Supporting Information

Structure variation of transition metal-organic frameworks using deep eutectic solvents with different hydrogen bond donors

Ming-Yu Zhao, Jian-Nan Zhu, Peng Li, Wei Li, Ting Cai, Fang-Fang Cheng* and Wei-Wei Xiong*

N_2 adsorption-desorption isotherms: Sample tubes were loaded with about 300 mg of sample and degassed at 120 °C in vacuum for 12 h on a Micromeritics ASAP 2460 analyzer until the outgas rate was less than 1 mTorr/min. The degassed sample and sample tube were weighed precisely and then transferred back to the analyzer. The outgas rate was again confirmed to be less than 1 mTorr/min. Measurements were performed at 77 K in a liquid nitrogen bath.

CO_2 adsorption-desorption isotherms: The adsorption isotherms of CO_2 at 273 K in a liquid nitrogen bath and gas pressure up to 800 mmHg were measured volumetrically in the Micromeritics ASAP 2020 adsorption apparatus. Before the measurement, the sample (300 mg) was activated at 120 °C in vacuum for 12 h.

Table S1 Summary of catalytic performance of **7** for the oxidation of styrene.

	Weight/ mg	TBHP/ μL	Temperature /°C	Time /h	Conversion/ %	Selectivity/ %
Amount of catalyst	4	72	75	24	51	53
	9	72	75	24	72	60
	15	72	75	24	85	54
Amount of TBHP	9	36	75	24	58	68
	9	72	75	24	72	60
	9	108	75	24	90	54
Temperature	9	72	55	24	46	85
	9	72	65	24	57	74
	9	72	75	24	72	60
Time	9	72	75	12	66	67
	9	72	75	24	72	60
	9	72	75	48	93	57

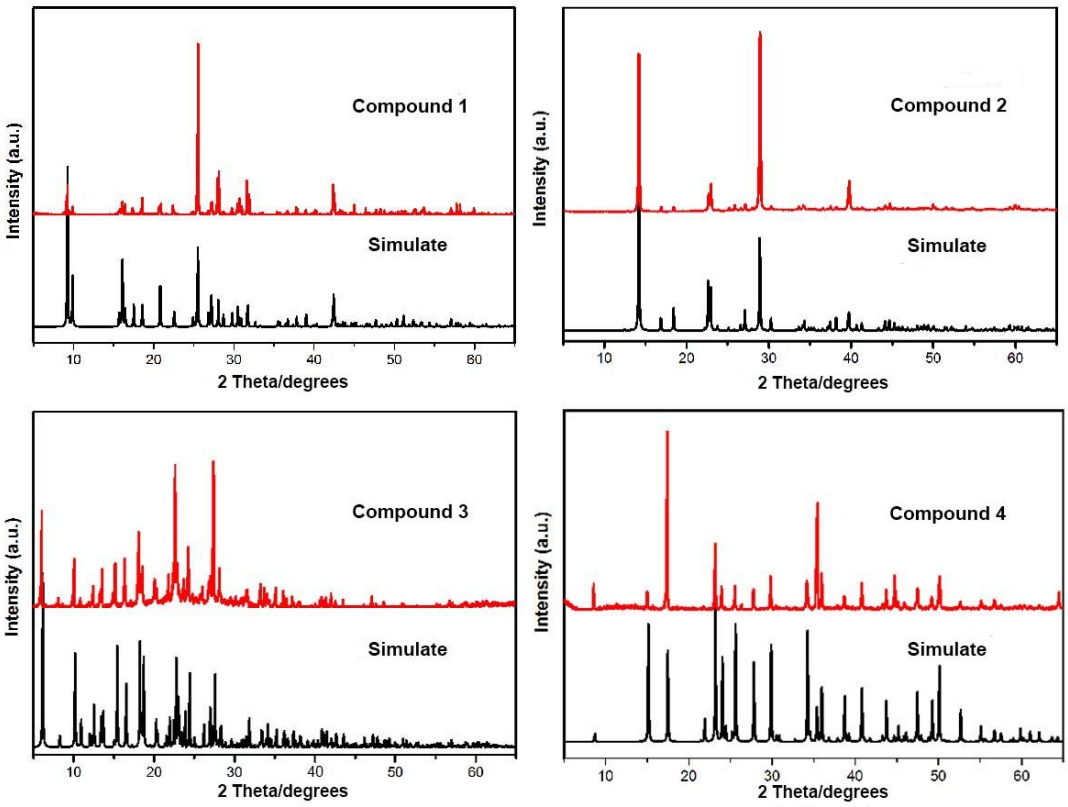

Figure S1. The experimental (red) and simulated (black) PXRD patterns of compounds **1-4**.

