

# MOFs Under Pressure: The Reversible Compression of a Single Crystal

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**Synthesis of ZAG-4:** In a typical experiment  $\text{Zn}(\text{Oac})_2 \cdot 2\text{H}_2\text{O}$  (0.1 mmol in 2 mL ddi  $\text{H}_2\text{O}$ ), in a 20 mL glass scintillation vial, was adjusted to a pH of  $\sim 1.8$  using glacial acetic acid. In a separate vial the 1,4-butanediol(phosphonic acid) (0.2 mmol) was dissolved in 2 mL of ddi  $\text{H}_2\text{O}$  and was subsequently layered on top of the zinc acetate solution and set undisturbed for two days to allow for crystal growth. The resulting large colorless crystals were filtered and washed with ethanol and dried at room temperature.

**Table S1. Results of equation of state calculations from eosfit<sup>1</sup>**

	$V_0$	$K_0$	$K'$	$K''$	$X^2_w$	$\text{delP}_{\text{max}}$
M	1160.173	9.38236	5.21098	-	1.049	0.077
BM2	1159.283	12.15152	4	-	12.7517	0.332
BM3	1160.174	8.73766	6.51476	-1.45664	0.9408	0.099
BM4	1160.096	11.66431	1.97567	1.3776	0.049	0.015
NS2	1158.199	16.09971	2	-	45.903	-0.585
NS3	1160.166	7.46254	10.24467	-10.3476	3.5833	0.134
NS4	1160.096	12.95447	-0.73121	3.21682	0.1571	0.027
V	1160.189	8.59717	6.71975	-	1.994	0.108

\*Murnaghan, Birch-Murnaghan (2nd, 3rd and 4th order), Natural Strain (2nd, 3rd, and 4th order) and Vinet

**Table S2. K. P. I's for the structures at each pressure**

	Ambient	1.65(10) GPa	2.81(9) GPa	5.69(3) GPa	7.32(7) GPa	Ambient post
<b>K. P. I.*</b>	69.7%	76.5%	80%	86.5%	87.5%	69.8%

