Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Self-Assembly of Bowl-Like Trinuclear Metallo-macrocycles

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Contents:

Table S1 Selected Bond Lengths (Å) and Angles (˚) for **4a**

Pd1-N1	2.013(4)	Pd1-N2	2.011(4)
Pd1-N7	2.007(3)	Pd1-N8	1.995(4)
Pd2-N3	2.040(3)	Pd2-N4	2.030(3)
Pd2-N9	2.013(3)	Pd2-N10	2.017(3)
Pd3-N5	2.047(3)	Pd3-N6	2.021(4)
Pd3-N11	2.038(4)	Pd3-N12	2.032(4)
N1-Pd1-N2	82.2(2)	N7-Pd1-N8	87.2(1)
N3-Pd2-N4	82.1(1)	N9-Pd2-N10	88.5(1)
N5-Pd3-N6	81.3(1)	N11-Pd3-N12	87.8(2)

Table S2 Hydrogen bond lengths (Å) and angles (º) for the complex **4a**

D−H···A	D(D-H)	D(H···A)	D(D···A)	∠(DHA)
C1-H1···N13	0.93	2.43	3.169(5)	136
C8-H8···F12[a]	0.93	2.40	3.277(4)	157
C103-H10H···F6	0.96	2.44	3.186(5)	135
C15-H15···F3[b]	0.93	2.43	3.189(4)	139
C26-H26···F1	0.93	2.41	3.081(5)	129
C47-H47···O10[b]	0.93	2.57	3.273(5)	133
C58-H58···O7[b]	0.93	2.45	3.249(5)	145
C69-H69···O8[b]	0.93	2.17	3.044(5)	156
C74-H74B···O2	0.93	2.20	2.558(5)	100
C79-H79A···O13[c]	0.93	2.47	3.142(5)	126
C80-H80B···O12[c]	0.93	2.42	3.317(5)	155
C83-H83A···F14[b]	0.93	2.54	3.483(5)	165
C89-H89A···F4[d]	0.93	2.41	3.226(5)	142
C95-H95C··N7	0.93	2.27	3.198(5)	163
C99-H99B···F6	0.93	2.46	3.209(5)	134

Symmetry codes: [a] x,-1+y,z; [b] 2-x,-y,1-z; [c] 1+x,-1+y,z; [d] 1-x,1-y,1-z.

Table S3 Selected Bond Lengths (Å) and Angles (˚) for **11**

Pd1-N1	2.033(5)	Pd1-N2	2.040(4)
Pd1-N7	2.006(5)	Pd1-N12	2.001(4)
Pd2-N3	2.020(4)	Pd2-N4	2.015(4)
Pd2-N8	2.028(4)	Pd2-N9	1.988(4)
Pd3-N5	2.016(4)	Pd3-N6	2.013(5)
Pd3-N10	2.003(4)	Pd3-N11	2.003(4)
N1-Pd1-N2	81.4(2)	N7-Pd1-N12	89.5(2)
N3-Pd2-N4	81.8(2)	N8-Pd2-N9	90.4(2)
N5-Pd3-N6	82.6(2)	N10-Pd3-N11	88.6(2)

Table S4 Hydrogen bond lengths (Å) and angles (º) for the complex **11**

D−H···A	D(D-H)	D(H···A)	D(D···A)	∠(DHA)
C1-H1···O19[a]	0.93	2.47	3.245(6)	140
C2-H2···O21[a]	0.93	2.41	3.205(8)	144
C9-H9···O17	0.93	2.38	3.171(7)	143
C10-H10···O16	0.93	2.36	3.194(7)	149
C13-H13···O16	0.93	2.49	3.341(6)	153
C21-H21···O22[a]	0.93	2.58	3.501(7)	170
C33-H33···O20[a]	0.93	2.48	3.382(7)	162
C34-H34···O19[a]	0.93	2.60	3.312(7)	134
C39-H39···O21[b]	0.93	2.55	3.428(7)	157
C43-H43···O16[a]	0.93	2.36	3.278(7)	168
C48-H48···O24[c]	0.93	2.48	3.330(7)	152
C52-H52···O23[c]	0.93	2.60	3.515(7)	170
C57-H57···O16[a]	0.93	2.40	3.317(7)	169
C64-H64B···O22	0.97	2.58	3.266(7)	128
C73-H73B···O7	0.97	2.44	3.381(8)	165
C74-H74A···O14	0.97	2.59	3.558(7)	174
C74-H74A···O15	0.97	2.26	2.770(7)	112