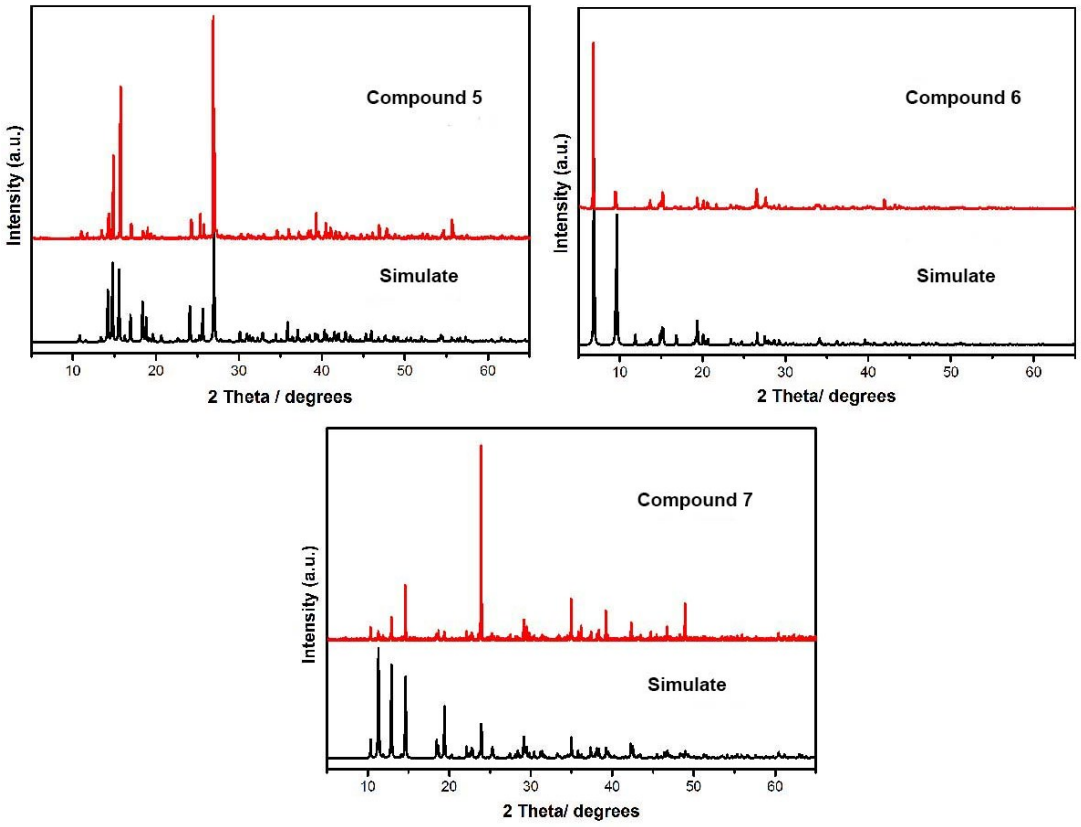

Figure S2. The experimental (red) and simulated (black) PXRD patterns of compounds **5-7**.

