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Supporting information for article:

Hydrogen bonding and fluorous weak interactions in the non-isomorphous {4,4′-bis[(2,2,3,3-tetrafluoropropoxy)methyl]-2,2′-bipyridine-κ^2N,N'}dibromidopalladium and -platinum complexes

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Supporting materials (SI)

There are three items in this SI. (A. Projection of 7 molecules of 1, B. Response to Alert level B in i15498LT, C. Response to Alert level C in i15498RT (at 295K) on missing FCF, and D. The fingerprint plot.)

A. Projection of 7 molecules of 1

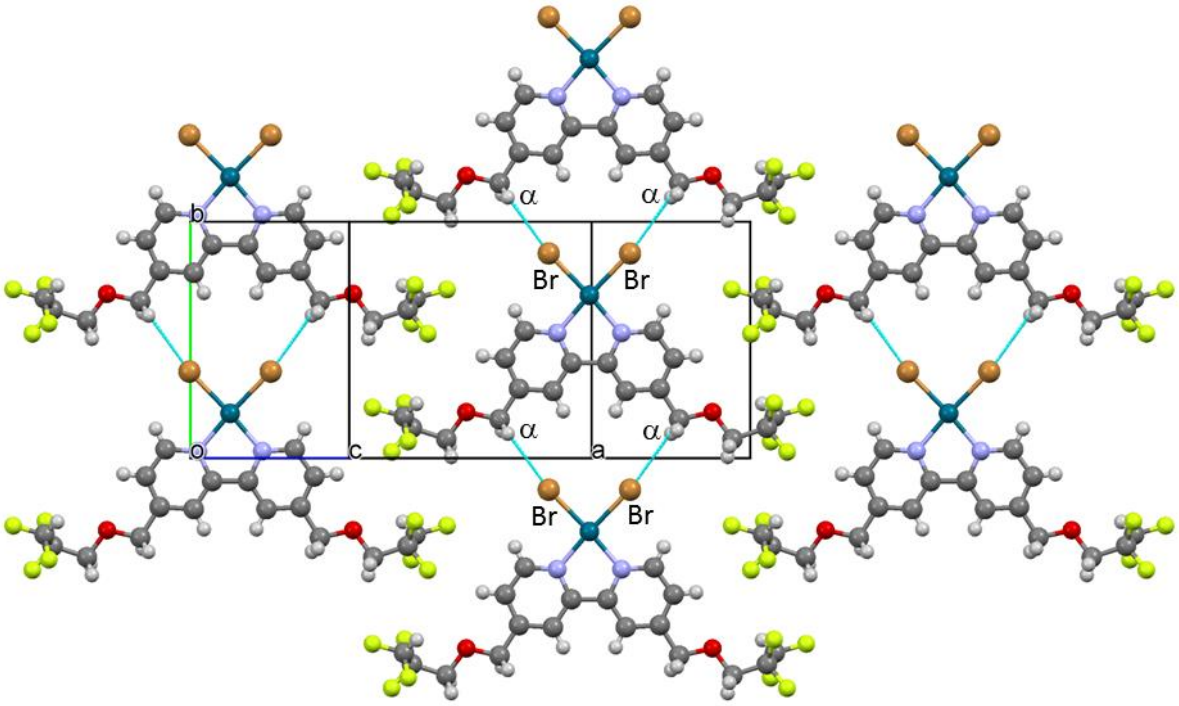


Figure S1. Projection of 7 molecules of **1** to form 3 belts, using double C–$H_{(\alpha)}$···Br hydrogen bonds that self-repeat along the crystallographic *b* axis. The layer steps between neighboring columns are 1.639(2) Å. Noted are that there are no fluorous C–H···F or C–F···F contacts. Color codes: Pd: dark blue; Br: brown; F: yellow-green; O: red; N: blue; C: gray; H: white.

B. Response to Alert level B in i15498LT CHECKCIF

Alert B: (from i15498LT)
Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 6 Check

Comments: The previous cif omitted the following 8 reflections to pass alert level B as follows:
(0 0 2), (0 1 6), (0 3 18), (-1 2 12) *, (-1 4 10), (-1 2 11), (1 2 0),
(1 2 11).
This version of cif put back reflections required by reviewer #2, limiting only (0 0 2) reflection that is low theta angle.

h k l	Fo^2	Fc^2	Error/esd	Fc/Fc(max)	Resolution (Å)
0 1 6	18957.07	9307.78	12.77	0.200	4.09
0 3 18	5776.04	11.17	12.36	0.007	1.36
-1 2 11	32695.72	18955.87	11.19	0.286	2.17
-1 4 10	1822.78	64.40	10.26	0.017	1.93
1 2 11	7957.85	2650.33	8.93	0.107	2.04
1 2 0	77237.63	58448.27	8.80	0.502	4.49

Note: * The (-1 2 12) is not listed in current cif file as one of the top (Iobs-Icalc)/SigmaW reflections.

