Supplementary Material (ESI) for Dalton Transactions


**Supporting Information for**

# Self-assembled half-sandwich Ir, Rh-based organometallic molecular boxes for reversible trapping of halocarbon molecules

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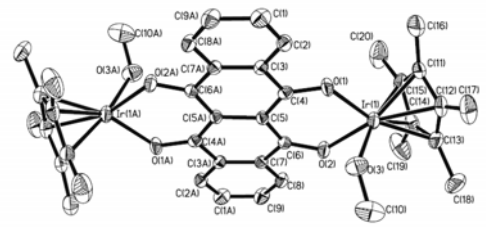

**Fig. S1** Complex cation of **2a** with thermal ellipsoids drawn at the 30% level. All hydrogen atoms and solvent molecules are omitted for clarity. Selected bond distances (Å) and angles (°): Ir(1)-O(1) 2.035(4), Ir(1)-O(2) 2.047(4), Ir(1)-O(3) 2.184(6), O(1)-C(4) 1.289(6), O(2)-C(6) 1.282(5), O(3)-C(10) 1.398(8), C(1)-C(2) 1.371(7), C(2)-C(3) 1.389(7), C(3)-C(4) 1.473(7); O(1)-Ir(1)-O(2) 85.48(14), O(1)-Ir(1)-O(3) 76.60(17), O(2)-Ir(1)-O(3) 81.70(19). Symmetry transformations used to generate equivalent atoms: -x+2,-y+1,-z+1.

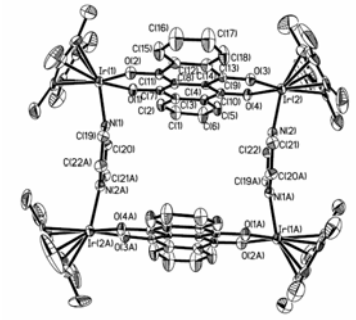

**Fig. S2** Complex cation of **3a** with thermal ellipsoids drawn at the 30% level. All hydrogen atoms and solvent molecules are omitted for clarity. Selected bond distances (Å) and angles (°): Ir(1)-O(1) 2.047(7), Ir(1)-O(2) 2.053(6), Ir(1)-N(1) 2.134(8), Ir(2)-O(3) 2.041(6), Ir(2)-O(4) 2.060(7), Ir(2)-N(2A) 2.129(8, O(1)-C(1) 1.298(11), O(2)-C(3) 1.301(10), O(3)-C(10) 1.283(11), O(4)-C(12) 1.299(11); O(1)-Ir(1)-O(2) 85.1(3), O(1)-Ir(1)-N(1) 84.4(3), O(2)-Ir(1)-N(1) 82.6(3), O(3)-Ir(2)-O(4) 84.4(3). Symmetry transformations used to generate equivalent atoms: -x+2,-y+1,-z.

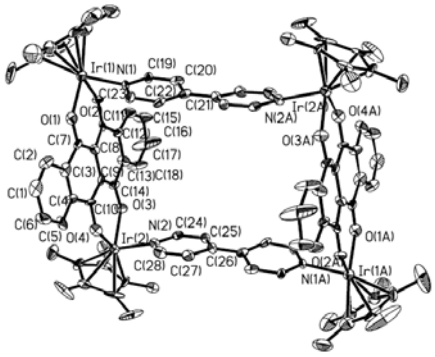

**Fig. S3** Complex cation of **4a** with thermal ellipsoids drawn at the 30% level. All hydrogen atoms and solvent molecules are omitted for clarity. Selected bond distances (Å) and angles (°): Ir(1)-O(2) 2.062(10), Ir(1)-O(1) 2.104(11), Ir(1)-N(1) 2.124(12), Ir(2)-O(3) 2.057(11), Ir(2)-O(4) 2.077(11), Ir(2)-N(2) 2.104(12), O(1)-C(7) 1.302(17), O(2)-C(11) 1.238(16), O(3)-C(14) 1.245(17), O(4)-C(10) 1.311(16); O(2)-Ir(1)-O(1) 84.3(4), O(2)-Ir(1)-N(1) 82.5(5), O(1)-Ir(1)-N(1) 83.2(5), O(3)-Ir(2)-O(4) 84.2(4), O(3)-Ir(2)-N(2) 83.2(5). Symmetry transformations used to generate equivalent atoms: -x+1,-y+1,-z+2.

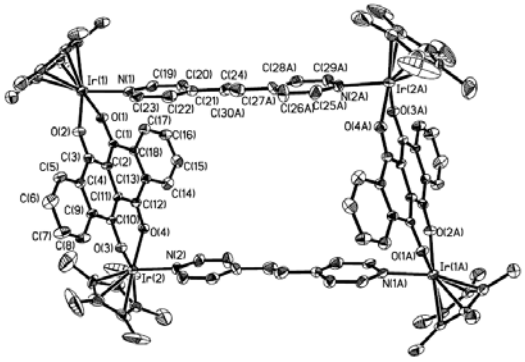


**Fig. S4** Complex cation of **5a** with thermal ellipsoids drawn at the 30% level. All hydrogen atoms and solvent molecules are omitted for clarity**.** Selected bond distances (Å) and angles (°): Ir(1)-O(2) 2.066(5), Ir(1)-O(1) 2.075(4), Ir(1)-N(1) 2.115(6), Ir(2)-O(3) 2.060(4), Ir(2)-O(4) 2.069(5), Ir(2)-N(2) 2.092(6), O(1)-C(1) 1.280(7), O(2)-C(3) 1.279(7), O(3)-C(10) 1.287(7), O(4)-C(12) 1.304(7); O(2)-Ir(1)-O(1) 84.93(17), O(2)-Ir(1)-N(1) 84.0(2), O(1)-Ir(1)-N(1) 80.4(2), O(3)-Ir(2)-O(4) 83.62(17), O(3)-Ir(2)-N(2) 84.3(2), O(4)-Ir(2)-N(2) 82.6(2), C(1)-O(1)-Ir(1) 128.8(4), C(3)-O(2)-Ir(1) 129.8(4). Symmetry transformations used to generate equivalent atoms: -x+1,-y+2,-z+2.