Electronic Supplementary Material (ESI) for Faraday Discussions.


# Supplementary information

## In-MOFs based on amide functionalised flexible linkers

J. Haddad, G. F. S. Whitehead, A. P. Katsoulidis, M. J. Rosseinsky

**Table S1.** Crystallographic data and structure refinement summary for **In(OH)CSA**.

| | |
|---|---|
| Identification code | C2_JH_CSA_36_4_twin1_hklf4 |
| Empirical formula | $C_{11}H_{12}InNO_7$ |
| Formula weight | 385.04 |
| Temperature/K | 100 |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 8.0483(8) |
| b/Å | 7.2282(3) |
| c/Å | 24.2472(18) |
| α/° | 90.0 |
| β/° | 93.708(8) |
| γ/° | 90.0 |
| Volume/Å$^3$ | 1407.62(18) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.817 |
| μ/mm$^{-1}$ | 1.708 |
| F(000) | 7602.0 |
| Crystal size/mm$^3$ | 0.2 × 0.2 × 0.05 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 5.072 to 53.02 |
| Index ranges | $-10 \leq h \leq 10$, $-9 \leq k \leq 9$, $-30 \leq l \leq 30$ |
| Reflections collected | 3669 |
| Independent reflections | 3669 [$R_{int}$ = 0.0929, $R_{sigma}$ = 0.0520] |
| Data/restraints/parameters | 3669/219/182 |
| Goodness-of-fit on F$^2$ | 1.094 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0867, $wR_2$ = 0.1869 |
| Final R indexes [all data] | $R_1$ = 0.1138, $wR_2$ = 0.1993 |
| Largest diff. peak/hole / e Å$^{-3}$ | 1.69/-2.05 |

