



Review

Halogen bonding: A powerful, emerging tool for constructing high-dimensional metal-containing supramolecular networks



Bo Li^{a,b}, Shuang-Quan Zang^{a,*}, Li-Ya Wang^{b,*}, Thomas C.W. Mak^{a,c}

^a College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou 450001, China

^b College of Chemistry and Pharmaceutical Engineering, Nanyang Normal University, Nanyang 473061, China

^c Department of Chemistry and Center of Novel Functional Molecules, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong Special Administrative Region

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ABSTRACT

Halogen bonding (XB), an attractive and valuable noncovalent interaction, has recently been exploited as an important tool in crystal engineering. The recent upsurge in crystal engineering has been prompted by the wide use of XB in the formation of liquid crystals and has implications for studies on non-linear optics (NLO), gels, anion recognition, magnetic and conducting materials, and porous and catalytic materials, among other topics. However, at present, most studies focus on XB-based organic supramolecular networks and do not consider metal-containing supramolecular networks. In this review, we provide an update on the recent advances in XB development to summarize the role of XB in the assembly

Abbreviations: apyz, 2-aminopyrazine; bbi, 1,1'-(1,4-butanediyl)bis(imidazole); *p*-bix, 1,4-bis(imidazol-1-ylmethyl)-benzene; *m*-bix, 1,3-bis(imidazol-1-ylmethyl)-benzene; BnOH, benzyl alcohol; bpa, 1,2-bis(4-pyridyl)ethane; bpe, 1,2-bis(4-pyridyl)ethene; bpp, 1,3-bis(4-pyridyl)propane; bpy, 4,4'-bipyridine; 3-CNpy, 3-cyanopyridine; 4-CNpy, 4-cyanopyridine; 4-ClpyH, 4-chloropyridinium; dabco, 1,4-diazabicyclo[2.2.2]octane; DBrETSe, dibromo(ethylenedithio)tetraselenafulvalene; dcb, 3,5-dichlorobenzoate; 3,5-diba, 3,5-diiodobenzoic acid; DIEDSS, 2-(5,6-dihydro[1,3]diselenolo[4,5-*b*][1,4]diselenin-2-ylidene)-4,5-diiodo-1,3-dithiole; DIEDSSe, 2-(4,5-diiodo-1,3-diselenol-2-ylidene)-5,6-dihydro[1,3]diselenolo[4,5-*b*][1,4]diselenine; DIETS, diiodo(ethylenedithio)diselenadithiafulvalene; DIETSe, 2-(4,5-diiodo-1,3-diselenol-2-ylidene)-5,6-dihydro[1,3]diselenolo[4,5-*b*][1,4]dithiine; DIET-STF, {2-(4,5-diiodo-1,3-diselenol-2-ylidene)-5,6-dihydro[1,3]dithiolo[4,5-*b*][1,4]dithiine}; DIP, diiodo(pyrazino)tetrathiafulvalene; DIPS, diiodo(pyrazino)diselenadithiafulvalene; DIPSe, diiodo(pyrazino)tetraselenafulvalene; DMAC, *N,N'*-dimethylacetamide; DMF, *N,N'*-dimethylformamide; dmit, 4,5-dithiolato-1,3-dithiole-2-thione anion; 2,6-DMP, 2,6-dimethylpyrazine; DMSO, dimethylsulfoxide; diiodo-PFA, 1,8-diiodoperfluorooctane; EDO-TTF₂, 4,5-diiodo-4',5'-ethylenedioxytetrathiafulvalene; EDT-TTFBr₂, 4,5-dibromo-4',5'-ethylenedithiotetrathiafulvalene; EDO-TTFBr₂, 4,5-dibromo-4',5'-ethylenedioxotetrathiafulvalene; HMTA, hexamethylenetetramine; HT, halothane; 3-ibz, 3-iodobenzoate; 4-ibz, 4-iodobenzoate; 5-iipa, 5-iodo-isophthalic acid; 4-XpyH, 4-halopyridinium (X = Cl, Br or I); IEIB, 1-iodoethyl-4-iodobenzene; Iqsal, 5-iodo-*N*-(8'-quinolyl)-salicylaldehyde; mnt, maleonitriledithiolate; NBS, *N*-bromosuccinimide; NIS, *N*-iodosuccinimide; PyDIPP, 5,15-bis(4'-pyridyl)-10,20-bis(4'-iodophenyl)porphyrin; PyTIPP, 5-(4-pyridyl)-10,15,20-tris(4-iodophenyl)porphyrin; pyz, pyrazine; qsal-X, 5-X-*N*quinolylsalicylaldehyde (X = F, Cl, Br); TBC[4], *p*-^tBu-calix[4]arene; TBrPP, 5,10,15,20-tetra(4-bromophenyl)porphyrin; TIPP, 5,10,15,20-mesotetrakis(4-iodophenyl)porphyrin; T3PyP, 5,10,15,20-tetrakis(3-pyridyl)-porphyrin; T4PyP, 5,10,15,20-tetrakis(4-pyridyl)-porphyrin; TRZ, 1,3,5-triazine.

