

Supporting Information

Monitoring thermally induced structural deformation and framework decomposition of ZIF-8 through *in-situ* temperature dependent measurements

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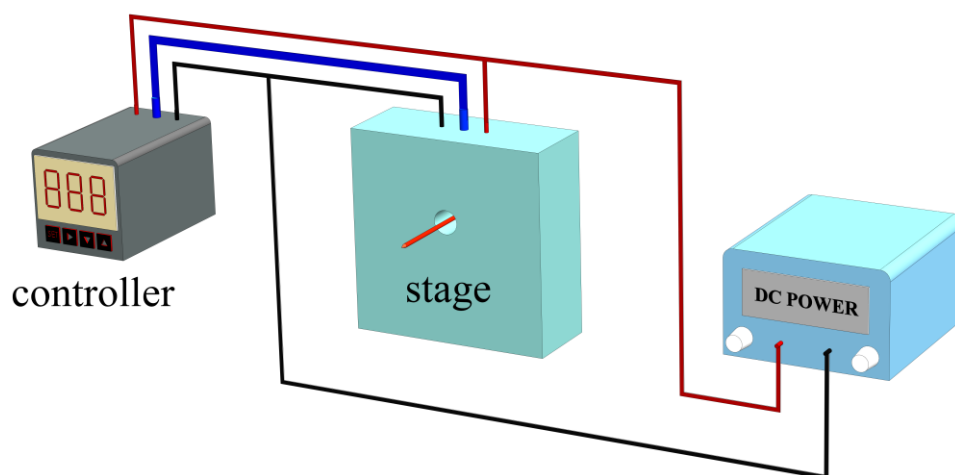


Fig. S1 Schematic of the *in situ* temperature controller stage for transmitting FTIR spectra collection. The blue wire is connected to the K-type thermocouple to measure the sample temperature. The aperture on the stage allows the transmitting of IR beam, which enables the spectra collection.

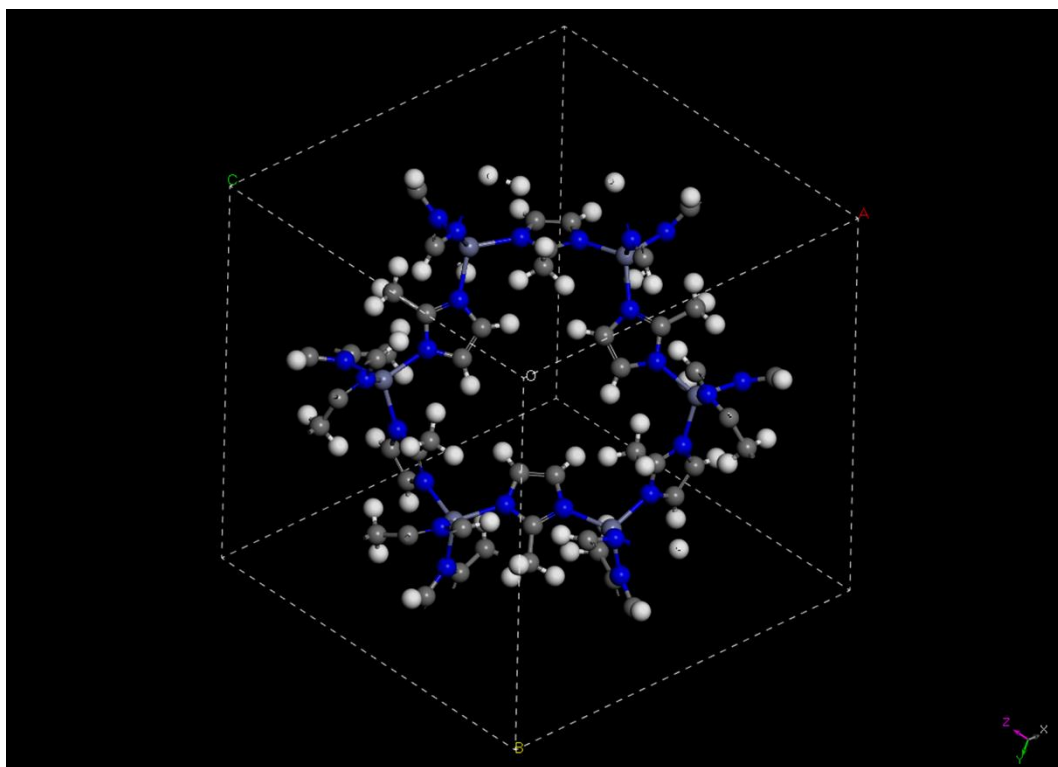


Fig S2 The ZIF-8 crystal model for DFT calculations.

