Microstructures

Open Access

Supplementary Material

First-principles study on the negative/zero area compressibility in Ag_3BO_3 with "wine-rack" architecture

Xingyu Zhang[1,3], Youquan Liu[1,3], Naizheng Wang[1,3], Xingxing Jiang[1,2], Zheshuai Lin[1,2]

[1]Functional Crystals Lab, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, China.
[2]Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China.
[3]University of the Chinese Academy of Sciences, Beijing 100049, China.

Correspondence to: Prof. Xingxing Jiang, Functional Crystals Lab, Technical Institute of Physics and Chemistry, 29 Zhongguancun East Road, Haidian District, Beijing 100190, China. E-mail: xxjiang@mail.ipc.ac.cn; Prof. Zheshuai Lin, Functional Crystals Lab, Technical Institute of Physics and Chemistry, 29 Zhongguancun East Road, Haidian District, Beijing 100190, China. E-mail: zslin@mail.ipc.ac.cn

Table S1. The calculated cell parameters and enthalpy of $Ag_3Co(CN)_6$-*I* and $Ag_3Co(CN)_6$-*II* with respect to pressure.

	$Ag_3Co(CN)_6$-*I*				**$Ag_3Co(CN)_6$-*II***					
Pressure (GPa)	a (Å)	c (Å)	V (Å^3)	H (eV)	a (Å)	b (Å)	c (Å)	Beta (°)	V (Å^3)	H (eV)
0	6.234390	7.599314	255.796	-6678.6130	6.294170	12.300578	6.596678	101.096425	501.179	-13356.7585
1	6.043281	7.690826	243.248	-6677.0575	6.284035	11.896045	6.637883	100.886952	487.285	-13353.6650
2	5.923171	7.736011	235.048	-6675.5653	6.068568	10.505781	6.791169	101.509813	424.264	-13350.9330
3	5.832755	7.764651	228.771	-6674.1177	5.926487	10.318975	6.866416	101.601636	411.338	-13348.3262
4	5.761712	7.780934	223.700	-6672.7054	5.818641	10.191172	6.918887	101.747580	401.688	-13345.7886
5	5.702537	7.792061	219.442	-6671.3223	5.730584	10.090016	6.958649	101.900261	393.713	-13343.3058
6	5.651829	7.798821	215.743	-6669.9642	5.657269	10.008507	6.988249	102.058293	386.950	-13340.8688
7	5.607291	7.800826	212.411	-6668.6279	5.592590	9.937269	7.013353	102.222236	380.933	-13338.4718
8	5.567981	7.800818	209.443	-6667.3113	5.537700	9.875631	7.031065	102.397463	375.551	-13336.1104
9	5.532687	7.799366	206.758	-6666.0122	5.489733	9.820168	7.044291	102.573155	370.651	-13333.7815
10	5.500658	7.795192	204.262	-6664.7293	5.447574	9.768793	7.053815	102.724154	366.159	-13331.4816

Table S2. The calculated cell parameters and enthalpy of Ag_3BO_3-*I* and Ag_3BO_3-*II* with respect to pressure.

	Ag_3BO_3-*I*				**Ag_3BO_3-*II***			
Pressure (GPa)	a (Å)	c (Å)	V (Å^3)	H (eV)	a (Å)	c (Å)	V (Å^3)	H (eV)
0	9.97276	3.01461	259.653	-13426.8533	9.94640	12.33943	1057.20	-53707.4132
1	9.96707	2.98961	257.205	-13425.2408	9.95372	12.19108	1046.03	-53700.9632
2	9.96021	2.96652	254.868	-13423.6431	9.96057	12.04875	1035.24	-53694.5724
3	9.95130	2.94652	252.697	-13422.0596	9.96223	11.93402	1025.72	-53688.2384
4	9.94209	2.92830	250.669	-13420.4888	9.96232	11.83234	1017.00	-53685.8794
5	9.93241	2.91188	248.778	-13418.9301	9.96073	11.74021	1008.76	-53675.7204
6	9.92292	2.89701	247.035	-13417.3829	9.95703	11.66024	1001.15	-53669.5316
7	9.91310	2.88283	245.340	-13415.8466	9.95341	11.58426	993.899	-53663.3864
8	9.90293	2.86972	243.723	-13414.3204	9.94711	11.51852	987.008	-53657.2816
9	9.89330	2.85711	242.181	-13412.8042	9.94215	11.45456	980.549	-53651.2168
10	9.88381	2.84532	240.719	-13411.2973	9.93624	11.39554	974.388	-53645.1892

Table S3. The calculated compressibility of Ag_3BO_3-*I* and Ag_3BO_3-*II*.

