and ionic Br···π(Cp*) bonds, respectively (Figure 1). Given larger covalent (1.39 Å)[19] and van der Waals (2.04 Å)[20] radii for iodine, as compared to those of bromine (1.20[19] and 1.86 Å,[20] respectively), the average distance between I and C atoms of a Cp ring in **1** (3.42 Å) is > 0.1 Å shorter than the average $Br\cdots C_{Cp*}$ distance in **2** (3.56 Å). Therefore, the distance between the x and $x + 1$ planes of Cp ligands in **1** is shorter than that in **2**; in general, the unit cell parameter a in **1** is ~0.3 Å shorter than that in **2**.

Complex **2** consists of $(C_5Me_5)_2Fe$ units in an oxidized form (decamethylferrocenium cations), which are responsible for its green colour in solution and a solid state. Pronounced green-brown dichroism of the cocrystals of **2** is the result of a parallel

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[†] *Preparation of the cocrystals of $(Me_5C_5)_2Fe/C_2I_2$* **1**. C_2I_2 (0.028 g, ~0.1 mmol) and $(Me_5C_5)_2Fe$ (0.033 g, ~0.1 mmol) were dissolved in hot heptane (0.3 ml) in a 5 mm test tube under moderate heating. The orange reaction mixture was allowed to cool down to room temperature and evaporated slowly for 12 h. The resulting yellow prismatic crystals were separated from mother liquor, washed with cold pentane, dried in a stream of argon and used for single crystal XRD analysis.

Crystal structure determination. A Bruker AXS Smart APEX CCD diffractometer with graphite-monochromated MoKα radiation (0.71070 Å) was used for the XRD analysis of compound **1**, space group *Cmcm*: $a = 14.837(7)$, $b = 12.639(7)$ and $c = 12.317(6)$ Å. The data were collected by standard θ,ω-scan techniques and scaled and reduced using the SHELXL-97 software. The structure was solved by direct methods and refined by full-matrix least-squares against F^2 using the SHELXL-97 and Olex2 software. Non-hydrogen atoms were refined with anisotropic thermal parameters. All hydrogen atoms were geometrically fixed and refined using a riding model.

CCDC 1528250 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* http://www.ccdc.cam.ac.uk.

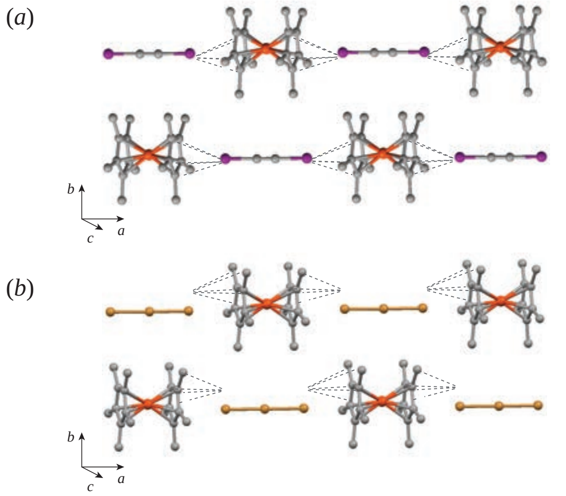

Figure 1 Isostructural packing patterns in the (*a*) cocrystal of $(C_5Me_5)_2Fe/C_2I_2$ **1**, *Cmcm*: *a* = 14.837(7), *b* = 12.639(7) and *c* = 12.317(6) Å and (*b*) ionic $[(C_5Me_5)_2Fe]^+[Br_3]^-$ **2**, *Cmcm*: *a* = 15.162(5), *b* =12.358(5) and *c* = 11.936(5) Å. Selected intermolecular distances in **1** (Å): I···C_{Cp*} 3.389, 3.331, 3.389, 3.496, 3.496; between Cp* planes, 11.5. Selected intermolecular distances in **2** (Å): Br···C_{Cp*} 3.447–3.667; between Cp* planes, 11.7. Hydrogen atoms are omitted for clarity.

linear chain packing. Typically for ionic CT complexes of ferrocenium cations, the Fe–$Cp_{centroid}$ distances in **2** (1.716 Å) are extended, as compared to 1.656 Å in neutral $(C_5Me_5)_2Fe$ (DMFERR01) and 1.650 Å in **1**. The almost negligible difference in Fe–$Cp_{centroid}$ distances for the latter two is in good agreement with the low contribution of charge transfer to the halogen bonding noted by Legon.[21,22]

Intermolecular I···C_{Cp} distances in **1** (3.331–3.496 Å) are significantly shorter than C/I van der Waals radii sum (3.81 Å),[20] while the range of Br···C_{Cp} distances in **2** (3.447–3.667 Å) is just matching or slightly exceeding the Br/C van der Waals radii sum (2.63 Å).[20] Even if we consider flexible maximum van der Waals radii for C_{sp2} (1.87 Å), Br (2,00 Å) and I (2.17 Å) reported recently,[23] the I···C_{Cp} distances in **1** appear even shorter, and the Br···C_{Cp} distance in **2** hardly reaches this upper limit for van der Waals interactions. The Hirshfeld surfaces for **1** and **2** are illustrative for closer I···Cp interaction in **1**, compared to Br···C_{Cp} in **2** (Figure 2).