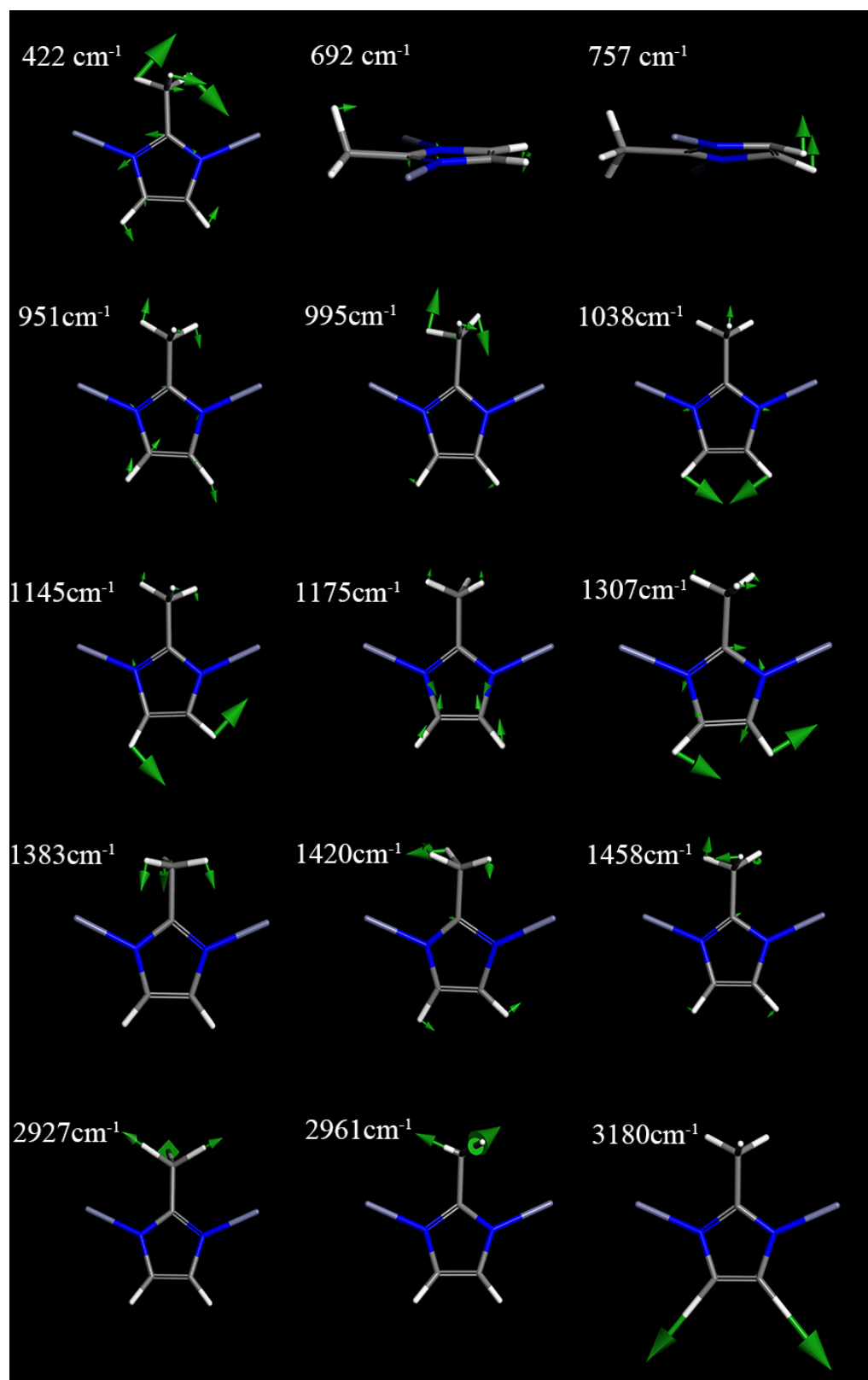


Fig. S3 Details of atomic moieties for each vibration of ZIF-8.