**Figure S1.** Asymmetric unit of **In(OH)CSA**, Dark grey = In, Light grey = C, Red = O, Blue = N, White = H

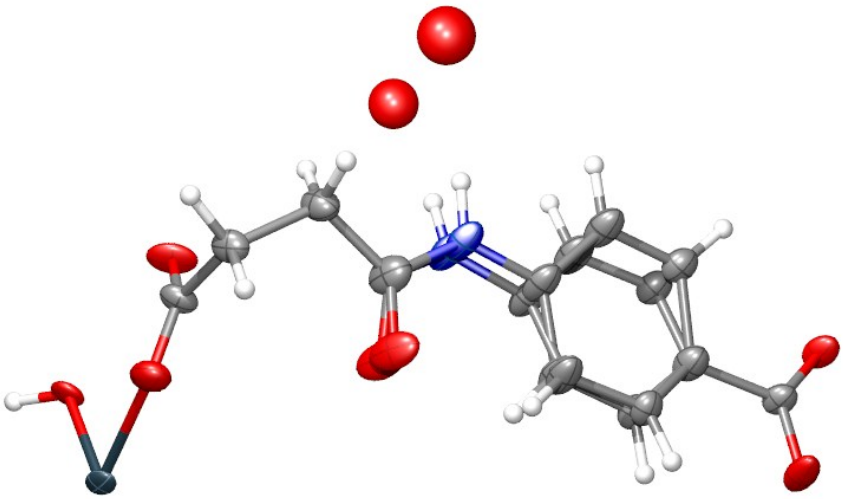

**Table S2.** Crystallographic data and structure refinement summary for **In(OH)PDG**.

| | |
|---|---|
| Identification code | C1_JH_PDG_47_2_sq |
| Empirical formula | $C_{12}H_{11}InN_2O_7$ |
| Formula weight | 410.05 |
| Temperature/K | 100 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 7.2372(4) |
| b/Å | 10.1596(8) |
| c/Å | 11.8645(8) |
| α/° | 77.815(7) |
| β/° | 78.748(5) |
| γ/° | 85.773(5) |
| Volume/Å$^3$ | 835.84(10) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.629 |
| μ/mm$^{-1}$ | 1.446 |
| F(000) | 404.0 |
| Crystal size/mm$^3$ | 0.2 × 0.05 × 0.05 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3.574 to 52.74 |
| Index ranges | $-9 \leq h \leq 6$, $-12 \leq k \leq 12$, $-14 \leq l \leq 14$ |
| Reflections collected | 9533 |
| Independent reflections | 3415 [$R_{int}$ = 0.0888, $R_{sigma}$ = 0.1213] |
| Data/restraints/parameters | 3415/24/202 |
| Goodness-of-fit on $F^2$ | 0.984 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0678, $wR_2$ = 0.1567 |
| Final R indexes [all data] | $R_1$ = 0.1162, $wR_2$ = 0.1809 |
| Largest diff. peak/hole / e Å$^{-3}$ | 2.58/-1.41 |

**Figure S2.** Asymmetric unit of **In(OH)PDG**, Dark grey = In, Light grey = C, Red = O, Blue = N, White = H

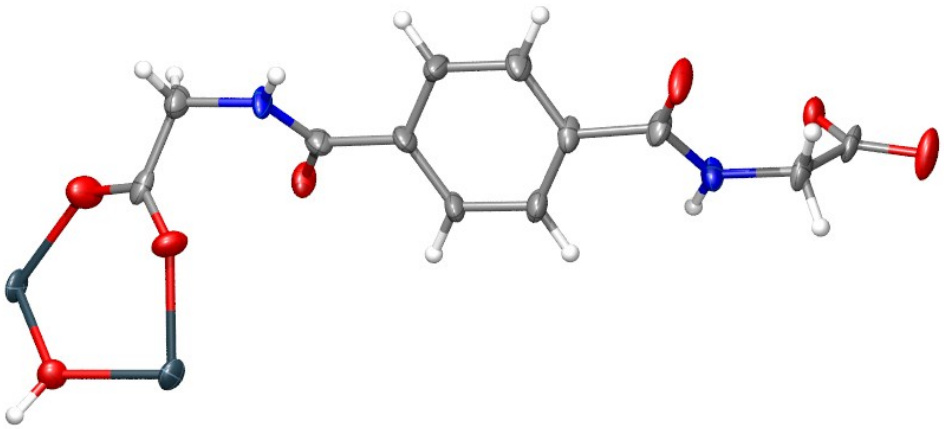

**Table S3** Unit cell parameters of bulk In(OH)CSA and Al(OH)CSA compared to the single crystal unit cell of In(OH)CSA

| | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) |
|---|---|---|---|---|---|---|
| In(OH)CSA bulk | 8.038(9) | 7.223(8) | 24.39(4) | 90 | 93.93(3) | 90 |
| Al(OH)CSA bulk | 8.05(5) | 7.25(2) | 24.3(1) | 90 | 92.64(8) | 90 |
| In(OH)CSA single crystal | 8.0483(8) | 7.2282(3) | 24.2472(18) | 90 | 93.708(8) | 90 |

**Table S4** Elemental analysis of the desolvated In(OH)CSA and Al(OH)CSA samples. $H_2O$ has been readsorbed in the pores of these samples prior to analysis.

| | | C (%) | H (%) | N (%) |
|---|---|---|---|---|
| In(OH)CSA•$H_2O$ | Theoretical | 34.31 | 3.14 | 3.64 |
| | Experimental | 33.96 | 2.75 | 3.54 |
| Al(OH)CSA•$H_2O$ | Theoretical | 44.46 | 4.07 | 4.71 |
| | Experimental | 44.09 | 3.84 | 4.81 |

**Table S5** Unit cell parameters of bulk In(OH)PDG compared to the single crystal unit cell of In(OH)PDG

| | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) |
|---|---|---|---|---|---|---|
| In(OH)PDC bulk | 7.24(2) | 10.17(4) | 11.88(6) | 78.178(5) | 78.522(6) | 85.992(6) |
| In(OH)PDG single crystal | 7.2372(4) | 10.1596(8) | 11.8645(8) | 77.815(7) | 78.748(5) | 85.773(5) |