Symmetry codes: [a] 1-x,1-y,1-z; [b] 2-x,1-y,1-z; [c] x,1+y,z.

Table S5 Selected Bond Lengths (Å) and Angles (˚) for complex **13**

Pd1-N1	2.005(6)	Pd1-N2	2.008(5)
Pd1-N7	1.992(5)	Pd1-N12	2.002(5)
Pd2-N3	2.027(5)	Pd2-N4	2.023(5)
Pd2-N8	2.008(5)	Pd2-N9	2.018(5)
Pd3-N5	2.019(5)	Pd3-N6	2.011(5)
Pd3-N10	2.004(5)	Pd3-N11	1.999(5)
N1-Pd1-N2	81.8(2)	N7-Pd1-N12	86.9(2)
N3-Pd2-N4	81.8(2)	N8-Pd2-N9	87.5(2)
N5-Pd3-N6	80.3(2)	N10-Pd3-N11	87.9(2)

Table S6 Hydrogen bond lengths (Å) and angles (º) for the complex **13**

D−H···A	D(D-H)	D(H···A)	D(D···A)	∠(DHA)
O10-H10A···O3	0.82	2.21	2.709(8)	119
O11-H11A···O6	0.85	2.30	2.738(9)	113
C11-H11···N8	0.93	2.59	3.106(8)	116
C11-H11···O2[a]	0.93	2.52	3.156(10)	126
C12-H12···O1[a]	0.93	2.56	3.318(10)	139
C17-H17···O9[b]	0.93	2.39	3.285(9)	160
C20-H20···O5[c]	0.93	2.51	3.288(8)	141
C21-H21···N10	0.93	2.60	3.116(8)	116
C21-H21···O5[c]	0.93	2.54	3.273(8)	136
C28-H28···O7[d]	0.93	2.55	3.304(7)	139
C30-H30···N11	0.93	2.62	3.121(10)	114
C44-H44···O5[e]	0.93	2.43	3.357(11)	173

Symmetry codes: [a] x,-y,1/2+z; [b]-x,1-y,1-z; [c]1/2-x,-1/2+y,1/2-z; [d]1/2-x,3/2-y,2-z; [e]x,1-y,1/2+z.

Table S7 Selected Bond Lengths (Å) and Angles (˚) for complex **14a**

Pd1-N1	2.007(4)	Pd1-N2	2.012(4)
Pd1-N3	2.011(4)	Pd1-N4	2.019(4)
Pd2-N5	2.002(4)	Pd2-N6	2.016(4)
N1-Pd1-N2	81.1(2)	N5-Pd2-N5A	86.4(2)
N3-Pd1-N4	87.9(2)	N6-Pd2-N6A	80.6(2)

Symmetry codes: -x, y, z

Table S8 Hydrogen bond lengths (Å) and angles (º) for the complex **14a**

D−H···A	D(D-H)	D(H···A)	D(D···A)	∠(DHA)
C1-H1···N4	0.93	2.58	3.103(6)	116
C13-H13···F1[a]	0.93	2.31	3.156(7)	151
C13-H13···F1[b]	0.93	2.31	3.156(7)	151
C17-H17···F4[a]	0.93	2.39	3.317(6)	171
C24-H24··N7	0.93	2.57	3.299(7)	135
C28-H28···F4[c]	0.93	2.40	3.330(7)	175
C31-H31B···F8[d]	0.96	2.40	3.355(7)	172

Symmetry codes: [a] x,y,-1+z; [b] -x,y,-1+z; [c] x,-y,1-z; [d] 1/2-x,-y,-1/2+z.