The outstanding conductivity of a ferrocene–diiodoacetylene hybrid organometallic–organic cocrystal (4×10^{-3} S cm^{-1}),[16] which is three orders of magnitude higher than an average of $\sim10^{-6}$ S cm^{-1} typically observed in regular elementoorganic and organic crystals, has prompted the electrochemical investigation of **1** and **2**. The conductivity measurement data for **1** and **2** demonstrated sample resistances of 1.75×10^6 and 1.2×10^6 Ω for **1** and **2**, respectively, resulting in typical 2.8×10^{-6} and 4×10^{-6} S cm^{-1} conductivities of the electron–hole type for **1** and **2**, respectively (Figure S1).

Note that the I···Cp* assisted chain assembly is not observed in $[(C_5Me_5)_2Fe]I_3$, which is a triiodide congener of **2**. Even sole I···C_{Cp*} contacts are absent from both of its polymorphs (*C*2/*c*[25] and $P\bar{1}$,[26] Figure 3), making us look closer at the geometry and energy of **1** and **2** packings.

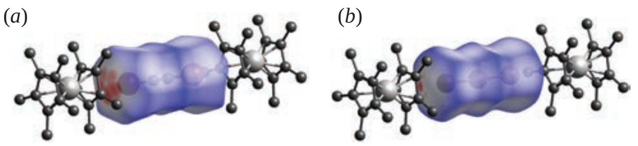

Figure 2 Hirshfeld surfaces for (*a*) the C_2I_2 molecule in **1** and (*b*) the $[Br_3]^-$ anion in **2**. Notice five I···C close contacts in **1** *vs.* just one Br···C in **2**.

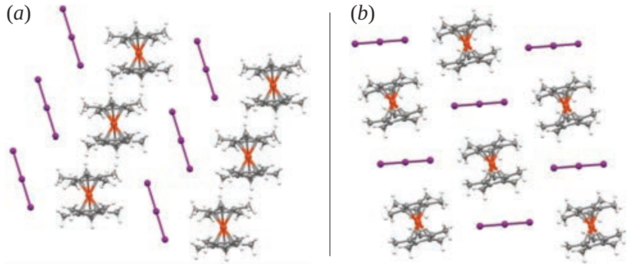

Figure 3 Fragments of the packing of two polymorphic forms of $[(C_5Me_5)_2Fe]I_3$: (*a*) *C*2/*c* and (*b*) $P\bar{1}$. Notice the absence of I···Cp* assisted chain assembly in both forms.

The energy frameworks[27] featured in the Crystal Explorer software package[28] combine the efficient quantum-chemical computational instrument for the energy of intermolecular interactions with the graphic representation of their magnitude. It is an effective tool for the visualization of supramolecular reactions,[29] structures,[30] physical properties[31] and topology of supramolecular recognition[32] in crystals. In the present case, the energy frameworks of **1** and **2** visualize the obvious difference in the hierarchy of their structures. The strongest intermolecular bonding in **1** is observed for two apical DMFc–C_2I_2 interactions (–29 kJ mol^{-1} each) [Figure 4(*a*)]. The sum of four equatorial DMFc–C_2I_2 interactions is 3 kJ mol^{-1} higher [–(13 + 13 + 11 + 15)/2 = = –26 kJ mol^{-1}][‡] [see Figure 4(*a*)]. However, the equatorial DMFc–C_2I_2 interactions are mostly driven, by dispersion forces while the apical has comparable contributed from dispersion and electrostatic interactions [Figures 4, 5, S2–S3(*a*–*c*), Tables S1, S2]. Note (citing a textbook by G. Desiraju *et al.*[33]) that these apical I···π(Me_5C_5) XBs in **1**, being predominantly electrostatically driven, are viable at distances that are much longer than the van der Waals limit and have a more gradual fall-off with distance (r^{-2}) than interactions with dispersive character (r^{-6}). Therefore, they have orienting effects on molecules prior to nucleation and crystallization. Their directional preferences are still retained in the final crystal structure even though these electrostatic interactions contribute to a lesser extent to the overall energy of the crystal.