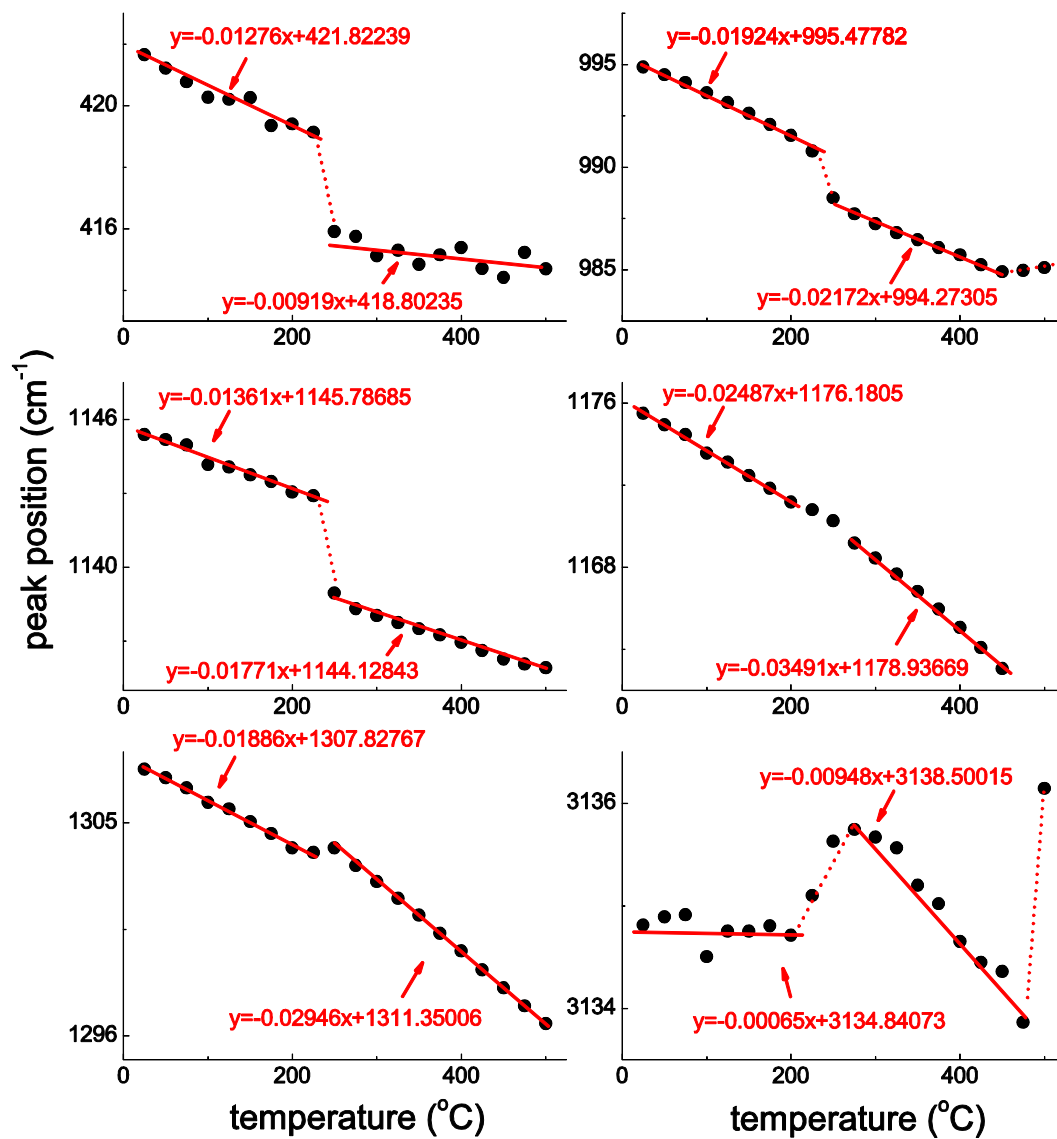


Fig. S4 Peak position changes due to temperature. The linear fitting was applied for each curve.