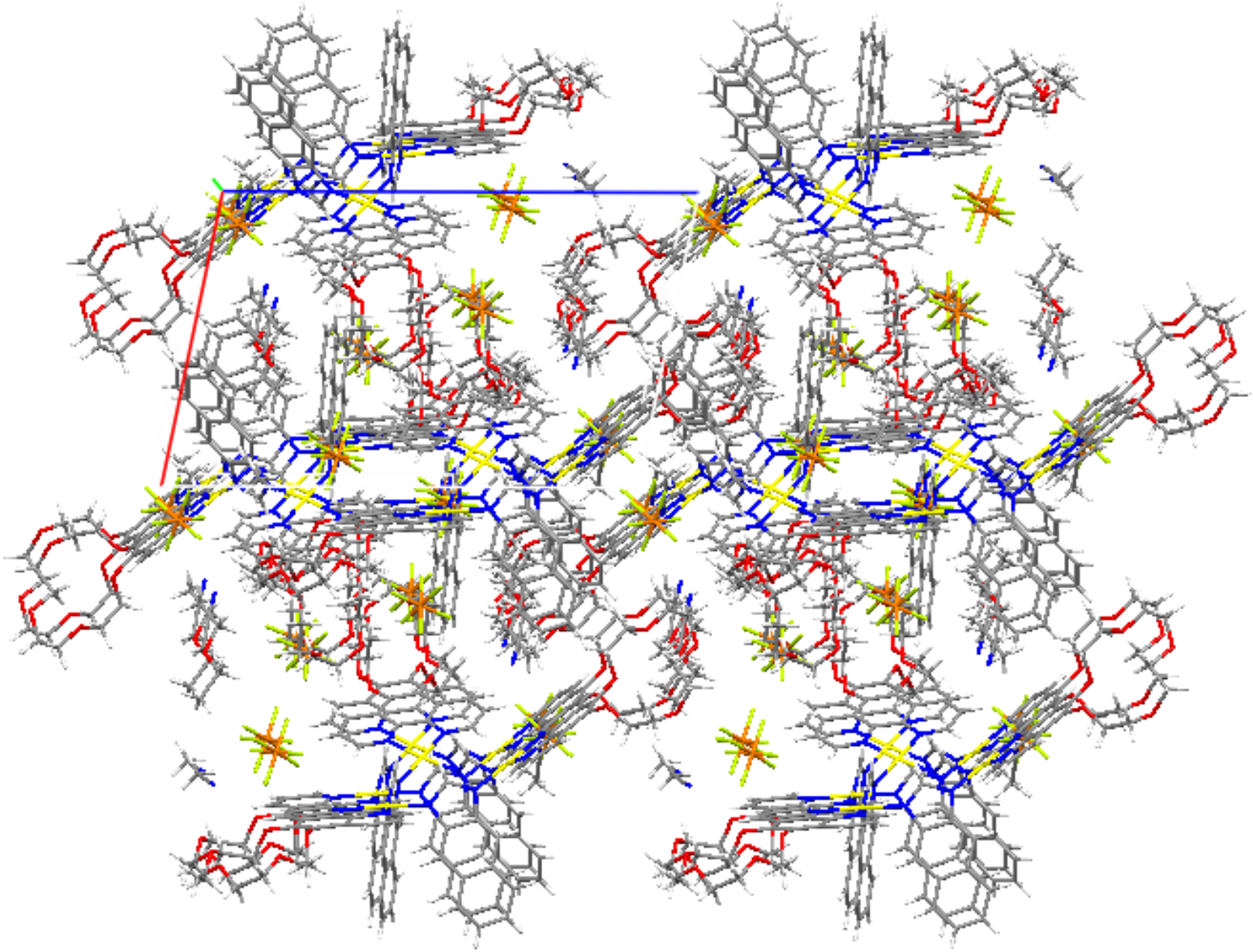

Figure S1 Packing diagram with channel formed by the cavity of complex **4a** viewed along the b axis.