Given a considerable difference in the energies of electrostatic interactions of charged particles with each other (hundreds of kJ mol^{-1}) and with neutral molecules (tens of kJ mol^{-1}), it is difficult to estimate the energy of the latter correctly at the background of the former [Figure 4(*b*)]. However, as noted recently,[26] the relatively weak HBs and XBs in the salt cocrystals are structure-forming interactions; thus, we can assume that Br_3···πCp anion-π interactions are more substantial than I_3···πCp, and they determine the observed structure of **2**, in contrast to both polymorphs of [DMFc][I_3].

The energetic structure of an ionic crystal of **2** is naturally dominated by electrostatic, and it consists of strongly associated

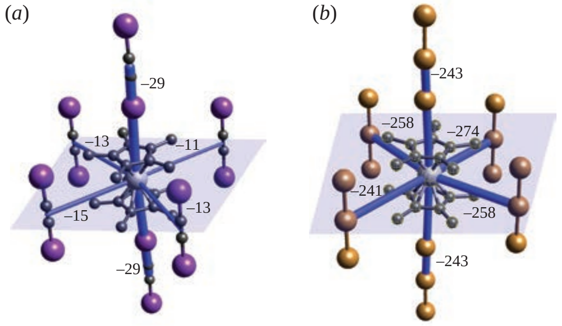

Figure 4 Intermolecular interaction energies in (*a*) **1** and (*b*) **2**.

[‡] Lattice energy was obtained as one-half the product of the number of molecular pairs and total enegy [https://crystalexplorer.scb.uwa.edu.au/wiki/index.php/Lattice_Energies].

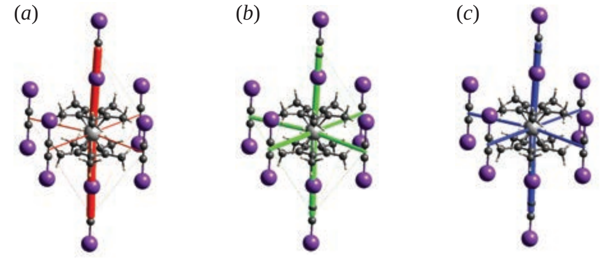

Figure 5 Graphic presentation of electrostatic (*a*, red) and dispersion (*b*, green) contributions to the total energy of intermolecular interactions (*c*, blue) in **1** (see Table S1 for energy values).

layers further assembled into a 3D structure [Figures 4(*b*), 6(*b*)]. This is in good agreement with data on the solid-state structure of **2**, which is comprised of layers of alternating cations, and no significant interactions between the layers are observed.[18] Although the latter statement was based on the conscious analysis of the intermolecular geometry and packing pattern (without quantum-chemical calculations), and thus it is not exact in the part mentioning the absence of significant interactions between the layers), it still suggests a better model of **2** than mere short intermolecular contacts analysis[34] (Figure S4), which suggests the chain architecture for both **1** and **2**, neglecting significant electrostatic attraction between the opposite charges in **2**.

Therefore, the given example of **1** and **2** demonstrates how completely different in nature and energy intermolecular forces can provide the formation of isomorphic crystals from the isometric coformers. Such a significantly different construction of the isostructural crystals of **1** and **2** makes an exciting alternative to a cocrystallization-based strategy for constructing isostructural solids, which exploits the same sort of noncovalent intermolecular interactions (XBs) in different combinations of XB-donor/acceptor pairs.[35] Methodologically, the isomorphic crystals of **1** and **2** exemplify the importance of calculating the energetics of intermolecular interactions rather than visually observed patterns. In this context, Gavezzotti[36] stated that no sensible journal should any more accept sentences like ‘the crystal structure consists of pairs/chains/layers held together by such and such interaction…’ and similar assertions when they are not supported by reliable energy numbers. Fortunately, the concept of energy frameworks brings energy calculations and their visual representation together and allows us to describe the crystal packing in terms of energetic chains, layers and more complex architectures.

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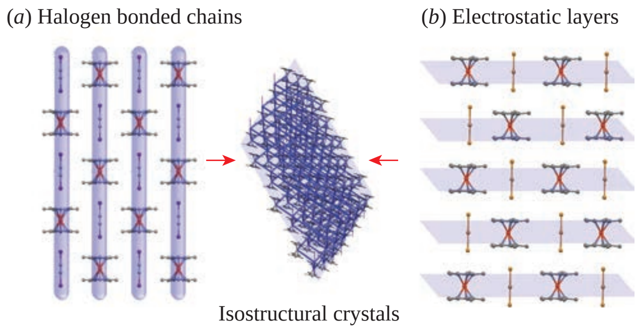
(*a*) Halogen bonded chains
(*b*) Electrostatic layers
Isostructural crystals

Figure 6 (*a*) Chains stabilized by I···Cp* XBs in **1** and (*b*) strongly electrostatically associated layers in **2**, both assembled into the isomorphic 3D structures.

Online Supplementary Materials

Supplementary data associated with this article can be found in the online version at doi: 10.1016/j.mencom.2021.01.017.

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