	Pressure range (GPa)	Princple axis	K (TPa^{-1})	a	b	c
Ag_3BO_3-*I*	0~10 GPa	X1	4.95 (11)	0	0	1
		X2	0.97 (1)	0.2588	0.9659	0
		X3	0.97 (1)	0.9659	0.2588	0
Ag_3BO_3-*II*	0~4 GPa	X1	9.26 (79)	0	0	1
		X2	-0.24 (22)	-0.8946	-0.8944	0
		X3	-0.24 (22)	-0.0005	1	0
	4~10 GPa	X1	5.51 (3)	0	0	1
		X2	0.53 (2)	-0.8944	-0.4472	0
		X3	0.53 (2)	-0.0001	1	0
	0~10 GPa	X1	6.56 (21)	0	0	1
		X2	0.09 (14)	-0.8944	-0.4473	0
		X3	0.09 (14)	-0.0001	1	0

Table S4. Elastic Stiffness Constants C_{ij} of $AgBO_3$-*I* and $AgBO_3$-*II*

		Ci1	Ci2	Ci2	Ci4	Ci5	Ci6
$AgBO_3$-*I*	C1j	236.61375	122.84546	83.08500	-26.73325	0.00000	0.00000
	C2j	122.84546	236.61375	83.08500	26.73325	0.00000	0.00000
	C3j	83.08500	83.08500	105.91086	0.00000	0.00000	0.00000
	C4j	-26.73325	26.73325	0.00000	20.49982	0.00000	0.00000
	C5j	0.00000	0.00000	0.00000	0.00000	20.49982	-26.73325
	C6j	0.00000	0.00000	0.00000	0.00000	-26.73325	56.88414
$AgBO_3$-*II*	C1j	229.34300	144.68043	101.23793	-22.10957	0.00000	0.00000
	C2j	144.68043	229.34300	101.23793	22.10957	0.00000	0.00000
	C3j	101.23793	101.23793	89.30071	0.00000	0.00000	0.00000
	C4j	-22.10957	22.10957	0.00000	24.68479	0.00000	0.00000
	C5j	0.00000	0.00000	0.00000	0.00000	24.68479	-22.10957
	C6j	0.00000	0.00000	0.00000	0.00000	-22.10957	42.33129

Table S5. The mechanical property of $AgBO_3$-*I* and $AgBO_3$-*II*.

	Direction	Young Modulus (GPa)	Bulk modulus (GPa)	Poisson Ratios	
$AgBO_3$-*I*	X	73.88421	101.54978	E_{xy}= 0.6775	E_{xz}= 0.2530
	Y	73.88421		E_{xy}= 0.6775	E_{xz}= 0.2530
	Z	67.50251		E_{zx}= 0.2311	E_{zy}= 0.2311
$AgBO_3$-*II*	X	68.69164	87.37082	E_{xy}= 0.5246	E_{xz}= 0.5390
	Y	68.69164		E_{xy}= 0.5246	E_{xz}=0.5390
	Z	34.49603		E_{zx}= 0.2707	E_{zy}=0.2707

Table S6. Pressure-dependent bond length and angle of Ag_3BO_3-*I*.

Pressure (GPa)	The bond length of B-O (Å)	The bond length of Ag-O (Å)	The angle of ∠O-Ag-O (Å)	Angle between O-Ag-O bar and *c*-axis	Angle between O-Ag-O bar and (*a*, *b*) plane
0	1.36648	2.14276	133.792	59.346	30.654
1	1.36510	2.13948	133.573	59.548	30.452
2	1.36400	2.13540	133.434	59.727	30.273
3	1.36308	2.13238	133.146	59.869	30.131
4	1.36206	2.12878	132.974	59.997	30.003
5	1.36088	2.12554	132.799	60.110	29.890
6	1.35978	2.12211	132.682	60.211	29.789
7	1.35870	2.11886	132.544	60.304	29.696
8	1.35766	2.11558	132.420	60.387	29.613
9	1.35662	2.11263	132.285	60.468	29.532
10	1.35554	2.10956	132.190	60.543	29.457

Table S7. Pressure-dependent bond length and angle of Ag_3BO_3-*II*.

