The first two examples of halogen bonding with a sigma hole-donating fluorine in C_{sp3} -F···O_{sp3} interaction from poly-fluorinated trans-dihalo-palladium(II) disubstituted pyridine complexes

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Electronic Supplementary Information (ESI)

Table of Contents

| 1. | Scheme S1. | ESI 4 |
|-----|--------------|---------------|
| 2. | Figure S1. | ESI 5 |
| 3. | Figure S2.1. | ESI 6 |
| 4. | Figure S2.2. | ESI 7 |
| 5. | Table S1. | ESI 8 |
| 6. | Table S2. | ESI 9 |
| 7. | Figure S3.1. | ESI 10 |
| 8. | Figure S3.2. | ESI 10 |
| 9. | Figure S4.1. | ESI 11 |
| 10. | Figure S4.2. | ESI 12 |
| 11. | Figure S5. | ESI 13 |
| 12. | Figure S6. | ESI 14 |
| 13. | Table S3. | ESI 15 |
| 14. | Reference | ESI 16 |

Experimental Sections

General procedures. Gas chromatographic/mass spectrometric data were obtained using an Agilent 6890 Series gas chromatograph with a series 5973 mass selective detector. Reactions were monitored with a HP 6890 GC using a 30 m 0.250 mm HP-1 capillary column with a 0.25 mm stationary phase film thickness. The flow rate was 1 mL/min and split-less. Samples analyzed by fast atom bombardment (FAB) mass spectroscopy were carried out by staff of the National Central University (Taiwan) mass spectrometry laboratory. Infrared spectra were obtained on a Perkin Elmer RX I FT-IR spectrometer. NMR spectra were recorded on Bruker AM 500 and 300 spectrometers using 5-mm o.d. sample tubes. CD₃OD, CD₂Cl₂, CDCl₃, deuterated DMF, and deuterated DMSO were the references for both ¹H and ¹³C NMR spectra, while Freon[®] 11 (CFCl₃) was the reference for ¹⁹F NMR spectra. Table S2 lists part of the parameters in X-ray studies employing a Bruker single-crystal diffractometer equipped with a CCD area detector and graphite-monochromatized Mo Ka radiation (λ 0.71073 Å). Chemicals, reagents, and solvents employed were commercially available and used as received.

Computational method for vibrational study

Theoretical calculations were performed using the Gaussian 16 packages.¹ For the geometry optimizations, the crystal geometries of two ligand molecules with interactions shown in Fig. 1a were taken for calculations and performed using the APFD DFT functional with a basis set of def2-SVP for all the atoms. The vibrational frequency analysis of the corresponding dimers were carried out while the optimized structure represented the local energy minimum.

Synthesis of 3-[(2,2,3,3-tetrafluoropropoxy)methyl]pyridine²**:** 2,2,3,3-Tetrafluoropropan-1-ol (0.83 g, 6.3 mmol) and 30% CH₃ONa/CH₃OH (5.1 mmol) were mixed in a double-necked flask and continuously stirred at 333 K under nitrogen for 4 hours. The methanol was removed using a vacuum system to shift the reaction to the product side. The obtained sodium fluorinated alkoxide was dissolved in dry THF (20 mL), and then 3-BrCH₂-pyridine (0.67 g, 3.9 mmol) was added, and the mixture was continuously stirred for 4 hours under a nitrogen atmosphere at 333 K. The resulting solution was extracted with dichloromethane and water to give 3-[(2,2,3,3-tetrafluoropropoxy)methyl]pyridine as a pale yellow liquid, and then a distillation system was applied to remove excess solvent to obtain pure 3-[(2,2,3,3-tetrafluoropropoxy)methyl]pyridine, which is the transparent liquid.

Synthesis of complex (1): 3-[(2,2,3,3-tetrafluoropropoxy)- methyl]pyridine (1.74 g, 7.8 mmol) was mixed with K2PdCl4 using dry DMSO in a round bottom flask and at 333 K under nitrogen for 4 hours. Then a distillation system was used to remove excess solvent to obtain a crude product. The crude product was dissolved in ethanol (10 mL), and then water was added (200 mL) to precipitate it out. After suction filtration, white powder was obtained. The yield of the white product (1) (833 mg, 1.2 mmol) was 92%.

Synthesis of complex (2): In the case of bromide complex, similar synthesis procedure was followed using K₂PdBr₂ to obtain a pale yellow powder. The yield of **t-[(3-4FH-py)₂PdBr₂]** (812 mg, 1.0 mmol) was 77%.

