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**Supporting information for article:**

**Structural analysis of interpenetrated methyl-modified MOF-5  
and its gas-adsorption properties**

**Koh Sugamata, Daichi Yanagisawa, Keiko Awano, Teruyuki Iihama and  
Mao Minoura**

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## 1. X-Ray structure analysis

The crystal data, data correction and selected refinement details are summarized in Table S1.

**Table S1** Crystal data and structure refinements of **Me2MOF-5-int**

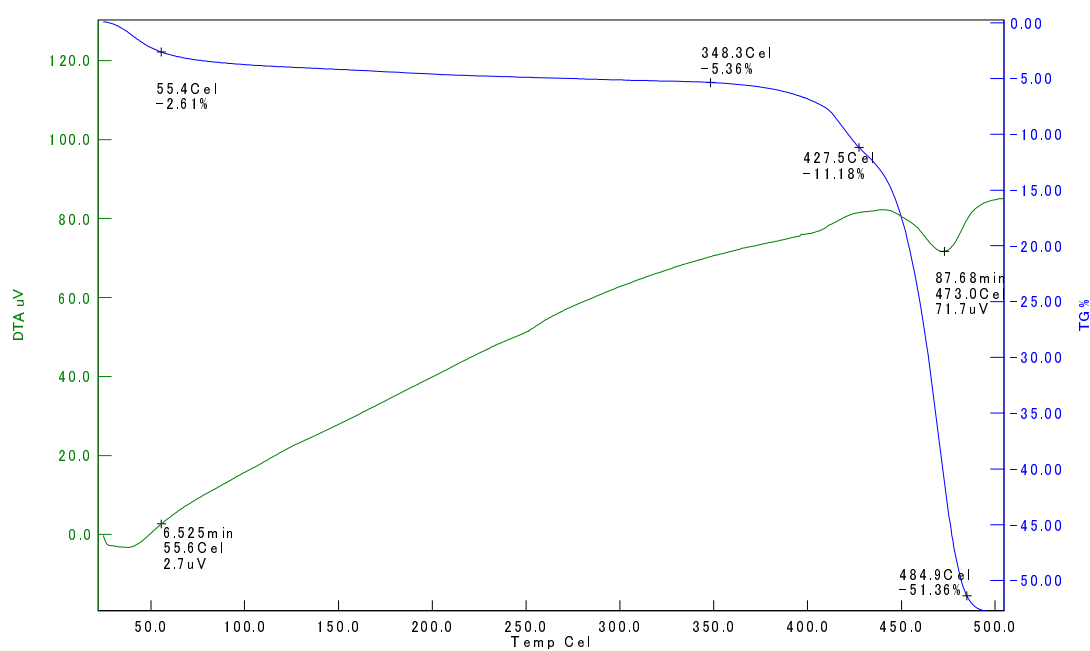
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empirical formula	C <sub>72</sub> H <sub>76</sub> N <sub>4</sub> O <sub>30</sub> Zn <sub>8</sub>
formula weight	2000.32
color	colorless
crystal system	monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i> (#14)
unit-cell dimensions ( <i>a</i> = Å), ( <i>b</i> = Å), ( <i>c</i> = Å)	<i>a</i> = 17.8530(9) <i>b</i> = 18.5810(11) <i>c</i> = 25.3020(15)
α (deg)	90.0000
β (deg)	91.504(2)
γ (deg)	90.0000
volume of unit cell (Å <sup>3</sup> )	8390.5(8)
<i>Z</i> value	4
<i>D</i> <sub>calc</sub> (g/cm <sup>3</sup> )	1.584
crystal size (mm)	0.1 x 0.1 x 0.1
temp (°C)	-173
λ(Å)	0.71073
Reflections collected	76309
Independent reflections	19165
Completeness (%)	99.8
Parameters	1064
<i>R</i> 1, <i>wR</i> 2	0.0424, 0.0969
goodness-of-fit on <i>F</i> <sup>2</sup>	1.032
CCDC	1972122