The remaining 6 out of the 7 reflections put back are listed above for information.

C. Response to Alert level C in i15498RT (at 295K) on missing FCF

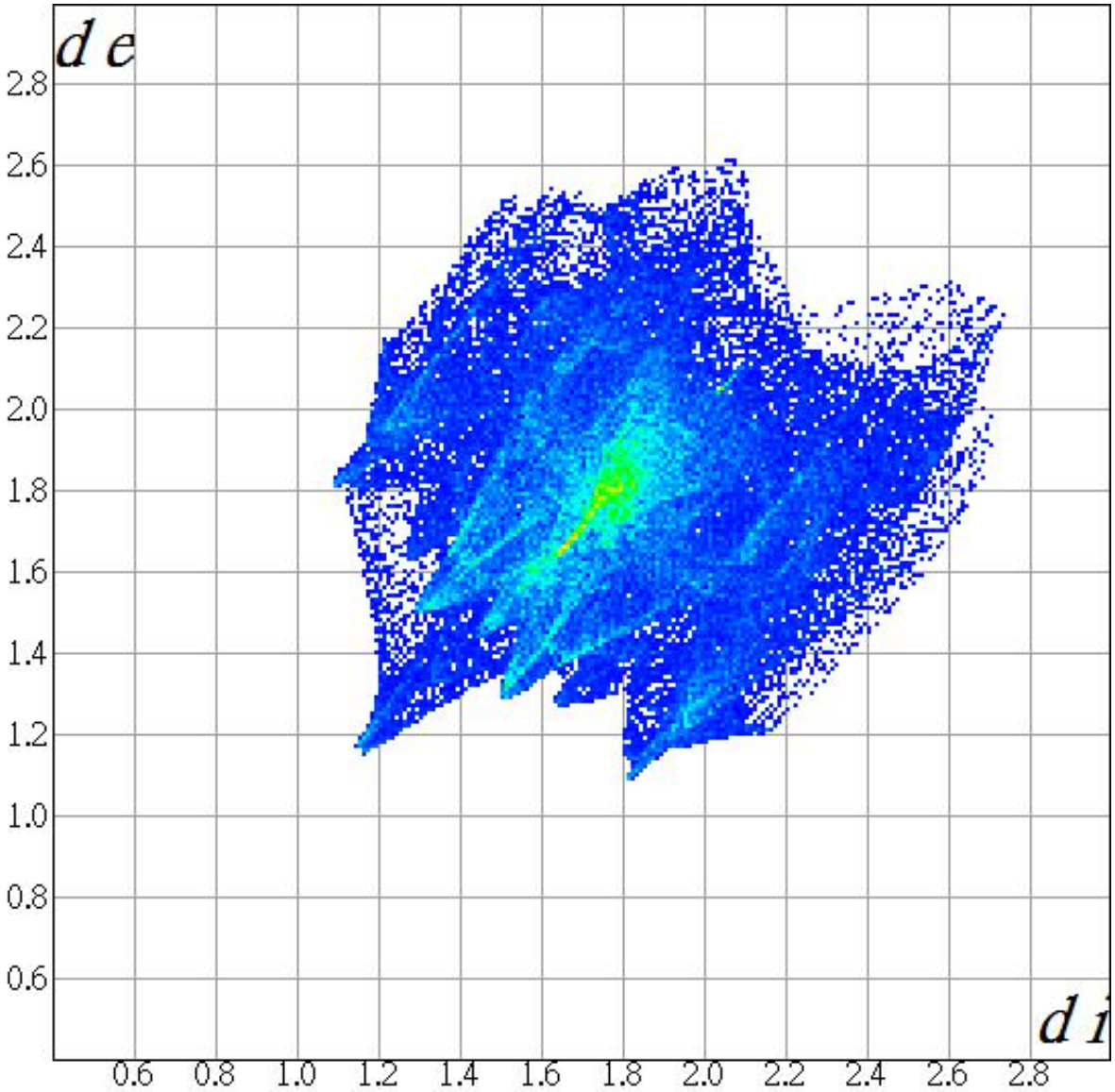
Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report

The low angle reflection 0 0 2 was manually omitted because of beam stop interference.
The list of missing FCF reflections is shown below, from section 3 of the FCF report.

