Supplementary Material (ESI) for Chemical Communications
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Supporting Information for

Sunlight induced photocycloaddition and host-guest property of self-assembled organometallic macrocycles based on a versatile building block

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Table 1. Crystal data and structure refinement of **1**−**4**

	1	**2**	**3**	**4**
Formula	$C_{106}H_{120}C_{l4}F_{12}Ir_4N_{12}O_{14}S_4$	$C_{100}H_{112}F_{12}Ir_4N_{12}O_{16}S_4$	$C_{146}H_{154}F_{18}Ir_6N_{24}O_{24}S_6$	$C_{186}H_{180}F_{18}Ir_6N_{24}O_{24}S_6$
F_w	3052.98	2863.06	4316.49	4823.10
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	C2/c	P2(1)/c	P2(1)/c	P2(1)/c
a (Å)	38.315(4)	13.0767(9)	20.861(3)	30.302(3)
b (Å)	14.4214(14)	23.9320(17)	33.223(5)	30.302(3)
c (Å)	22.307(2)	18.5594(14)	28.731(4)	41.215(4)
α (°)	90	90	90	90
β (°)	104.0090(10)	98.0130(10)	107.195(2)	90
γ (°)	90	90	90	120
V (Å ^{3})	11959(2)	5751.5(7)	19022(4)	32774(6)
Z	4	2	4	6
D_c (Mg / m^3)	1.696	1.653	1.507	1.466
μ(Mo-Kα)(mm^{-1})	4.677	4.768	4.326	3.775
F(000)	6000	2808	8440	14256
θ range (°)	1.10~27.01	1.40~27.81	0.96~25.01	0.92~27.59
Limiting indices (hkl)	-48, 32; -17, 18; -28, 26	-17, 17; -31, 31; -16, 24	-24, 23; -39, 39; -34, 34	-39,39; -39,36; -53,39
Reflections collected	33546	42266	103769	80769
Independent reflections	12890	13510	32977	16790
R_{int}	0.0568	0.0281	0.0782	0.0727
Completeness to θ (°)	98.7 %	99.1 %	98.3 %	99.4 %
Data / restraints / parameters	12890 / 40 / 683	13510 / 49 / 714	32977/ 254 / 1515	16790 / 21 / 778
Goodness-of-fit on F^2	1.044	1.087	0.974	0.990
R_1[a],wR_2[a] [I> 2σ(I)]	0.0605, 0.1572	0.0395, 0.1121	0.0936, 0.2510	0.0643, 0.1708
R_1, wR_2 (all data)	0.1025, 0.1740	0.0533, 0.1192	0.1535, 0.2840	0.1007, 0.1938

In complexes **1**, **2**, **3**, **4**, there are disorder solvents (in **3**, triflate anions are also disordered) in the asymmetric units and the SQUEEZE algorithm was used to omit them. In complex **3**, one of six pentamethylcyclopentadienyl ligands in the cation were disordered and it was refined to two idealized positions (53:47); C3, C4, C89, C99, C100, C109, C110, C111, C119, C124, C130, C130, C135, C136, O4 and O5 were refined isotropically because of non-positive definition and other non-hydrogen atoms were refined anisotropically. In complex **4**, C48, C61, C62, O7 and O8 were also refined isotropically because of non-positive definition and other non-hydrogen atoms were refined anisotropically. In complex **2**, two of four triflate anions in the asymmetric unit were disordered and it was refined to two idealized positions (57:43). In complex **1**, C48, C50 -53 and O7 were refined isotropically because of non-positive definition and other non-hydrogen atoms were refined anisotropically. In all complexes, hydrogen atoms were placed in the geometrically calculated positions with fixed isotropic thermal parameters. However, hydrogen atoms of the solvent water and methanol molecules could not be found.