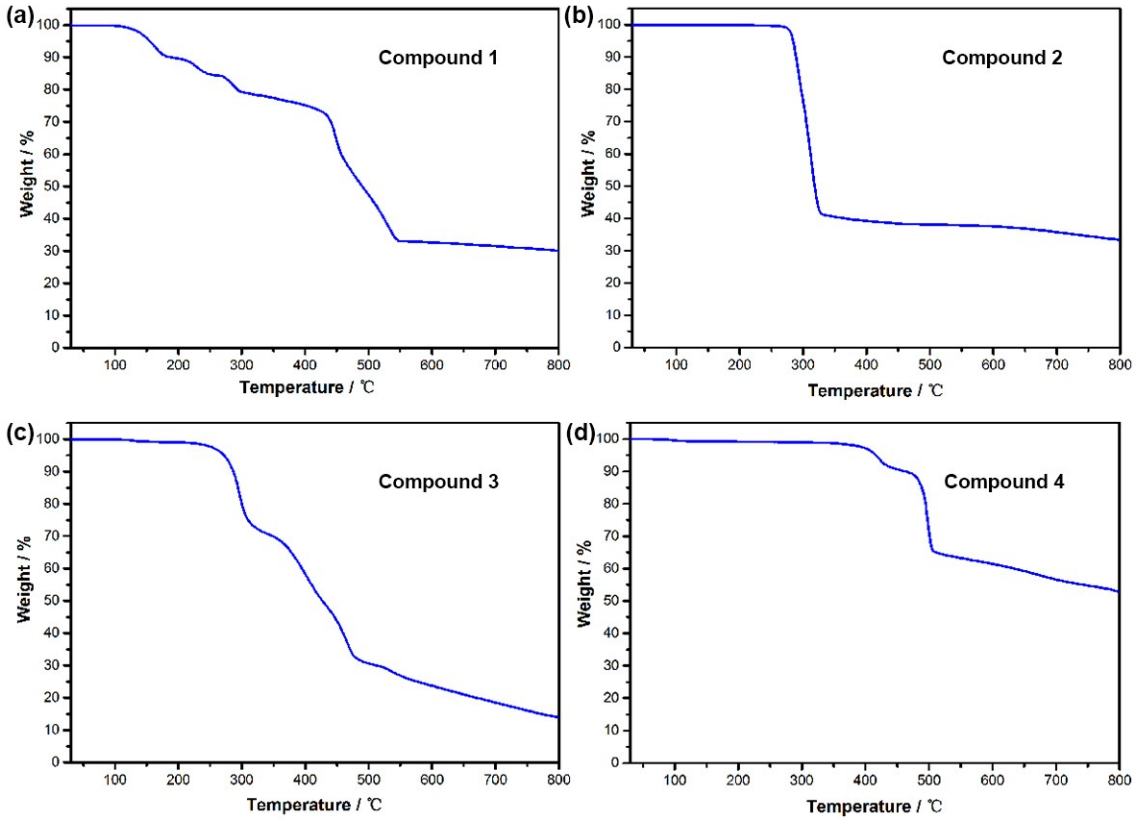

Figure S3. Thermogravimetric analysis curves of compounds **1-4**.

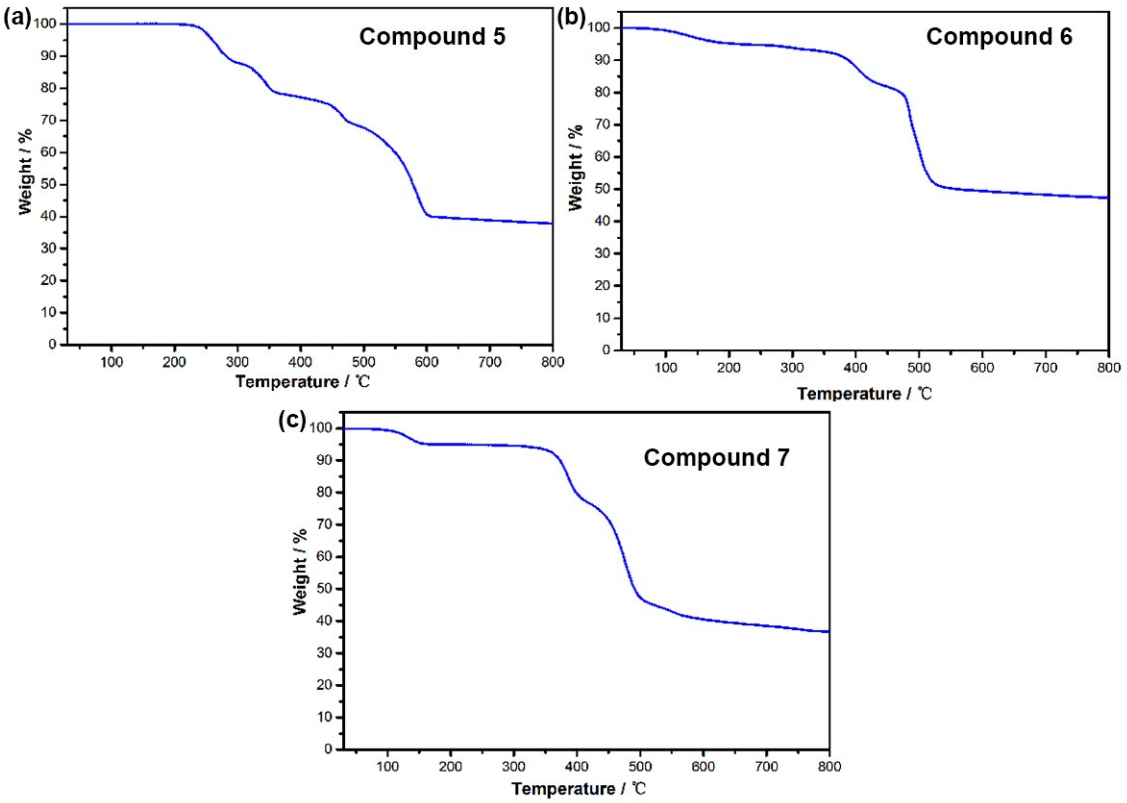

Figure S4. Thermogravimetric analysis curves of compounds **5-7**.