* Corresponding authors.

E-mail addresses: zangsqzq@zzu.edu.cn (S.-Q. Zang), wly@nynu.edu.cn (L.-Y. Wang).

of metal-containing supramolecular networks. We begin by introducing the reader to halogen-related interactions by highlighting a selection of typical organic supramolecular networks. Next, we present an overview of metal-containing supramolecular networks based on XB in metal halide/pseudohalide, metal 2,2'-dipyridylamino/s-triazine, metal quinolylsalicylaldehyde, metal thiocalixarene, metal tetrathiafulvalenium (TTF), metal porphyrin, and metal iodo-benzenecarboxylic acid systems. The conclusions describe the potential applications of halogen-bonded supramolecular networks. A major goal of this review is to provide an organized and illustrative account of the recent work on XB-based, high-dimensional supramolecular networks, particularly metal-containing supramolecular networks. Finally, prospective directions for research involving XB in high-dimensional supramolecular architectures will be discussed.

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1. Introduction

The design and synthesis of metal-containing supramolecular networks has been an active field in recent years [1–7]. In the construction of such frameworks, coordinate covalent bonding [4,5] and noncovalent interactions (hydrogen bonding and $\pi \cdots \pi$ interactions) [6,7] are two well-established essentials of crystal engineering. As is well known, hydrogen bonding is by far one of the major and the most frequently occurring cohesive interaction in crystal engineering for the construction of supramolecular assemblies with predefined architectures. Some characteristics of the complexes are related to the noncovalent interactions that determine their networks [8–12]. Recently, several groups have realized that it is feasible to utilize hydrogen bonding interactions to construct new, porous materials with permanent porosity and highly selective gas separation [13]. Compared to the assembly of supramolecular networks with conventional noncovalent interactions (hydrogen bonding and $\pi \cdots \pi$ interactions), designed crystal engineering with halogen bonding (XB) has not been given sufficient attention.

XB is an emerging noncovalent interaction involving polarizable chlorine, bromine, or iodine molecular substituents. XB can be described as $Y-X \cdots D$, where $Y-X$ is the halogen bond donor, X is any halogen atom with an electrophilic (electron-poor) region, Y is a group covalently bound to X , and D is a neutral oxygen, nitrogen, or sulfur atom, an olefinic or aromatic unsaturated system, or a halide or acetate anion [14–16]. After the seminal paper entitled “Halogen Bonding: A Paradigm in Supramolecular Chemistry” was published by Metrangolo and Resnati [17], published work on the topic grew exponentially (Fig. 1). XB has been widely used to drive molecular self-assembly and has developed considerably as an intermolecular force analogous to hydrogen bonding in the last five years. The great potential for the development of high-value, functional materials based on the formation of XB is already known. Particularly important reviews [18–24] have primarily focused on the effectiveness of such interactions in crystal engineering and have thereby drawn widespread interest in many fields, most notably in connection with biological systems [25], magnetic and conducting materials [26], liquid crystals [27], nonlinear optics (NLO) [28], porous materials [29], catalysis [30], solar cells [31], nanomaterials [32], and molecular recognition and assembly [33]. The effectiveness of XB interactions in the crystal engineering of low-dimensional supramolecular networks has been widely documented [34].