Pressure (GPa)	The bond length of B-O (Å)	The bond length of Ag-O1 (Å)	The bond length of Ag-O2 (Å)	The angle of ∠O-Ag-O (Å)	Angle between O-Ag-O chain and *c*-axis	Angle between O-Ag-O bar and (*a*, *b*) plane
0	1.36840	2.09401	2.09607	176.406	60.590	29.410
1	1.36681	2.09061	2.09252	176.427	60.925	29.075
2	1.36550	2.08740	2.08952	176.266	61.248	28.752
3	1.36404	2.08349	2.08689	176.220	61.498	28.502
4	1.36267	2.08012	2.08375	176.210	61.714	28.286
5	1.36130	2.07690	2.08059	176.182	61.907	28.093
6	1.35989	2.07350	2.07751	176.171	62.068	27.932
7	1.35857	2.07023	2.07462	176.185	62.221	27.779
8	1.35735	2.06710	2.07241	176.081	62.352	27.648
9	1.35613	2.06394	2.06951	176.096	62.475	27.525
10	1.35485	2.06086	2.06665	176.106	62.586	27.414

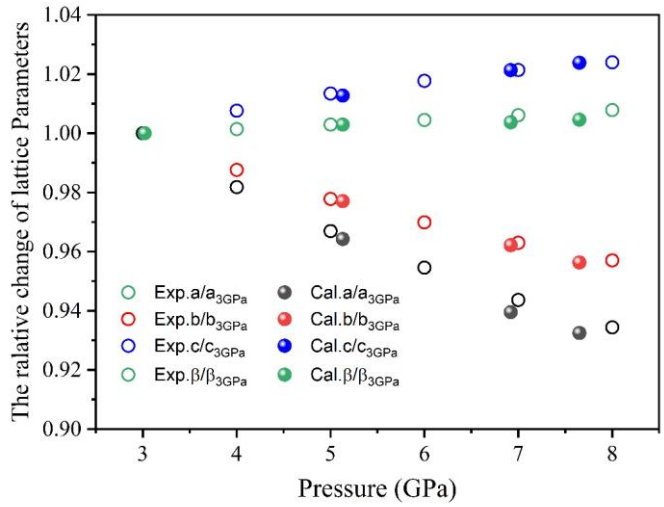


Figure S1. The relative change of lattice parameters of $Ag_3Co(CN)_6$-*II*. The experimental lattice parameters in graph were reproduced from Goodwin et al[1].

