

## SUPPLEMENTARY MATERIAL

# **ZIF-75 under pressure: Negative linear compressibility and pressure-induced instability**

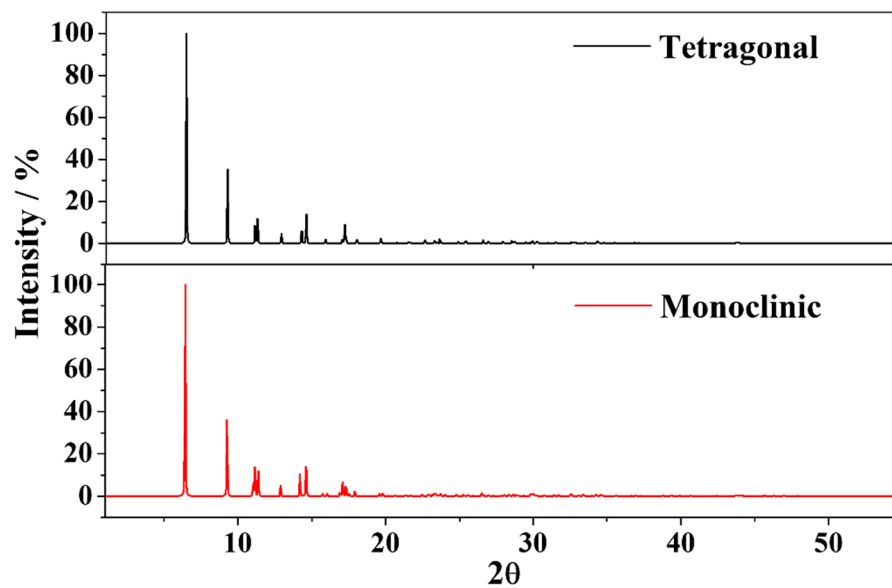
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Contents:	Page
Figure S1. X-ray diffraction patterns of ZIF-75 derived from the tetragonal and monoclinic structures	S.2
Table S1. Most intense reflections in the X-ray diffraction pattern of tetragonal ZIF-75	S.3
Table S2. Unit cell volume and lattice parameters of ZIF-75 under the effect of different external pressures.	S.4
References	S.5

**Figure S1.** X-ray diffraction patterns of ZIF-75 derived from the computed tetragonal ( $I41/a$ ) and monoclinic structures ( $C2/c$ ).



**Table S1.** Most intense reflections in the X-ray diffraction pattern of ZIF-75 (a) X-ray pattern derived from the tetragonal experimental crystal structure [1]; (b) X-ray pattern derived from the calculated tetragonal crystal structure.

$[h\ k\ l]$	Exp. [1]			Calc.		
	$2\theta$ (deg)	$d$ (Å)	I (%)	$2\theta$ (deg)	$d$ (Å)	$\Delta$ ( $2\theta$ )
[0 1 1]	6.662	13.257	100.000	6.44	13.717	0.22
[0 2 0]	9.612	9.195	41.613	9.24	9.568	0.38
[-1 2 1]	11.704	7.555	23.109	11.27	7.847	0.44
[0 3 1]	15.166	5.837	18.668	14.59	6.068	0.58
[1 1 2]	11.476	7.705	12.778	11.11	7.956	0.36
[0 1 3]	14.692	6.024	12.405	14.27	6.203	0.43
[-1 3 2]	17.837	4.969	9.780	17.19	5.154	0.65
[0 2 2]	13.347	6.628	5.762	12.90	6.858	0.45
[0 0 4]	18.539	4.782	5.044	18.02	4.918	0.52
[1 2 3]	17.586	5.039	3.892	17.02	5.205	0.56
[2 2 2]	16.473	5.377	3.638	15.89	5.574	0.59
[1 4 1]	20.43	4.344	3.517	19.64	4.517	0.79
[0 3 5]	27.459	3.246	3.376	26.60	3.349	0.86
[1 5 4]	31.034	2.879	3.316	29.93	2.983	1.11
[3 4 1]	24.629	3.612	3.314	23.67	3.757	0.96
[1 3 2]	17.837	4.969	3.037	17.19	5.154	0.65
[-2 5 3]	29.653	3.010	2.892	28.55	3.124	1.11
[-1 5 2]	26.391	3.375	2.328	25.38	3.506	1.01
[1 3 4]	24.074	3.694	2.274	23.29	3.817	0.79
[2 3 1]	17.985	4.928	2.125	17.29	5.124	0.69
[-2 3 3]	22.303	3.983	2.102	21.52	4.125	0.78
[0 2 6]	29.633	3.0122	1.716	28.76	3.1016	0.87

**Table S2.** Unit cell volume and lattice parameters of ZIF-75 (I41/*a*) under the effect of different external isotropic pressures.

<b>P (GPa)</b>	<b>Vol. (Å<sup>3</sup>)</b>	<b><i>a</i> (Å)</b>	<b><i>b</i> (Å)</b>	<b><i>c</i> (Å)</b>	<b><i>α</i> (deg)</b>	<b><i>β</i> (deg)</b>	<b><i>γ</i>(deg)</b>
-1.0000	9145.8664	21.5555	21.5555	19.6837	90.00	90.00	90.00
-0.7509	8766.0596	21.1826	21.1826	19.5365	90.00	90.00	90.00
-0.5000	8472.7248	20.9067	20.9067	19.3844	90.00	90.00	90.00
-0.2500	8211.1779	20.5558	20.5558	19.4328	90.00	90.00	90.00
-0.1256	7757.1256	20.1081	20.1081	19.1848	90.00	90.00	90.00
-0.0629	7524.3086	19.9030	19.9030	18.9946	90.00	90.00	90.00
-0.0003	7203.3094	19.1356	19.1356	19.6719	90.00	90.00	90.00
0.0626	6962.3737	18.6261	18.6261	20.0685	90.00	90.00	90.00
0.0939	6797.0337	18.2930	18.2930	20.3119	90.00	90.00	90.00
0.1094	6771.1421	18.2582	18.2582	20.3117	90.00	90.00	90.00
0.1147	6764.3872	18.2444	18.2444	20.3222	90.00	90.00	90.00
0.1249	3437.9886	13.2513	13.2513	19.5789	90.00	90.00	90.00
0.2498	3389.9991	13.1684	13.1684	19.5494	90.00	90.00	90.00
0.5000	3291.0852	12.9585	12.9585	19.5987	90.00	90.00	90.00
0.7499	3240.5895	12.8790	12.8790	19.5370	90.00	90.00	90.00
0.9998	3180.9584	12.7789	12.7789	19.4791	90.00	90.00	90.00

## References

- [1] Tian, Y. Q.; Zhao, Y. M., Chen, Z. X. Zhang, G. N., Weng, L. H.; Zhao, D. Y. Design and Generation of Extended Zeolitic Metal–Organic Frameworks (ZMOFs): Synthesis and Crystal Structures of Zinc(II) Imidazolate Polymers with Zeolitic Topologies. *Chem. Eur. J.* **2007**, *13*, 4146 – 4154.