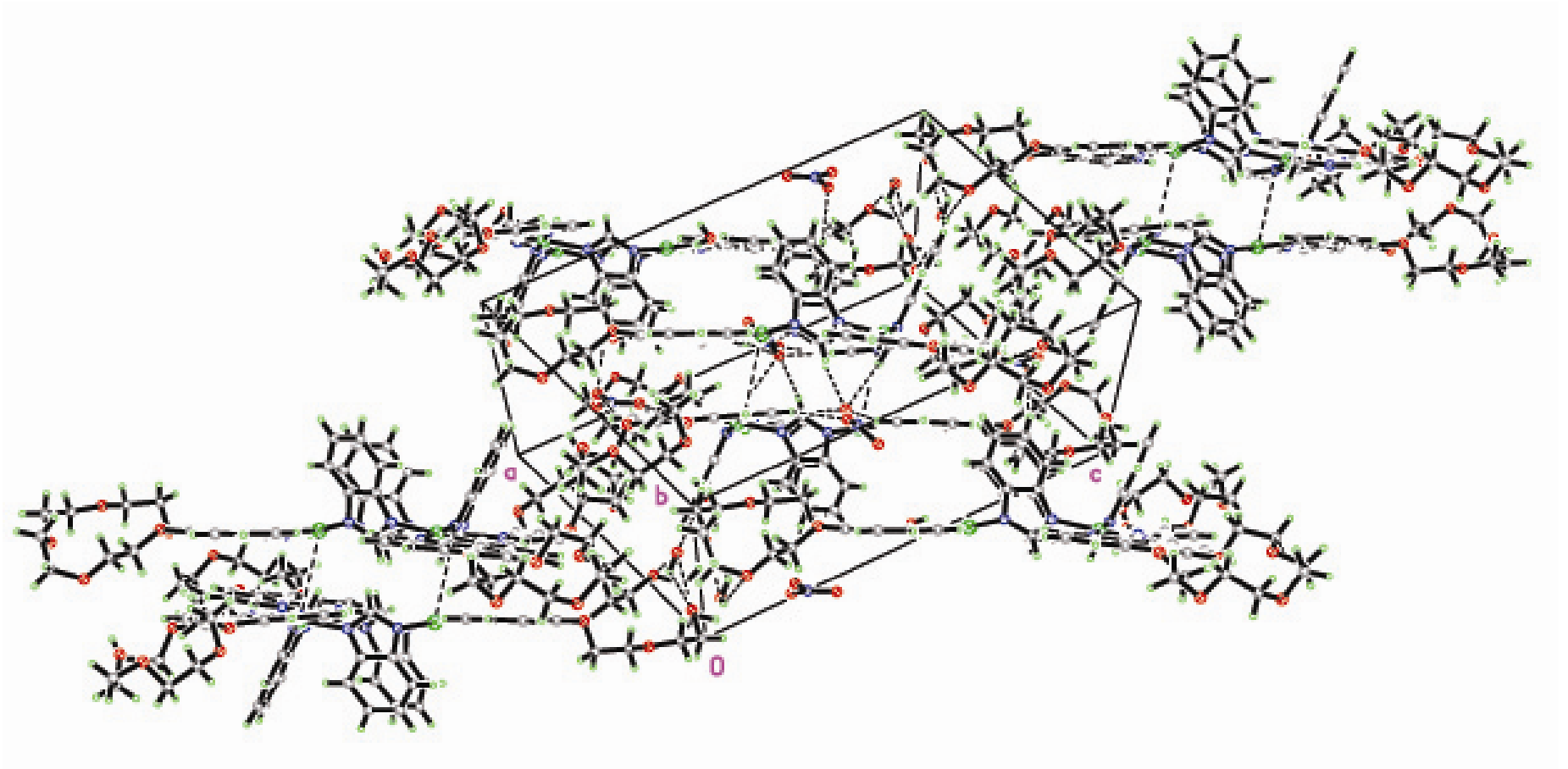

Figure S2 Packing diagram with channel formed by the cavity of complex **11** viewed along the b axis.