Analytical data of t-[(3-4FH-py)₂PdCl₂] (1)

m.p. 138 °C, ¹H-NMR (500 MHz, CDCl₃), δ (ppm)= 8.77 (2H, d, ³J_{HH}=6.0 Hz, H₆), 8.77 (2H, s, H₂), 7.77 (2H, d, ³J_{HH}=8.0 Hz, H₄), 7.35 (2H, dd, ³J_{HH}=8.0Hz, ³J_{HH}=5.8Hz, H₅), 5.93 (2H, tt, ²J_{HF}=53.5 Hz, ³J_{HF}= 5.0 Hz, terminal H), 4.65 (4H, s, py-**CH**₂ OCH₂CF₂CF₂H, H7), 3.91 (4H, tt, ³J_{HF}=13Hz, ⁴J_{HF}= 2.0 Hz, py-CH₂OC**H**₂CF₂CF₂H, H8); ¹³C-NMR (125 MHz, CDCl₃), δ (ppm)=152.9, 152.0, 137.6, 134.5, 124.8, (10C, s, py), 117.0~106.9, (4C, py-CH₂OCH₂CF₂CF₂H) 70.7, (2C, s, py-CH₂OCH₂CF₂CF₂H) 67.7, (2C, ³J_{CF}= 27.88 Hz, py-CH₂OCH₂CF₂CF₂H); ¹⁹F-NMR (500 MHz, CDCl₃), δ (ppm)= -124.37, (4F, s, py-CH₂OCH₂CF₂CF₂H) -138.90, (4F, s, py-CH₂OCH₂CF₂CF₂H). FT-IR: ν (cm⁻¹) = 1614, 1587, 1471, 1447 (vpy, m), 1135, 1092 (C-F, stretch); HR-FAB [(M-Cl)⁺; m/z=] C₁₈H₁₈³⁵ClF₈N₂O₂Pd calcd m/z 586.9964, found 586.9962 C₁₈H₁₈³⁷ClF₈N₂O₂Pd calcd m/z 588.9968, found 588.9936.

Analytical data of t-[(3-4FH-py)₂PdBr₂](2):

m.p.= 141 °C; ¹H-NMR (500 MHz, CDCl₃), δ (ppm)= 8.82 (2H, s, H₂) 8.79 (2H, d, ³J_{HH}= 5.5 Hz, H₆), 7.75 (2H, d, ³J_{HH}= 7.0 Hz, H₄), 7.34 (2H, dd, ³J_{HH}= 7.0 Hz, ³J_{HH}= 6.0 Hz, H₅), 5.93 (2H, tt, ²J_{HF}= 53.5 Hz, ³J_{HF}= 5.0 Hz, terminal H), 4.65 (4H, s, py-**CH**₂OCH₂CF₂CF₂H), 3.92 (4H, t, ³J_{HF}=12Hz, py-CH₂O**CH**₂CF₂CF₂H); ¹³C-NMR (125 MHz, CDCl₃), δ (ppm)= 153.9, 152.9, 137.4, 134.5, 124.9, (10C, s, py), 117.0~106.9, (4C, py-CH₂OCH₂CF₂CF₂H) 70.6, (2C, s, py-CH₂OCH₂CF₂CF₂H) 67.7, (2C, ³J_{CF}=27.9 Hz, py-CH₂OCH₂CF₂CF₂H); ¹⁹F-NMR (500 MHz, CDCl₃), δ (ppm)= -124.36 (4F, s, py-CH₂OCH₂CF₂CF₂H), -138.87 (4F, s, py-CH₂OCH₂CF₂CF₂H); FT-IR: υ (cm⁻¹)= 1613, 1586, 1472, 1446 (vpy, m), 1136 1094 (C-F, stretch); FAB (M+; m/z=) C₁₈H₁₈⁷⁹Br₂F₈N₂O₂Pd calcd m/z 709.8642, found 709.8632; C₁₈H₁₈⁸¹Br₂F₈N₂O₂Pd calcd m/z 713.8626, found 713.8585; C₁₈H₁₈⁷⁹Br⁸¹Br F₈N₂O₂Pd calcd m/z 711.8622, found 711.8620.

Deuterated t-[(3-4FH-py)_2PdCl_2]: the deuterated compound of **t-[(3-4FH-py)_2PdCl_2]** is was also similarly prepared.