\*As calculated by the program Platon.<sup>2</sup>

Figure S1. Full-size Figure 1 from main body of work

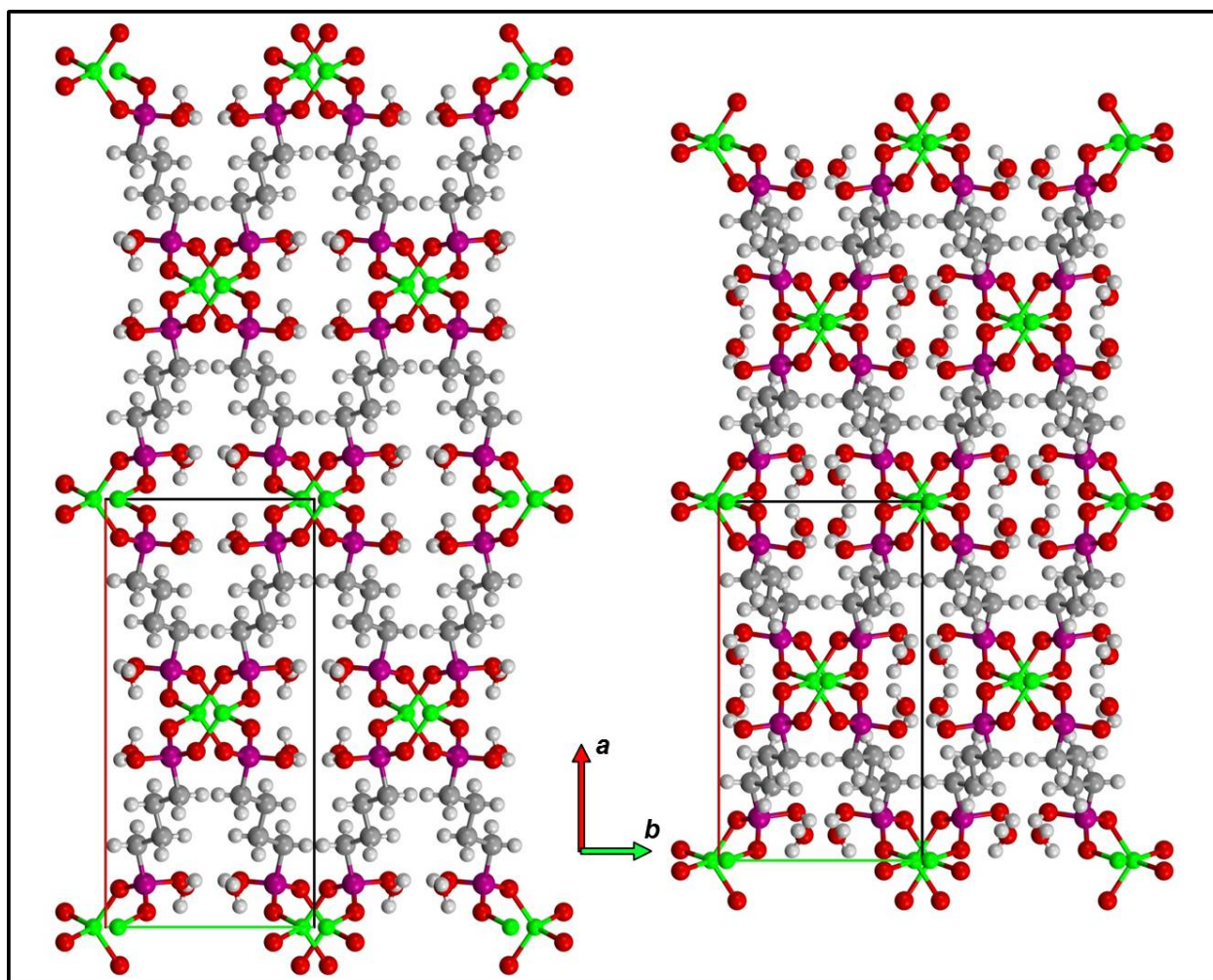


Figure S2. Full-size Figure 4 from main body of work