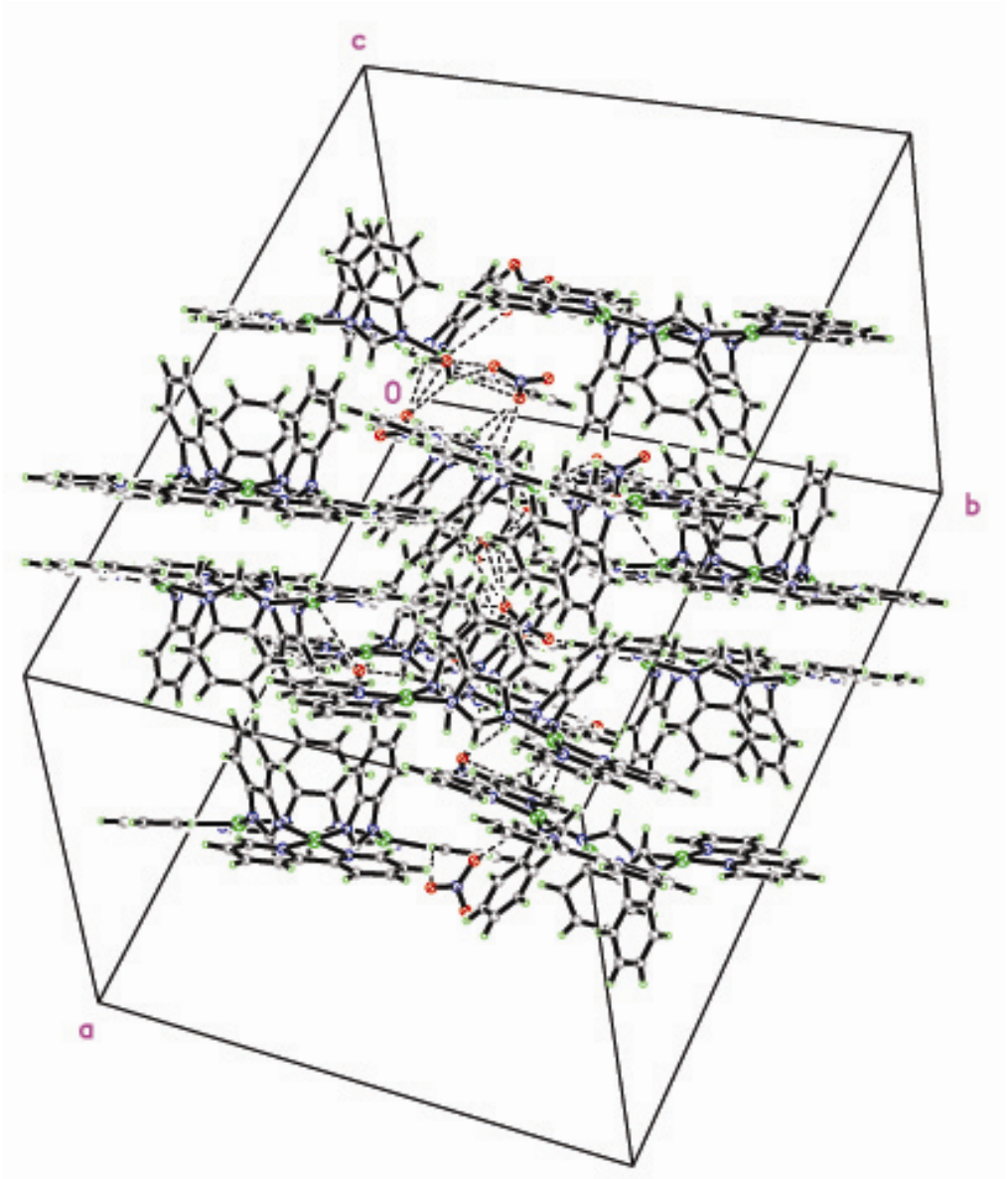

Figure S3 Packing diagram with channel formed by the cavity of complex **13** viewed along the c axis.