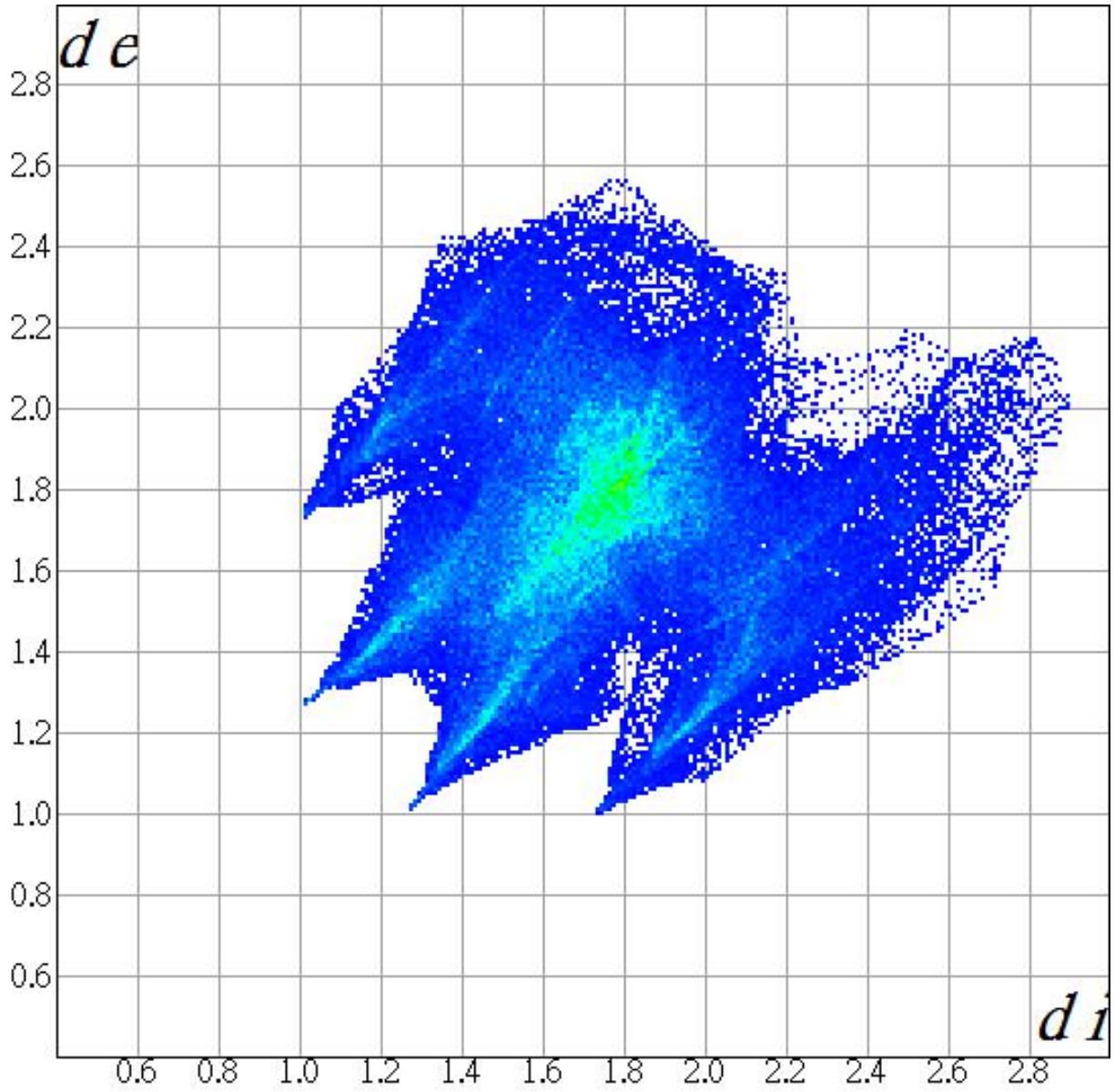
Nr	H	K	L	sin(th)/lambda	Theta	I(calc)	I(calc)/I(max)
1	0	0	2	0.038	1.53*	110043.67	0.48718
2	-7	0	5	0.499	20.77	10419.21	0.04613
3	-1	0	5	0.111	4.52	51074.96	0.22612
4	1	0	7	0.158	6.44	77363.95	0.34250
5	-1	0	15	0.282	11.57	2365.18	0.01047
6	-2	0	22	0.421	17.40	4827.08	0.02137

D. The fingerprint plot

The fingerprint plots of **1** and **2** mono-molecules are shown in Figures S2a and S2b. The small red dots along the pseudo d_i=d_e axis of Figures S2a are believed to be due to the C–F···π interactions. No such observable red colored areas could be located in Figure S2b. The fingerprint plots not only give the evidence to weak C–H···π, π···π, H-bonding, van der Waals interactions, etc., but also **the presence of C–F···π interactions**, as revealed in the structurally related complexes 1 and **2** in this study.



(a)



(b)

Figure S2a,b. The fingerprint plots of **1** (a; top) and **2** (b; bottom).

(Note: The small red dots along the pseudo d_i=d_e axis are only present in Figure S2a.)