Some analytical data are shown below:

¹H-NMR (300 MHz, CDCl₃) δ (ppm)= 8.86 (1H, d, ³J_{HH}= 5.5 Hz, H₆), 8.84 (1H, s, H₂), 7.78 (1H, d, ³J_{HH}= 8.1 Hz, H₄), 7.33 (1H, t, ³J_{HH} = 6.9 Hz, H₅), 5.93 (1H, tt, ²J_{FH}= 52.8, ³J_{FH}= 4.5 Hz, -OCH₂CF₂CF₂H), 3.92 (2H, t, ³J_{FH} = 12.3 Hz, -OCH₂CF₂CF₂H); FT-IR: υ (cm⁻¹) = 2932, 2889, 2780 (HC₂F₄-CH₂-O-CD₂ stretch), 2184, 2164, 2078 (CH₂-O-CD₂ stretch), 1614, 1587, 1471, 1447 (vpy, m), 1136, 1092 (C-F, stretch).

Crystallization:

The samples of **t-[(3-4FH-py)₂PdCl₂]** and **t-[(3-4FH-py)₂PdBr₂]** (30 mg) were dissolved in dry DMF (2 mL), and its top was layered with about water (about 3 mL). After approximately 2 weeks of diffusion crystallization, the resulted single crystal was suitable for X-ray crystallographic studies.



Scheme S1. The schematic drawing of t-[(3-4FH-py)₂PdX₂] where X=CI, Br with the labeling.

1. Molecular packing



Figure S1. Molecular packing diagrams of t-[(3-4FH-py)₂PdBr₂](**2**) (a) showing C8*-F2*...O1 halogen bond (in green dash) and two weak interactions involving C8*-F2*...F4-C9 (in orange dash) and tetrel bonding (in blue dash); (b) its stacking piles arranged in the herringbone pattern. [Note: C, O, N, F, Br and Pd are in grey, red, blue, yellow, brown and dark green color, respectively.]. The r(C8*-F2*...O1), r(F2*...F4) and r(F2*...C6) are 2.839(2), 2.817 and 3.094Å, respectively. Furthermore, C8* and F2* are at an equivalent position (0.5+x, 1.5-y, 0.5+z).]

2. FT-IR spectra I



Figure S2.1. Experimental FT-IR spectra of (X) solid t-[$(3-4FH-py)_2PdBr_2$], and (Y) t-[$(3-4FH-py)_2PdBr_2$] dissolved in C₆D₆; both show the CH₂ vibrational stretches and their shifts. [Note: A description of the shifting of CH₂ groups: when comparing the IR spectrum in solid state (trace X, —) with that in d-benzene solution (trace Y, —), the asymmetric and symmetric CH₂ stretches have red shifted from 2980, 2934 and 2831 to 2916, 2886 and 2769 cm⁻¹, respectively.

3. FT-IR spectra II



Figure S2.2. FT-IR spectra of solid t-[$(3-4FH-py-d_2)_2PdCl_2$] (trace X—) and t-[$(3-4FH-py-d_2)_2PdCl_2$] dissolved in benzene (trace Y—) showing the asymmetric and symmetric stretches of CD₂ group². Note: When comparing the IR spectrum in solid state (trace X) with that in benzene solution (trace Y), the asymmetric and symmetric CD₂ stretches are red-shifted from 2198, 2175 and 2092 to 2184, 2164 and 2078 cm⁻¹, respectively.

4. Vibrational table

| | | t-[(3-4FH-py) ₂ PdCl ₂] solid | t-[(3-4FH-py) ₂ PdCl ₂] in benzene | deuterated t-[(3-4FH-py) ₂ PdCl ₂] solid | |
|----------------------|------------|--|--|---|--|
| | | CH ₂ Stretching frequencies (cm ⁻¹) | | | |
| CH ₂ next | Asymmetric | 2917 | 2978 | NA ⁱ | |
| to the ring | Asymmetric | 2889 | 2931 | NA^{i} | |
| | Symmetric | 2770 | 2830 | NA^{i} | |
| CH ₂ next | Asymmetric | 2932 | 2931 | 2932 | |
| to the chain | Asymmetric | 2889 | 2884 | 2889 | |
| | Symmetric | 2780 | 2780 | 2780 | |

Table S1. The FT-IR studies of CH_2 (or CD_2) stretches of solid and dissolved t-[(3-4FH-py)₂PdCl₂] and its solid deuterated species.

Note: ⁱ NA= not available. (and the stretches of CD₂ group appear at 2184, 2164 and 2078 cm⁻¹ shown in Fig. S.2.2.). t-[(3-4FH-py)₂PdCl₂]= trans-[PdCl₂(3-HCF₂CF₂CH₂OCD₂py)₂].