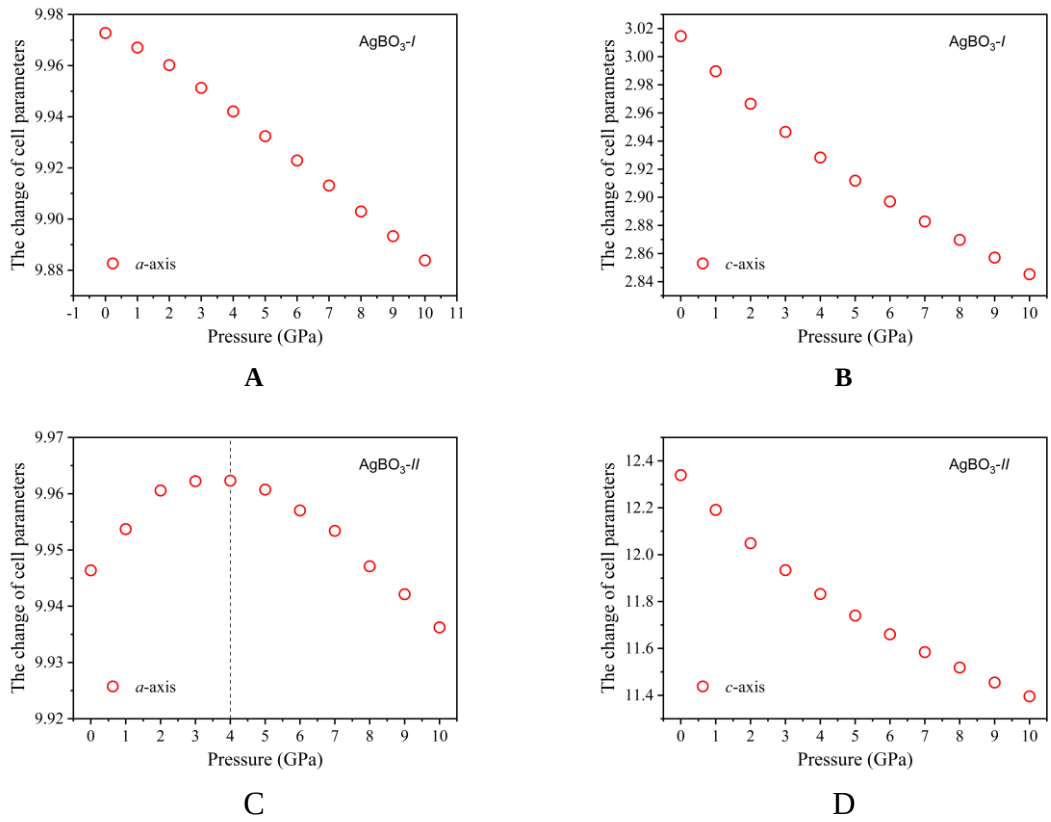


Figure S2. The cell parameters of $AgBO_3$-*I* and $AgBO_3$-*II* with respect to pressure. (A) a-axis in $AgBO_3$-*I*. (B) c-axis in $AgBO_3$-*I*. (C) a-axis in $AgBO_3$-*II*. (D) c-axis in $AgBO_3$-*II*.