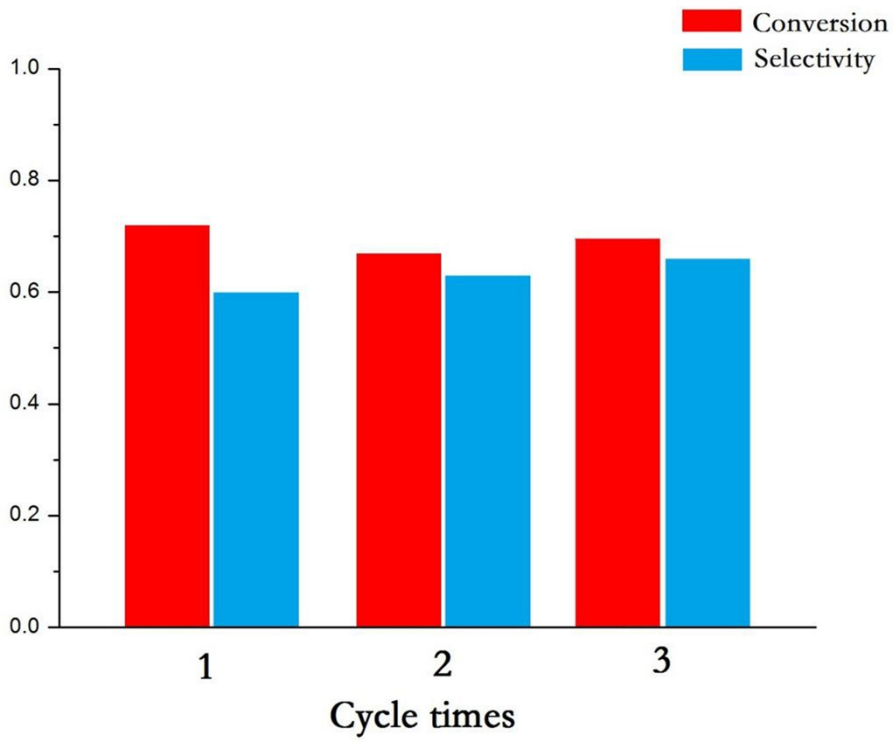

Figure S5. The conversion and selectivity of compound **7** in cyclic experiment.

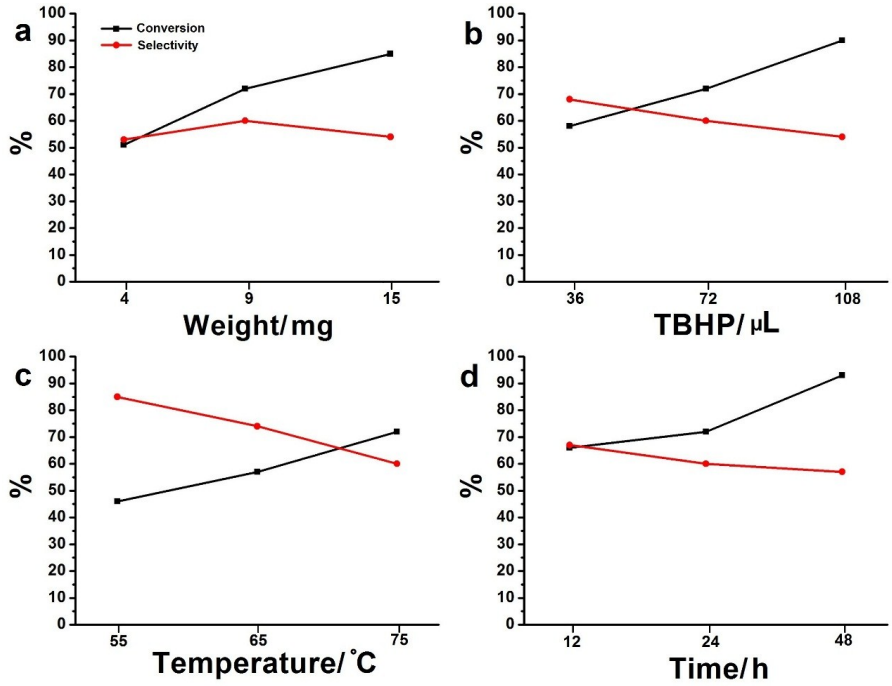

Figure S6. Linear relationship diagrams for the oxidation of styrene with compound **7** as catalyst: (a) Weight of catalyst *vs* Conversion/Selectivity; (b) amount of TBHP *vs* Conversion/Selectivity; (c) Temperature *vs* Conversion/Selectivity; (d) Time *vs* Conversion/Selectivity.