This review does not aim to exhaustively cover the field of XB-based, metal-containing supramolecular networks. Instead, we highlight several important research groups' efforts to rationally synthesize metal-containing supramolecular networks based on XBs in metal halide/pseudohalide, metal 2,2'-dipyridylamino/s-triazine, metal quinolylsalicylaldehyde, metal thiocalixarene, metal tetrathiafulvalenium (TTF), metal porphyrin, and metal iodo-benzenecarboxylic acid systems. The effective design of intermolecular recognition processes requires a thorough understanding of all interactions and mechanisms that may be used. At

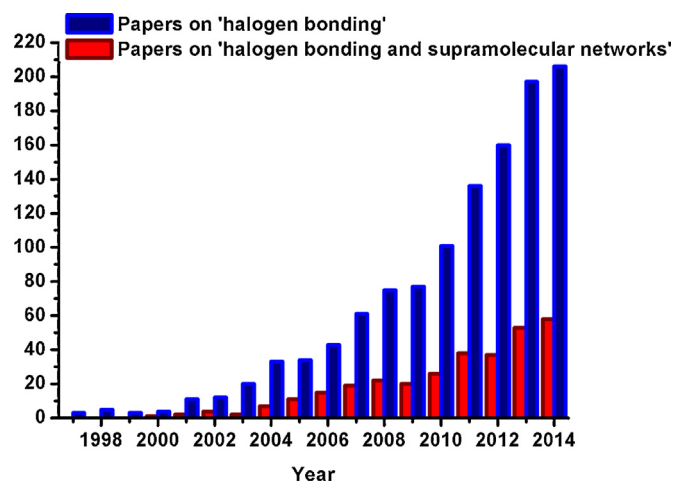


Fig. 1. Number of publications featuring the term 'halogen bonding' and 'halogen bonding and supramolecular' in their topics.

Data obtained from ISI Web of Science until April 6th, 2015.

the beginning of this review, some general geometries of halogen-related interactions in some typical supramolecular networks will be described. From this, it is easy to predetermine the structures of the supramolecular networks based on XBs.

2. Halogen-related interactions

Understanding the unique nature of XB is critical to the creation of supramolecular networks that use XB interactions as design elements in their crystal engineering. XB is a strong, specific and highly directional interaction capable of driving the self-assembly of supramolecular networks [35]. These interactions include many halogen \cdots halogen interactions ($X \cdots X$) and nearly all halogen \cdots heteroatom interactions ($X \cdots D$). Theoretical and experimental data prove that all four halogens can be XB donors, and the tendency to form strong interactions follows the trend $I > Br > Cl \gg F$ (a fluorine atom can act as a XB donor only when attached to a particularly strong electron-withdrawing group [35f]). Over the last decade, systematic studies have revealed that halogen-related interactions, such as halogen $\cdots N$ (O, S), halogen $\cdots \pi$ and halogen \cdots halogen interactions, are ubiquitous, noncovalent interactions in crystal engineering. In this section, we highlight a selection of typical organic supramolecular networks to demonstrate the generality of the interactions.

2.1. Halogen $\cdots N$ (or O, S) interactions

Nitrogen, oxygen or sulfur atoms are often better XB acceptors than other atoms; accordingly, a variety of nitro, hexamethylenetetramine, pyridine, pyrazine, triazine, imidazole, and pyridine derivatives and other related groups have been widely used in crystal engineering to obtain halogen $\cdots N$ (or O, S) interactions

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