5. Computation section

The DFT functional have been used for calculations. The IR comparison table of CH_2 groups are shown in Table S2 below. The numbers marked in yellow (both EXP and factored) represent the CH_2 group whose stretches are influenced by C-F^{...}O and tetrel bond interactions. The numbers marked in green (EXP) represent the CH_2 groups without intermolecular C-F^{...}O and tetrel bond interactions because the complex is dissolved in benzene. The numbers marked in pink (factored) represent the CH_2 groups without intermolecular C-F^{...}O and tetrel bond interactions because this CH_2 has not affected by C-F^{...}O and tetrel bond intermolecular interactions. Clearly, from the calculated results, the respective symmetric and two asymmetric stretches of CH_2 group (next to py ring) which is affected by C-F^{...}O and tetrel bond interactions are 2829, 2888, 2910 cm⁻¹. The respective symmetric and two asymmetric stretches of CH_2 group (next to py ring) which have no C-F^{...}O and tetrel bond interactions are 2863, 2934, 2948 cm⁻¹. Thus, based on theoretical calculations, the symmetric and asymmetric CH_2 stretches have red shifted from 2863, 2934 and 2948 to 2829, 2888, and 2910 cm⁻¹, respectively. In other words, the red shifting of CH_2 group (next to py ring) has been confirmed by DFT calculations.

| - | | | | |
|------|-------------------|-------------------|----------|--|
| item | EXP | factored* | unfactor | |
| | | (factor=0.95) | | |
| 1 | <mark>2770</mark> | <mark>2829</mark> | 2978.3 | Symmetric CH ₂ stretch with intermolecular |
| | | | | interaction |
| 2 | (2830) | <mark>2863</mark> | 3013.3 | Symmetric CH ₂ stretch w/o interaction. |
| | $(in C_6H_6)$ | | | |
| 3 | <mark>2889</mark> | <mark>2888</mark> | 3040.1 | asymmetric CH ₂ stretch with intermolecular |
| | | | | interaction |
| 4 | <mark>2917</mark> | <mark>2910</mark> | 3062.7 | asymmetric CH ₂ stretch with intermolecular |
| | | | | interaction |
| 5 | (2931) | <mark>2934</mark> | 3088.6 | asymmetric CH ₂ stretch w/o interaction. |
| | $(in C_6H_6)$ | | | |
| 6 | (2978) | <mark>2948</mark> | 3103.0 | asymmetric CH ₂ stretch w/o interaction. |
| | $(in C_6H_6)$ | | | |

Table S2. The IR CH₂ stretch comparison from both experiment and DFT calculations

Note: 1. The two fluorous pyridine ligands, which have the C-F^{...}O bond, C-F^{...}F-C interaction and tetrel bond shown in Fig. 1a, have been used for this DFT calculations. The stretch of pyridyl CH₂ group from the left pyridine molecule (in Fig. 1a) which serves as F-atom donor is considered as the free CH₂ group. Thus, their calculated CH₂ stretches (next to py) are similar to those from the complex-dissolved benzene solution.

2. w/o: without; EXP: experiment.

6. Crystal packing



Figure S3.1. (a) Single molecule of trans-dichloro-palladium(II) bis(pyridine) complex; (b) Parallel arrangement of the molecules in the crystal packing.



Figure S3.2. (a) Single molecule of trans-dibromo-palladium(II) bis(pyridine) complex, trans-[PdBr₂(py)₂]; (b) Parallel arrangement of the molecules in the crystal packing (without formation of the herringbone type of packing).³

7. Hirshfeld surface analysis



Figure S4.1. Hirshfeld surface⁴ analysis mapped with d_{norm} for t-[(3-4FH-py)₂PdBr₂](**2**) (a) Hirshfeld surface of single molecule and the main interactions formed in the herringbone structure. Three interactions are marked inside the red circle, C_{sp3} -F^{...}O_{sp3} interaction pointed by a yellow arrow; (b) (enlarged image of S4a) Intermolecular interactions indicated with connecting lines between two related atoms.

8. Hirshfeld surface analysis of d_i and d_e of t-[(3-4FH-py)₂PdCl₂]



Figure S4.2. The d_i (S4.2a) and d_e (S4.2b) Hirshfeld surface of t-[(3-4FH-py)₂PdCl₂]; for the d_i mapping (Fig. S4.2a), the red spots pointed by arrows show the distance of atom (C6, O1 or F4) to the surface less than the van der Waals radius; for the d_e mapping (Fig. S4.2b), the ESP surface near F2* atom can be seen as uniformly distributed area with light red color which shows the distance of F2* to surface is shorter than its van der Waals radius. [Note: In order to show the surface better, only one F atom (F2*) from the other molecule is shown.]