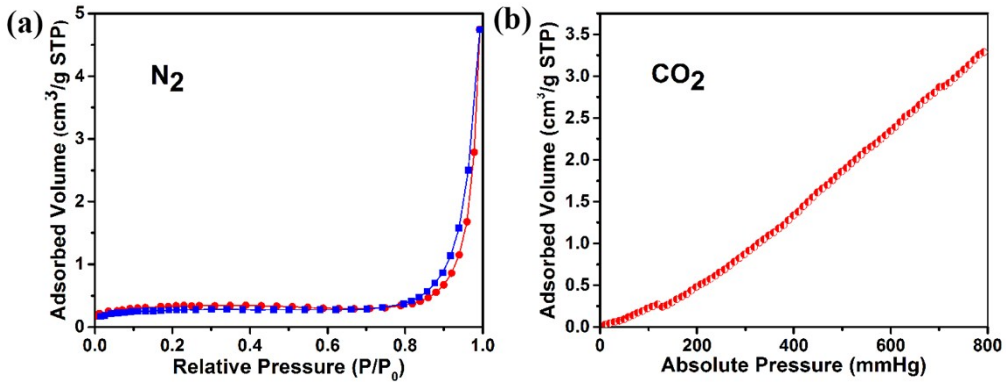

Figure S7. (a) N_2 adsorption-desorption isotherms and (b) CO_2 adsorption isotherms.

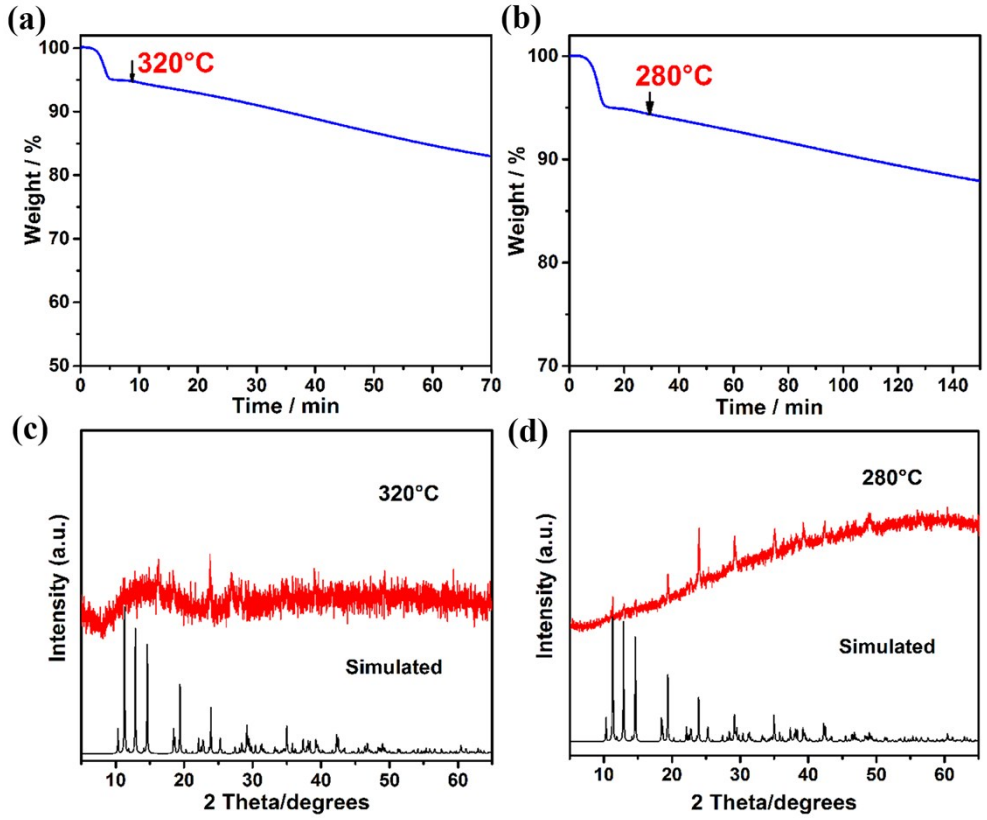

Figure S8. TGA curves of compound **7** heated at 320°C (a) and 280°C (b); comparison between simulated (black) PXRD pattern and experimental (red) PXRD pattern of samples heated at 320°C (c) and 280°C (d).