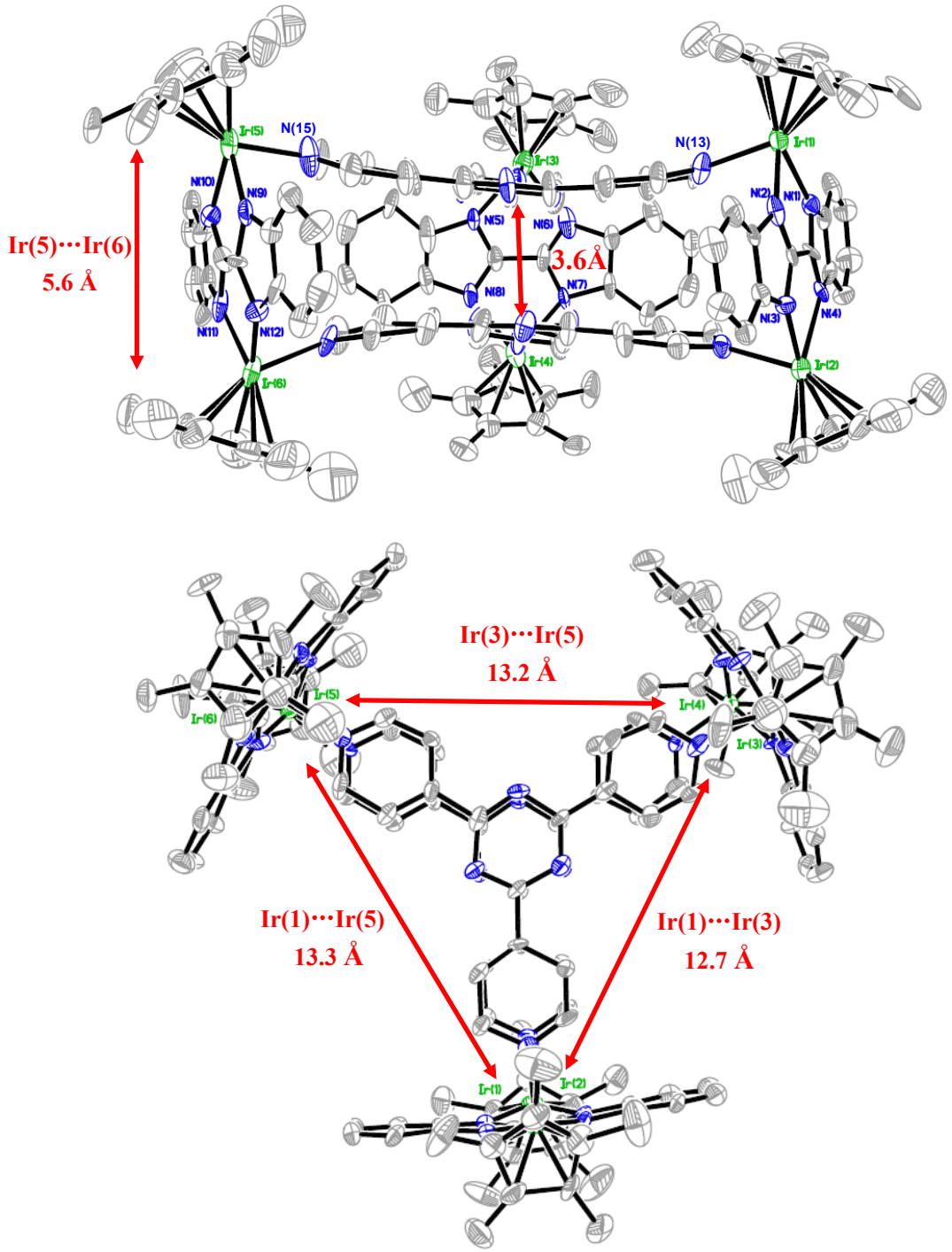

Figure S1. Cation structure of **3** with thermal ellipsoids drawn at the 30% level. Hydrogen atoms are omitted for clarity. Selected distances (Å) and angles (°): Ir(1)-N(1) 2.174(11), Ir(1)-N(2) 2.125(12), Ir(1)-N(13) 2.129(13), N(1)-Ir(1)-N(2) 77.4(5), N(1)-Ir(1)-N(13) 84.8(5), N(2)-Ir(1)-N(13) 85.6(5). The centre to centre of triazine is 3.6 Å.