Hirshfeld surface analysis of complex (1) mapped with d_i (Fig. S4.2a) and d_e (Fig. S4.2b) represents the proximity of the atom from the mapped surface, from inside of the surface and outside of the surface, respectively. The distance of the atom to the surface is less than van der Waals radius of specific atom, and then the color of the surface is shown in red color. Here the d_i plot shows the three red spots, which correspond to the C6, O1 and F4 atoms (clockwise from the bottom), are indicated with arrows (their respective distance to the surface is smaller than van der Waals radius). For the d_e plot shown in Fig. S4.2b, the ESP surface near F2* atom can be seen as uniformly distributed area with light red color which shows the distance of F2* to surface of the other molecule is shorter than its van der Waals radius. Additionally, the d_i and d_e Hirshfeld surface maps of complex (2) is similar to those of complex (1).

9. Deformation density analysis and Laplacian map



Figure S5. (a) Deformation density⁶ analysis ((+ve and –ve values indicated by red and blue colors); and (b) Laplacian map⁷ of the interaction region of t-[(3-4FH-py)₂PdBr₂](**2**), +ve and –ve values represented by black and pink (where vscc is.) colors. [Note: Deformation density iso-surfaces are drawn at 0.001 au; the vscc region, which is shown as pink rings, just closely surrounds the central O atom (in red color) in (b).]

10. Electrostatic Potential Analysis



Figure S6. Electrostatic potential (ESP) contours⁸ for (a) t-[(3-4FH-py)₂PdCl₂](1); and (b) t-[(3-4FH-py)₂PdBr₂] (2), showing the presence of electron negative region (red concentric circles area) between the fluorine and oxygen. [Note: C, O, N, F, Cl, Br and Pd are in grey, red, blue, yellow, green, brown and dark green color, respectively. The method of B3LYP/LANL2DZ level of theory is used for all the ESP related calculations.

| | t-[(3-4FH-py)2PdCl2](1) | t-[(3-4FH-py)2PdBr2](2) |
|--|--|---|
| CCDC No. | 1948936 | 1948937 |
| Chemical formula <i>M_r</i> Crystal system, space group Temperature (K) | C ₁₈ H ₁₈ Cl ₂ F ₈ N ₂ O ₂ Pd 623.64 Monoclinic, <i>P2</i> ₁ / <i>n</i> 100.0(2) | C18H18Br2F8N2O2Pd 712.56 Monoclinic, <i>P21/n</i> 100.0(2) |
| <i>a, b, c</i> (Å) | 7.0691 (2), 18.6278 (5), | 7.2992 (3), 18.6059 (7), 8.7965 |
| | 8.7985 (3) | (4) |
| β | 109.625 (1) | 110.215 (2) |
| V (Å ³) | 1091.30 (6) | 1121.05 (8) |
| Ζ | 2 | 2 |
| Radiation type | Mo $K\alpha$ | Mo $K\alpha$ |
| $\mu (\mathrm{mm}^{-1})$ | 1.18 | 4.48 |
| Crystal size (mm) | 0.44 	imes 0.40 	imes 0.06 | 0.24 	imes 0.22 	imes 0.16 |
| Data collection | | |
| Diffractometer | Bruker APEX-II CCD | Bruker APEX-II CCD |
| Absorption correction | Multi-scan Bruker <i>SADABS</i> , 1996 | Multi-scan Bruker <i>SADABS</i> , 1996 |
| Tmin, Tmax | 0.844, 0.971 | 0.713, 0.971 |
| No. of measured, independent, and | 11039, 2398, 2195 | 27252, 2473, 2394 |
| observed $[I > 2\sigma(I)]$ reflections | | |
| R _{int} | 0.040 | 0.041 |
| $(\sin\theta/\lambda)_{max},$ (Å ⁻¹) | 0.641 | 0.641 |
| Refinement $R[F^2 > 2\sigma(F^2)], wR(F^2), S$ | 0.021, 0.050, 1.05 | 0.015, 0.037, 1.06 |
| No. of reflections | 2398 | 2473 |
| No. of parameters | 152 | 153 |
| $\Delta \rho_{\rm max}, \Delta \rho_{\rm min} (e {\rm A}^{-3})$ | 0.45, -0.60 | 0.46, -0.64 |

11. Crystal data

Table S3. Crystal data of both compounds

Computer programs: Bruker Instrument Service v2012.12.0.3, *SAINT* V8.35A (Bruker AXS Inc., 2015), XT, VERSION 2014/4, *SHELXL2013* (Sheldrick, 2013), shelXle (C.B. Huebschle, rev 740), *WinGX* publication routines (Farrugia, 1999).

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