Table S1 Band assignments of ZIF-8 based on DFT calculations

Band assignment ^a	Exp. (cm ⁻¹)	Cal. (cm ⁻¹)
IP δ_{C2-M}	422	414
δ_{M-H} +Ring puckering+OP R-H wagging	692	667
OP R-H wagging	757	734
δ_{M-H+VR}	951	940
δ_{M-H} +IP R-H wagging	995	981
δ_{M-H+VR} +R-H scissoring	1038	1011
δ_{M-H+VR} +IP R-H wagging	1145	1141
δ_{M-H+VR}	1175	1192
δ_{M-H+VR} +IP R-H wagging	1307	1308
Sym. δ_{M-H}	1383	1369
δ_{M-H+VR} +IP R-H wagging	1420	1403
δ_{M-H+VR} +IP R-H wagging	1458	1465
Sym. ν_{M-H}	2927	2951
Asym. ν_{M-H}	2961	3013
ν_{C-H} (R)	3135	3180

Table S2 Fitting results for each peak in the regions below 200°C and above 250°C.

Peak position (cm ⁻¹)	<200°C		>250°C	
	slope	y-intercept	slope	y-intercept
422	-0.01276	421.82239	-0.00919	418.80235
995	-0.01924	995.47782	-0.02172	994.27305
1146	-0.01361	1145.78685	-0.01771	1144.12843
1176	-0.02487	1176.1805	-0.03491	1178.93669
1308	-0.01886	1307.82767	-0.02946	1311.35006
1380	-0.01529	1384.70623	-0.02354	1385.89411
2926	0.00743	2927.27005	-0.00148	2926.76792
3135	-0.00065	3134.84073	-0.00948	3138.50015

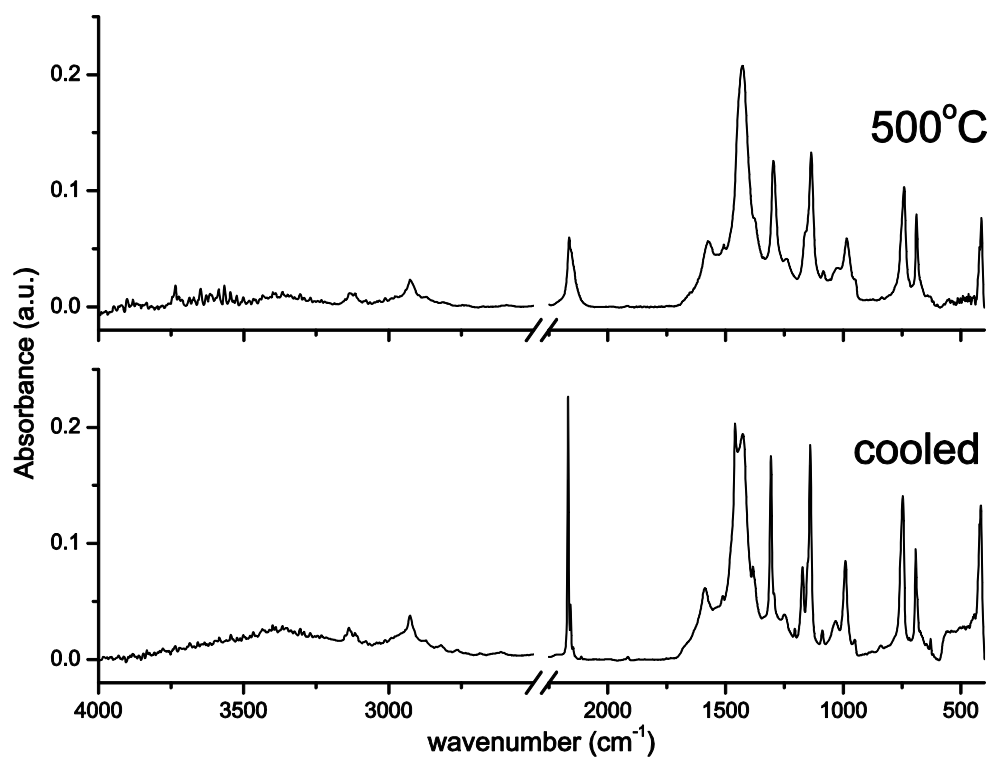


Fig. S5 IR spectra of ZIF-8 under 500 °C and cooled back to 100 °C. The sharp and narrow peak at 2170 cm⁻¹ is typical for -C≡N vibration.