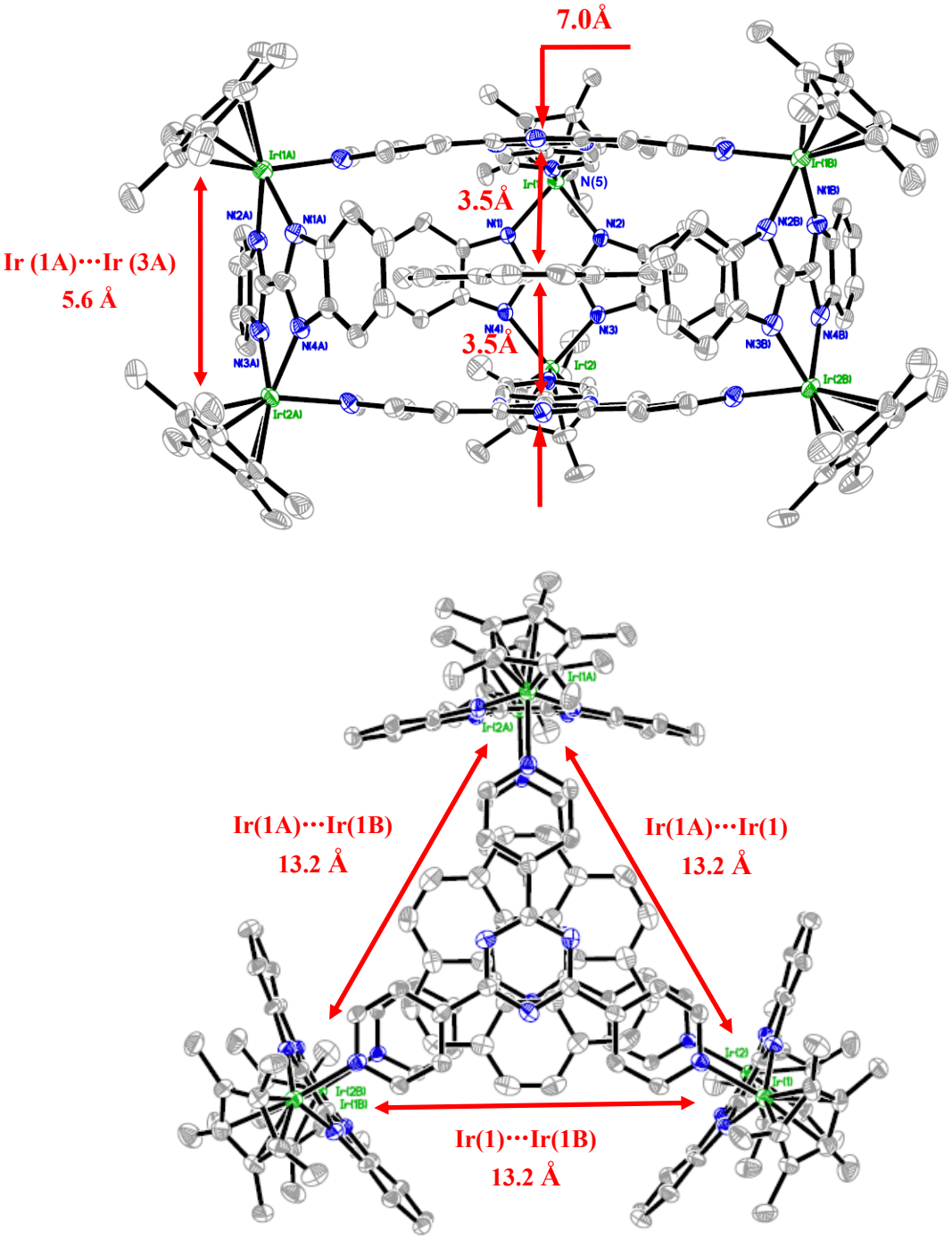

Figure S2. Cation structure of **4** with thermal ellipsoids drawn at the 30% level. Hydrogen atoms are omitted for clarity. Selected distances (Å) and angles (°): Ir(1)-N(1) 2.163(6), Ir(1)-N(2) 2.186(7), Ir(1)-N(5) 2.108(6), N(1)-Ir(1)-N(2) 78.6(2), N(5)-Ir(1)-N(1) 87.9(2), N(5)-Ir(1)-N(2) 88.4(2). The centre to centre of triazine is 7.0 Å

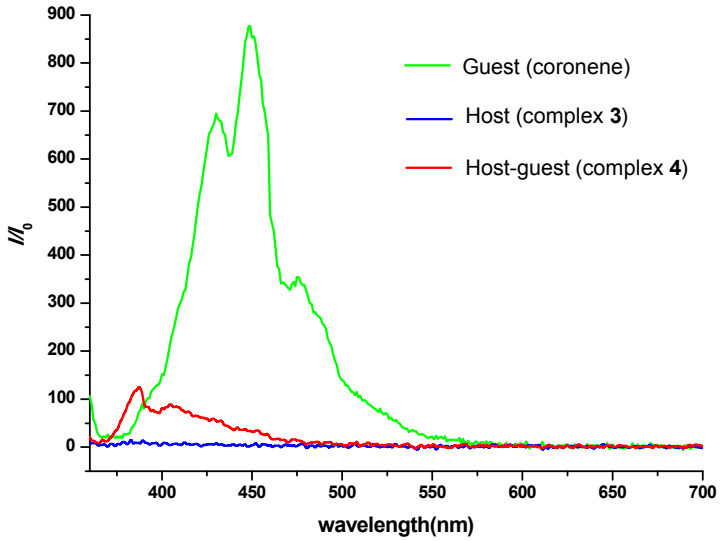

Figure S3. Fluorescence emission spectra of $[\mathbf{3}]^{6+}$ and [coronene⊂**3**]$^{6+}$ as solution(10^{-5}M) in methanol and coronene as solution(10^{-5}M) in toluene. Excitation at 350 nm. All solvents have no effection to the results.

Fluorescence emission spectra showed us that the polyaromatic compounds with strong fluorescence can be quenched after being encapsulated by complex **3** when the excitation was at 350 nm.