# Supplementary Material (ESI) for Chemical Communications


## Syntheses of compounds 1-4

### 1. Synthesis of $[Cd_3(bbtz)_6(H_2O)_6](BF_4)_6 \cdot 2H_2O$ (1)

A methanolic solution (20 ml) of 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene (bbtz) (0.096 g, 0.4 mmol) was added slowly to an aqueous solution (10 ml) of $Cd(BF_4)_2 \cdot 6H_2O$ (0.394 g, 1.0 mmol) with stirring. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature. After one week, the well-shaped colourless single crystals $[Cd_3(bbtz)_6(H_2O)_6](BF_4)_6 \cdot 1.75H_2O$ (**1**) were obtained. Yield: 0.136 g (83%). Found: C, 35.31; H, 3.57; N, 20.46. Calcd. for $C_{72}H_{87.5}B_6Cd_3F_{24}N_{36}O_{7.75}$ (**1**): C, 35.45; H, 3.62; N, 20.68%.

### 2. Synthesis of $[Cd(bbtz)_2(H_2O)_2](BF_4)_2 \cdot 3DMF$ (2)

$[Cd_3(bbtz)_6(H_2O)_6](BF_4)_6 \cdot 2H_2O$ (**1**) (0.073 g, 0.03 mmol) was dissolved in 10 ml DMF. After two weeks, the well-shaped colourless single crystals $[Cd(bbtz)_2(H_2O)_2](BF_4)_2 \cdot 3DMF$ (**2**) were obtained. Yield: 0.086 g (93%). Found: C, 38.67; H, 4.72; N, 20.38. Calcd. for $C_{33}H_{49}B_2CdF_8N_{15}O_5$ (**2**): C, 38.79; H, 4.83; N, 20.56%.

### 3. Synthesis of $[Cd(bbtz)_2(H_2O)_2](ClO_4)_2 \cdot 2H_2O$ (3)

A methanolic solution (20 ml) of 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene (bbtz) (0.096 g, 0.4 mmol) was added slowly to an aqueous solution (10 ml) of $Cd(ClO_4)_2 \cdot 6H_2O$ (0.419 g, 1.0 mmol) with stirring. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature. After several days, the well-shaped colourless single crystals $[Cd(bbtz)_2(H_2O)_2](ClO_4)_2 \cdot 2H_2O$ (**3**) were obtained. Yield: 0.149 g (86%). Found: C, 33.29; H, 3.71; N, 19.42. Calcd. for $C_{24}H_{32}CdCl_2N_{12}O_{12}$ (**3**): C, 33.37; H, 3.73; N, 19.46%.

### 4. Synthesis of $[Cd(bbtz)_2(H_2O)_2](ClO_4)_2 \cdot 3DMF$ (4)

$[Cd(bbtz)_2(H_2O)_2](ClO_4)_2 \cdot 2H_2O$ (3) (0.086 g, 1.0 mmol) was dissolved in 10 ml DMF. After two weeks, the well-shaped colourless single crystals $[Cd(bbtz)_2(H_2O)_2](ClO_4)_2 \cdot 3DMF$ (**4**) were obtained. Yield: 0.097 g (93 %). Found: C, 37.78; H, 4.67; N, 19.95. Calcd. for $C_{33}H_{49}CdCl_2N_{15}O_{13}$ (**4**): C, 37.85; H, 4.72; N, 20.07%.