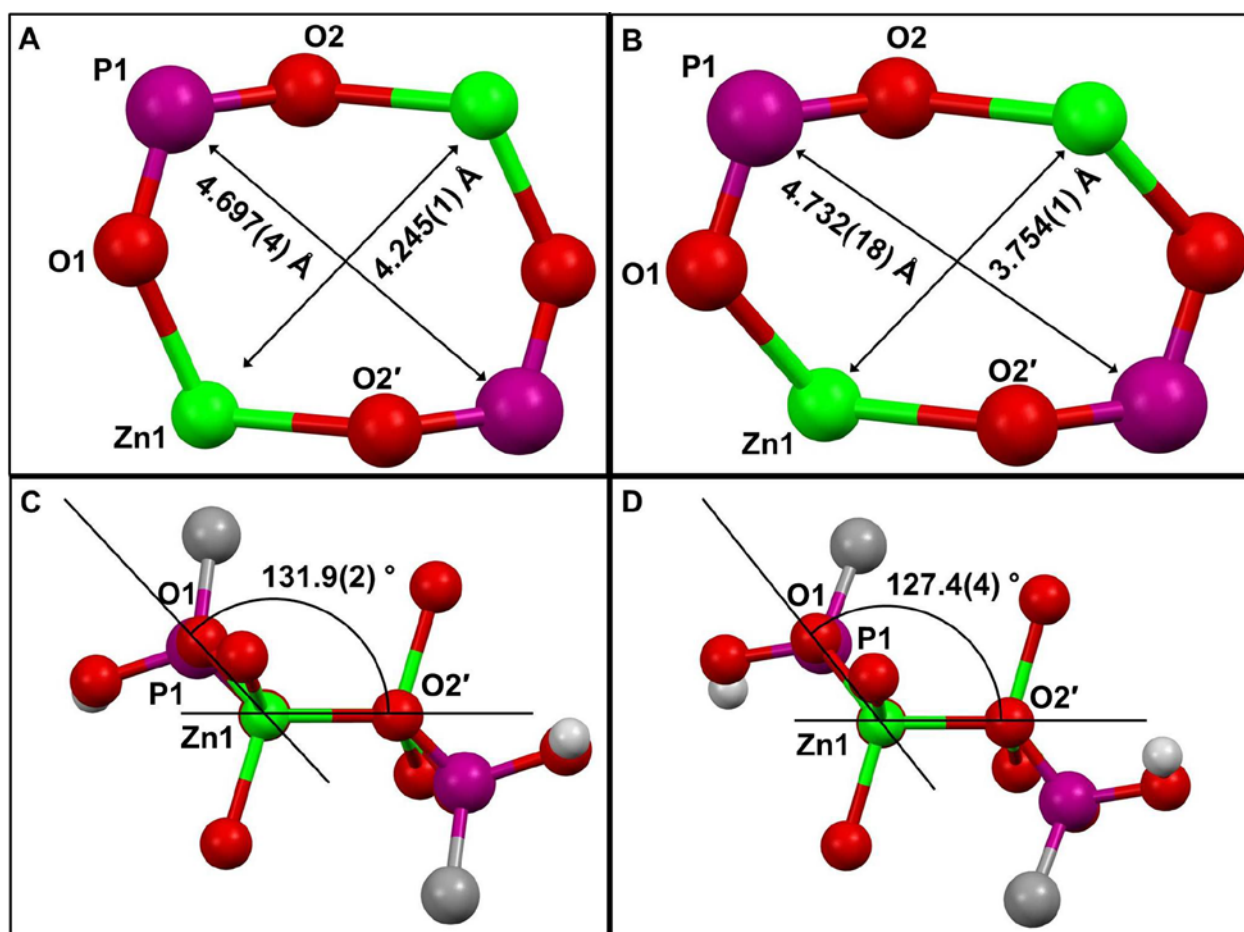
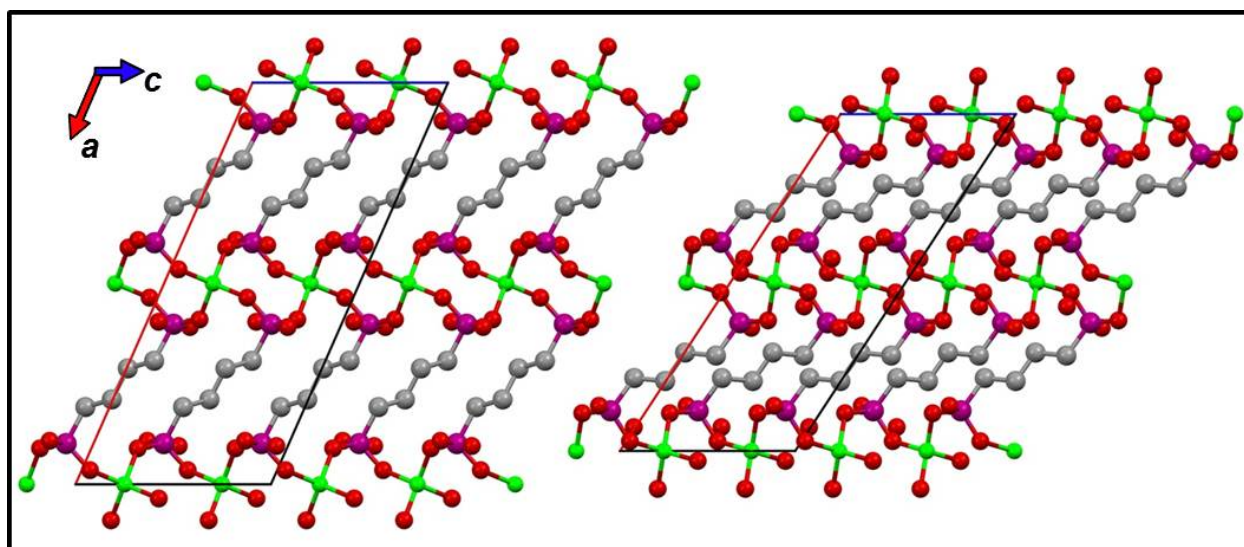
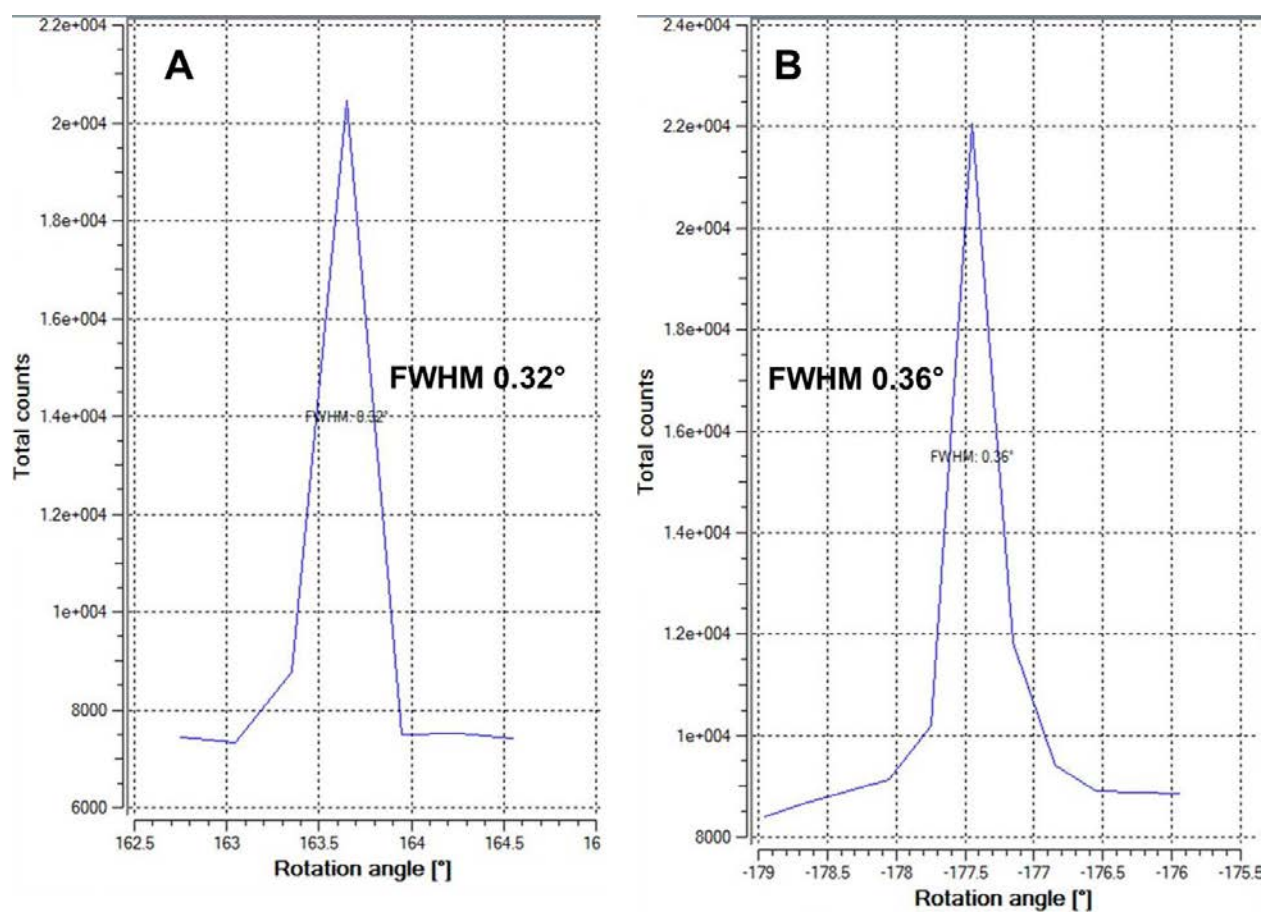


Figure S3. Full-size Figure 5 from the main body of work



**Figure S4. Rocking curves of reflection -6 2 8 with the FWHM of each peak in the pre (A) and post (B) pressure ambient data**



## References

1. Angel, R. J., *Reviews in Mineralogy and Geochemistry* 2000, 41 (1), 35-59.
2. A.L.Spek, *Acta Cryst.* 2009, D65, 148-155.