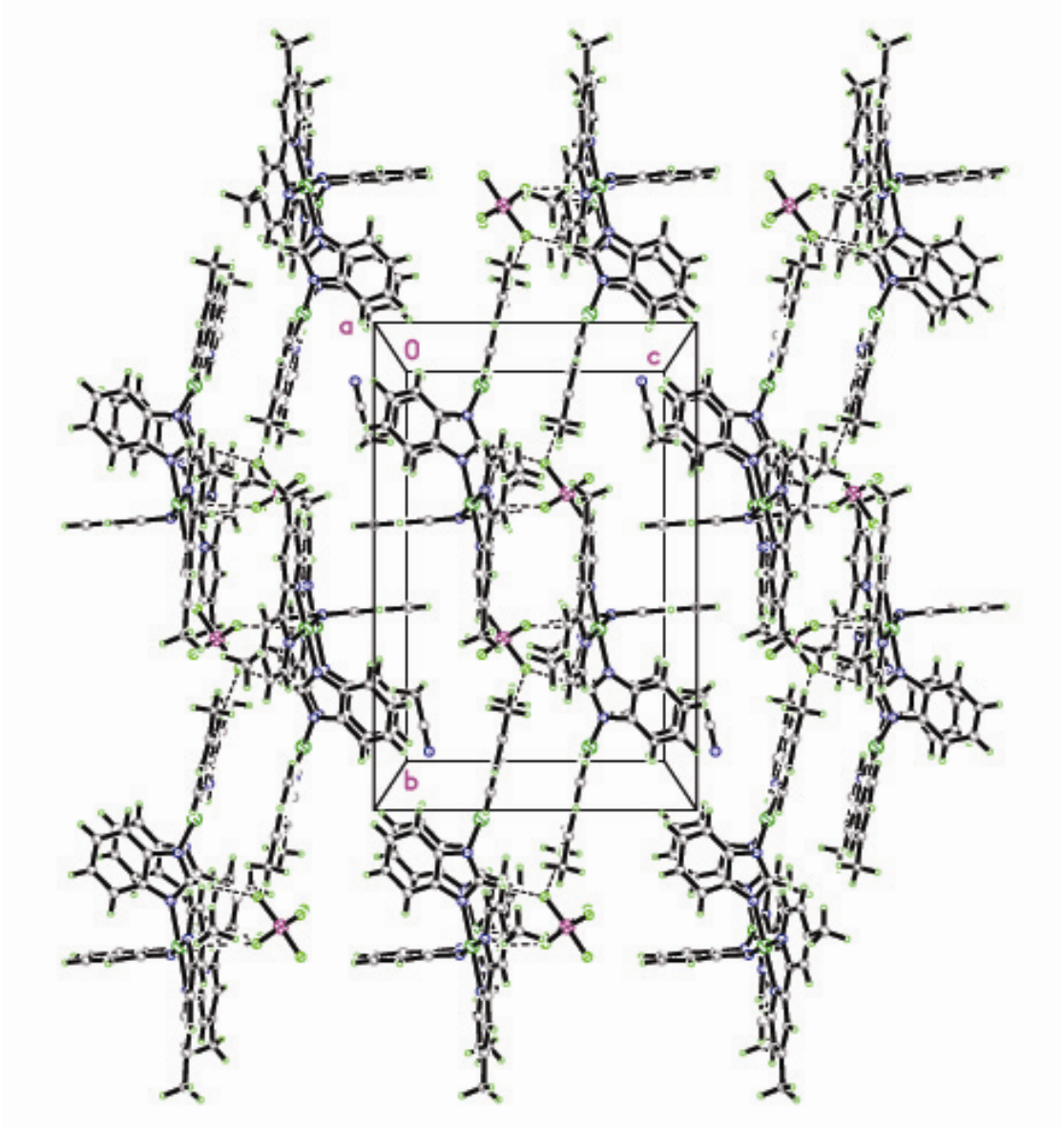

Figure S4 Packing diagram with channel formed by the cavity of complex **14a** viewed along the a axis.