**Co-existence of distinct supramolecular assemblies in solution and in the solid state**

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**Figure 2**  1D one-pulse 1H NMR data

|  |  |  |
| --- | --- | --- |
| Complex | Solution-state 1H NMR data in CDCl3 | Solid-state 1H NMR data (75 kHz MAS) |
| GaceC10 KPic (1, 2 and 3) | Recorded 14/05/2015 | Recorded 28/12/2013 |
| GaceC10 Sr Pic (4)  | Recorded 14/05/2015 | Recorded 16/05/2015 |
| GaceC10 KI (5, 6 and 7)  | Recorded 07/05/2015 | Recorded 15/05/2015 |
| GaceC10 KEth (8, 9 and 10)  | Recorded 21/05/2016 | Recorded 29/04/2015 |

**Figure 3 and S3 (Circular Dichroism, CD)**

Experimental CD data of GaceC10 KPic, KI, KEth and Sr(Pic)2 complexes in excel format (recorded 11/05/2016 – 12/05/2016)

**Figures 3**

2D solution-state PFG 1H NMR data

GaceC10 KPic 8:1 complex (recorded on 19/05/2015)

GaceC10 Sr(Pic)2 8:1 complex (recorded on 18/05/2015)

**Figure 4** 2D solid-state 1H DQ-SQ and 2D 1H spin-diffusion NMR data (see also Figure S6)

GaceC10 KPic 8:1 complexes (recorded on 28/12/2013)

Gacec10 Sr(Pic)2 8:1 complex (recorded 16/05/2015)

**Figure 5** 2D solid-state 1H DQ-SQ correlation NMR data

GaceC10 (recorded 23/02/2015)

GaceC10 KPic 8:2 and 8:4 complexes (recorded on 18/05/2015)

GaceC10 KI complexes (recorded on 15/05/2015)

GaceC10 KEth complexes (recorded on 29/04/2015)

**Figure 6** 1D combined solution and solid-state NMR data of GaceC10 KPic 8:1 complex (recorded 08/05/2015)

**Figure S1** 1D solution-state 1H and 13C NMR data of GaceC10 in DMSO-*d*

(recorded 14/03/2016 – 15/03/2016**)**

**Figure S2** Time course 1H NMR data

1D NMR data of GaceC10 KPic 8:2 complex (recorded on 19/11/2015)

1D NMR data of GaceC10 KPic 8:4 complex (recorded on 20/11/2015)

2D PFG NMR data of GaceC10 KPic 8:2 complex (recorded on 01/06/2015)

2D PFG NMR data of GaceC10 KPic 8:4 complex (recorded on 01/06/2015)

**Figure S4** Powder X-ray diffraction data of GaceC10 and GaceC10 KPic complex

(recorded on 12/08/2016)

**Figure S6** 2D1H spin-diffusion NMR data

GaceC10 KPic 8:1 (at four different mixing times, recorded on 28/12/2013)

Gacec10 KI 8:1 complexes (recorded on 13/05/2015)