

## Supporting Information

### Organoamine-induced isomerism of calixarene- based complexes: from 1D to 2D

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**Table S1.** Crystal data and structure refinement for compounds **CIAC-236-238**.

Compounds	<b>CIAC-236</b>	<b>CIAC-237</b>	<b>CIAC-238</b>
Formula	C <sub>76</sub> H <sub>74</sub> ClCo <sub>4</sub> N <sub>7</sub> O <sub>12</sub> S <sub>4</sub>	C <sub>76</sub> H <sub>74</sub> ClCo <sub>4</sub> N <sub>7</sub> O <sub>12</sub> S <sub>4</sub>	C <sub>76</sub> H <sub>74</sub> ClFe <sub>4</sub> N <sub>7</sub> O <sub>12</sub> S <sub>4</sub>
Formula eight	1676.83	1676.83	1664.51
Crystal system	Monoclinic	Tetragonal	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>m</i>	<i>P</i> 42 <sub>1</sub> 2	<i>P</i> 2 <sub>1</sub> / <i>m</i>
<i>a</i> /Å	11.5232(2)	20.549(3)	11.5257(2)
<i>b</i> /Å	21.9302(4)	20.549(3)	21.7684(4)
<i>c</i> /Å	20.4472(4)	15.790(3)	20.6414(4)
<i>α</i> /°	90	90	90
<i>β</i> /°	93.0370(10)	90	92.7150(10)
<i>γ</i> /°	90	90	90
<i>V</i> /Å <sup>3</sup>	5159.88(16)	6667(2)	5173.03(16)
<i>Z</i>	2	2	2
<i>D<sub>c</sub></i> /g cm <sup>-3</sup>	1.079	0.798	1.069
<i>μ</i> /mm <sup>-1</sup>	6.336	4.887	5.794
<i>F</i> (000)	1728	1642	1720
θ range/°	3.841-49.553	2.798-33.905	2.952-59.050
No. of reflections	5382/4355	1322/901	7646/5812
<i>R<sub>int</sub></i>	0.0387	0.1684	0.0549
GoF	1.013	1.028	0.946
<i>R</i> <sub>1</sub> <sup>a</sup> , <i>wR</i> <sub>2</sub> <sup>b</sup> [ <i>I</i> >2σ( <i>I</i> )]	0.0378, 0.0870	0.0509, 0.0948	0.0446, 0.1123
<i>R</i> <sub>1</sub> , <i>wR</i> <sub>2</sub> <sup>b</sup> (all data)	0.0522, 0.0925	0.0944, 0.1091	0.0643, 0.1220

$$^aRI = \sum ||F_0| - |F_c|| / \sum |F_0|; ^bwR2 = \{ \sum [w(F_0^2 - F_c^2)^2] / \sum [w(F_0^2)^2] \}^{1/2}$$

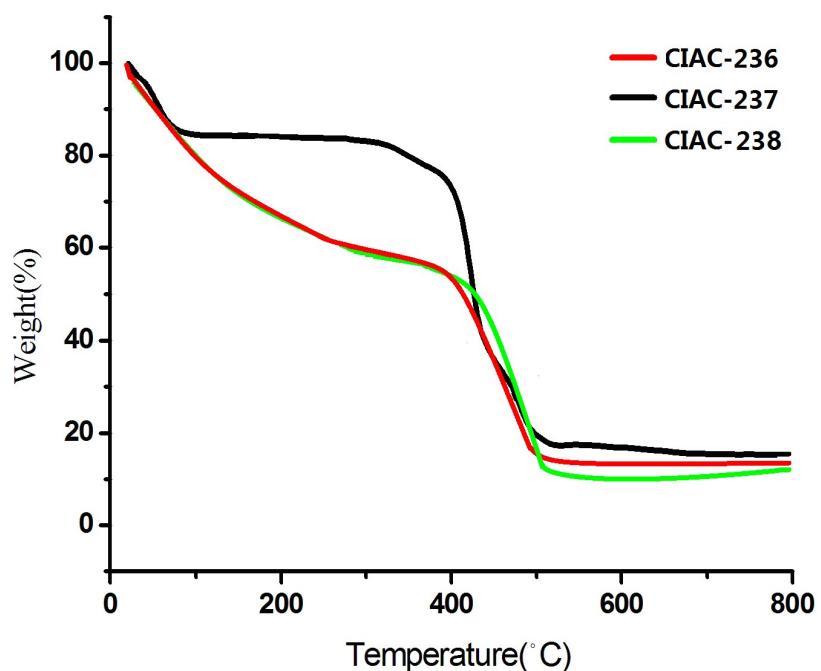


Fig S1 TGA of **CIAC-236–238**.