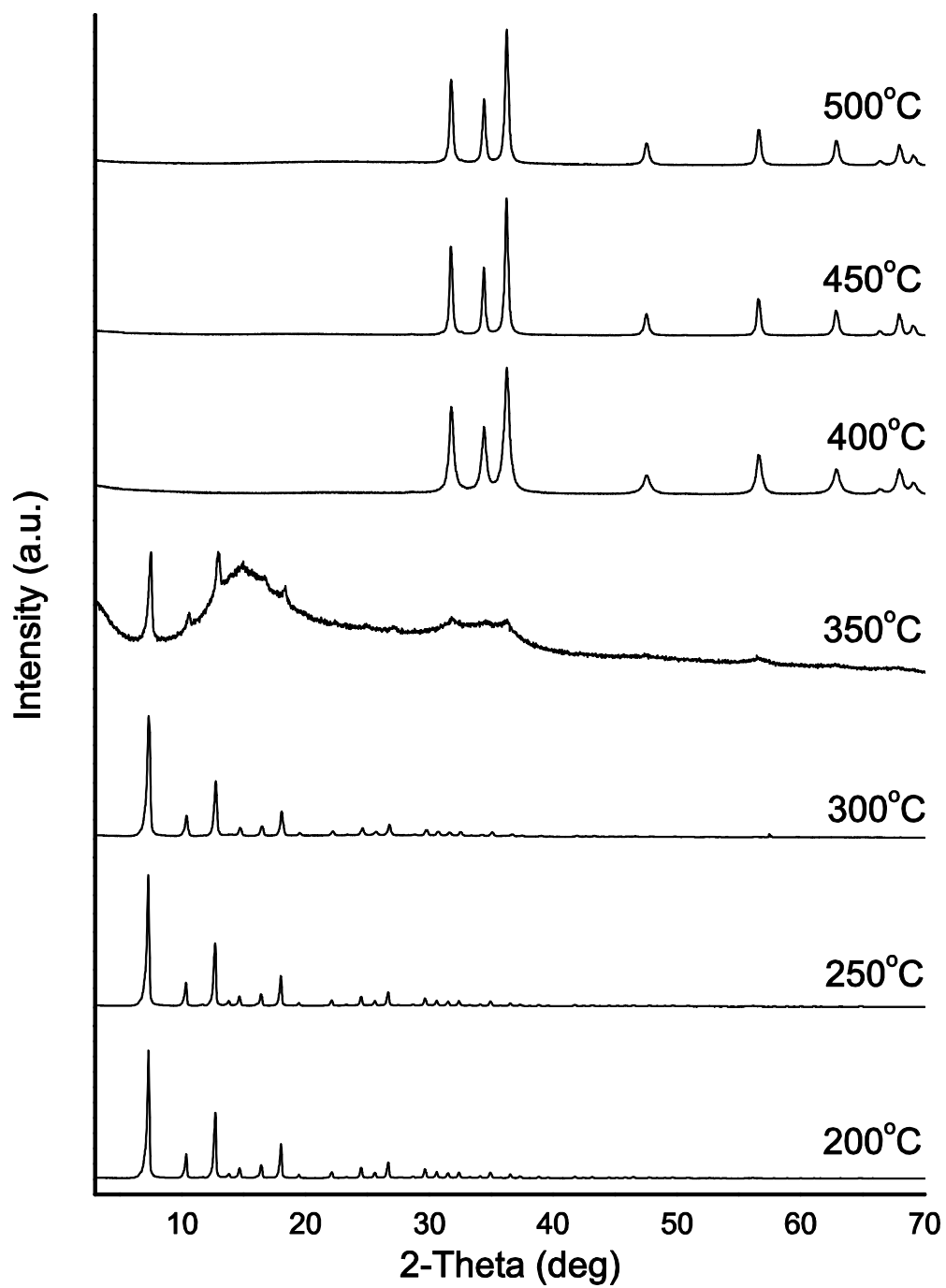


Fig. S6 XRD patterns for ZIF-8 powders heated at different temperatures.