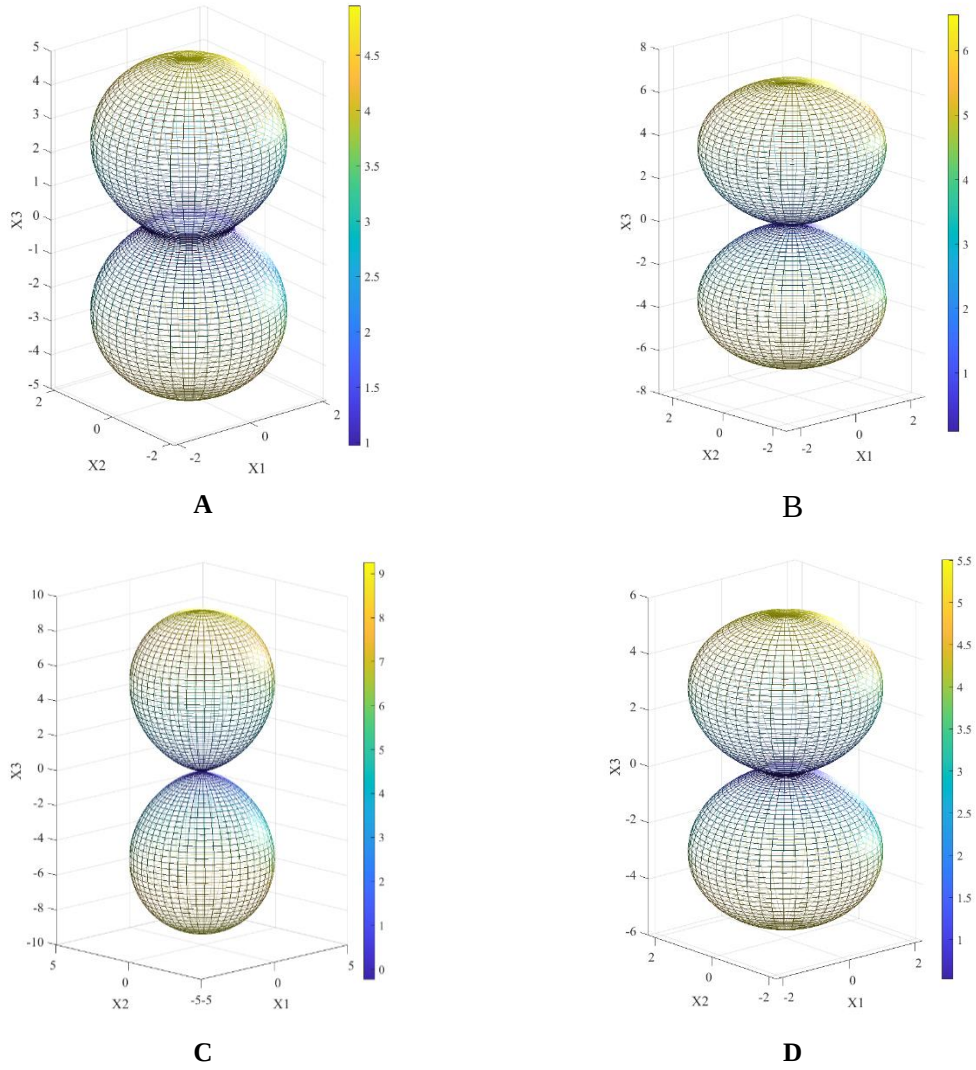


Figure S3. The steric compressibility of Ag_3BO_3-*I* and Ag_3BO_3-*II*. (A) the compressibility of Ag_3BO_3-*I* in the range from 0 GPa to 10 GPa. (B) the compressibility of Ag_3BO_3-*II* in the range from 0 GPa to 10 GPa; (C) the compressibility of Ag_3BO_3-*II* in the range from 0 GPa to 4 GPa; (D) the compressibility of Ag_3BO_3-*II* in the range from 4 GPa to 10 GPa.

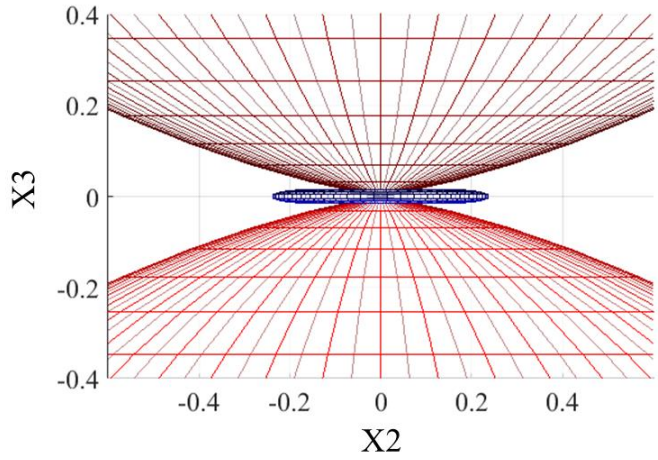
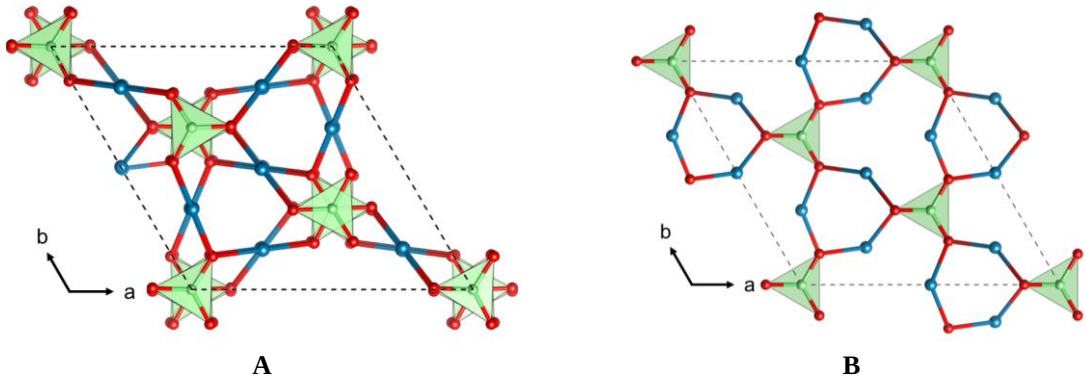


Figure S4. The compressibility of Ag_3BO_3-*II* viewed along X1 direction (0~4 GPa). The red and blue line are represented of positive and negative values.



A **B**

Figure S5. The top-view of $AgBO_3$. (A) $AgBO_3$-*I*. (B) $AgBO_3$-*II*.

REFERENCES

1. Goodwin A. L., Keen D. A., Tucker M. G., Large negative linear compressibility of $Ag_3[Co(CN)_6]$. Proc. Natl. Acad. Sci. U.S.A. 2008; 150: 18708–18713. [DOI: http://doi.org/10.1073/pnas.0804789105]