**Table S6** Elemental analysis of the desolvated In(OH)PDG and Al(OH)PDG samples. $H_2O$ has been readsorbed in the pores of these samples prior to analysis.

| | | C (%) | H (%) | N (%) |
|---|---|---|---|---|
| In(OH)PDG•$H_2O$ | Theoretical | 33.67 | 3.06 | 6.54 |
| | Experimental | 33.64 | 2.74 | 6.86 |
| Al(OH)PDG•$H_2O$ | Theoretical | 44.40 | 3.73 | 8.94 |
| | Experimental | 43.99 | 3.77 | 8.71 |

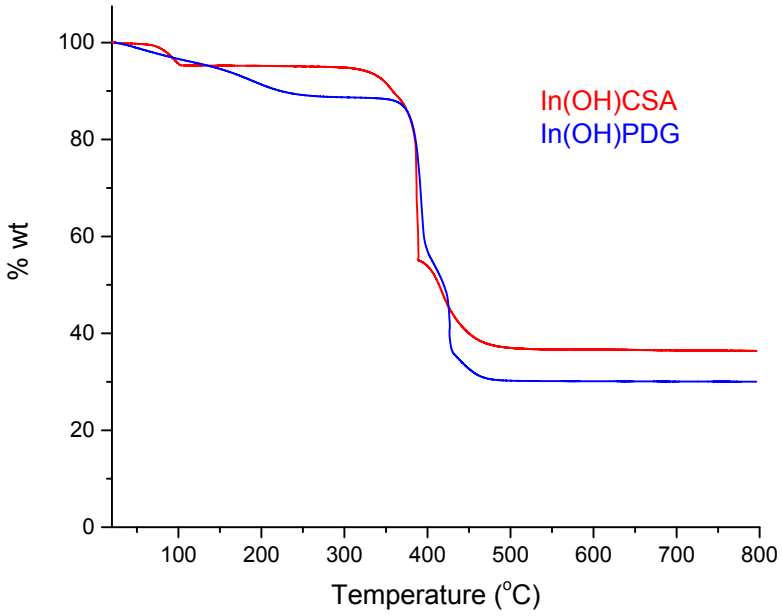


**Figure S3** Thermogravimetric analysis of In(OH)CSA and In(OH)PDG under flow of air

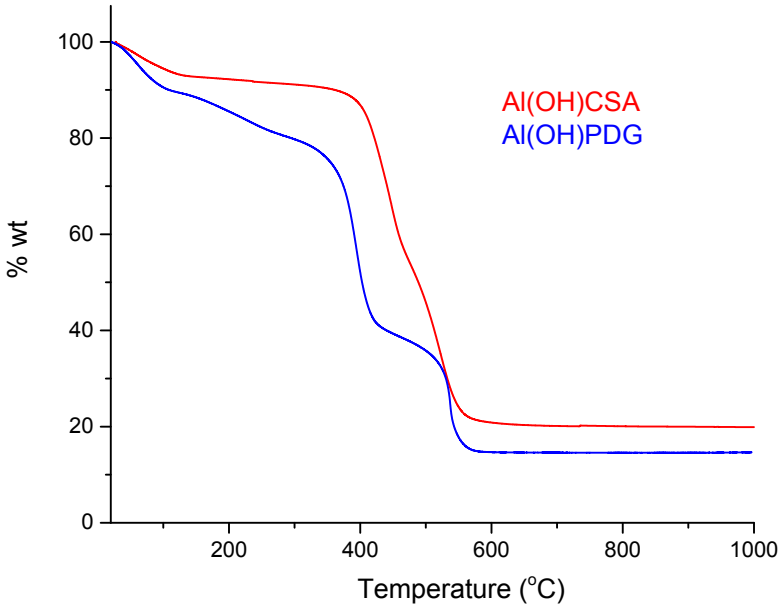


**Figure S4** Thermogravimetric analysis of Al(OH)CSA and Al(OH)PDG under flow of air