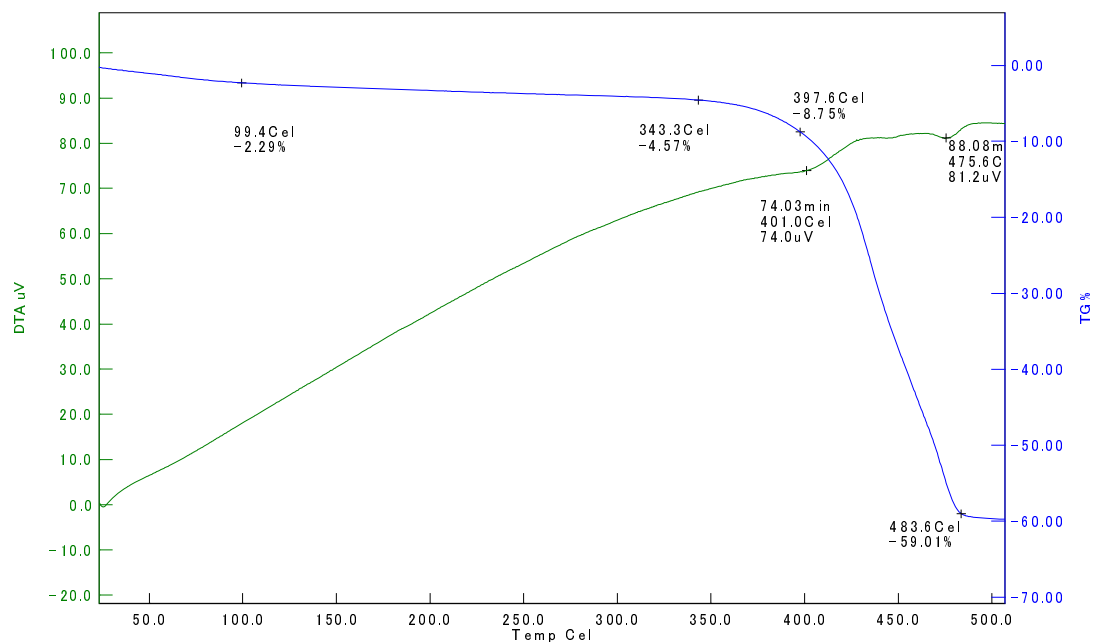
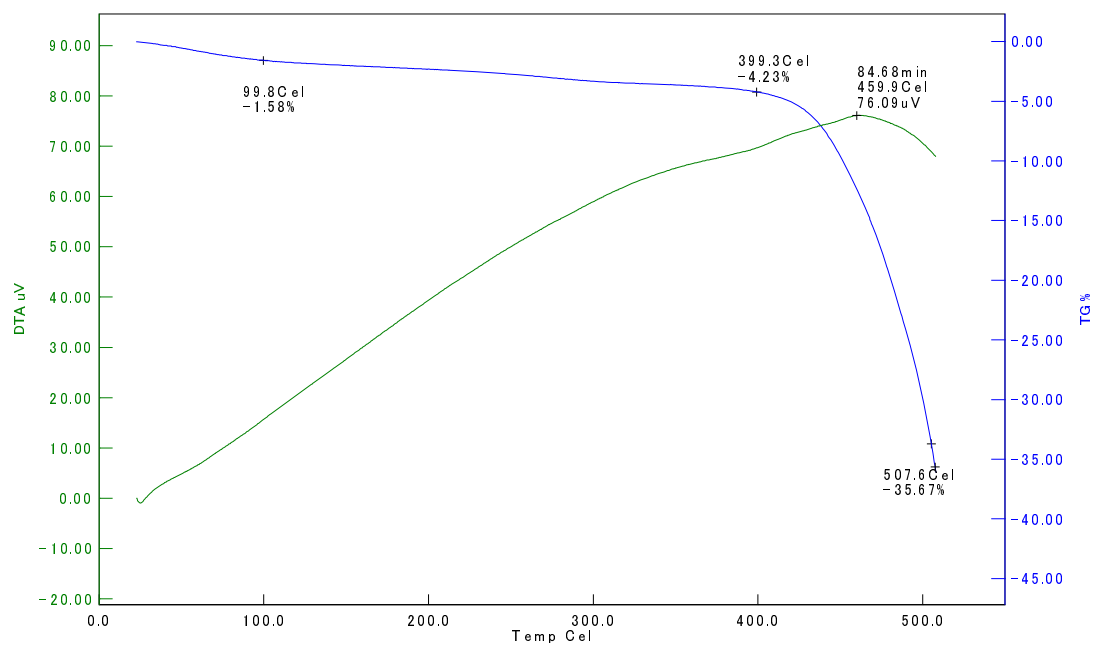
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## 2. Thermogravimetric Analyses

The thermal stability of **Me<sub>2</sub>MOF-5-int**, **Me<sub>2</sub>MOF-5**, and **MOF-5** was evaluated using TGA (r.t. to 500 °C) (Figs. S7 and S8). All **MOFs** exhibited high thermal stability up to 400 °C. The first weight loss (<100 °C) is due to the removal of solvent molecules from the pores.



**Fig. S1** TG/DTA curve of bulk **Me<sub>2</sub>MOF-5-int**.

**Fig. S2** TG/DTA curve of bulk **Me<sub>2</sub>MOF-5**.**Fig. S3** TG/DTA curve of bulk **MOF-5**.