Supporting information for

High Pressure and Elastic properties of a Guanidinium-formate Hybrid Perovskite

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Table S1 Mechanical properties and linear compressibility of MGF are summarized.

		E			***H***			***Compressibility***		
$[C(NH_2)_3]Mn$ [1-3]		010	10-1	101	010	10-1	101	K_a	K_b	K_c
	orthorhombic	28.6(4)	23.5(6)	24.5(5)	1.25(4)	1.11(5)	1.18(5)	26.6(6)	15.4(3)	0.11(8)
								26.7(4)	15.2(2)	0.03(16)
	trigonal							2.4(2)		29.1(5)
								2.04(15)		27.3(5)
$[C(NH_2)_3]Co$ [2-4]		010	10-1		010	10-1		K_a	K_b	K_c
	orthorhombic	32.6(7)	23.6(7)		1.54(7)	1.16(5)		19.8(3)	11.77(21)	0.80(5)
								19.5(3)	11.4(2)	1.10(8)
	trigonal							3.3(3)		18.2(3)
								2.34(10)		21.9(7)
$[C(NH_2)_3]Cu$ [5]		110	-11-1	011	110	-11-1	011	K_a	K_b	K_c
	orthorhombic	21.3(6)	17.5(6)	16.2(4)	1.28(5)	1.01(5)	0.8(0)	28.7(29)	4.0(36)	11.9(72)
$[C(NH_2)_3]Zn$ [5]		-1-10	-11-1	011	-1-10	-11-1	011	K_a	K_b	K_c
	orthorhombic	29.3(6)	26.6(8)	24.1(6)	1.45(4)	1.26(5)	0.97(5)	0	3.6(42)	8.4(61)

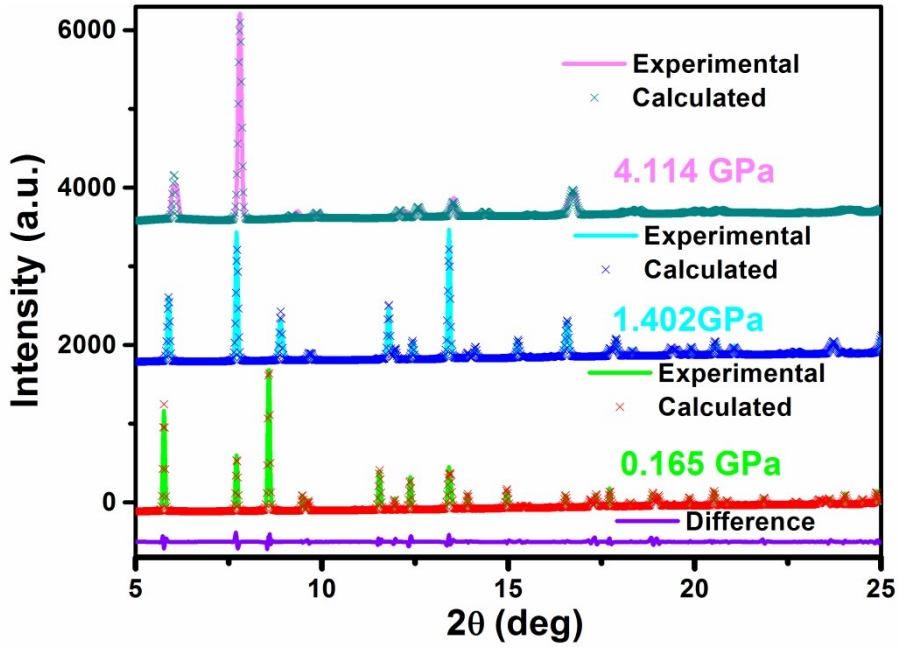

Figure S1 The representative synchrotron powder X-ray diffraction patterns of CdGF at 1.165，1.402 and 4.114 GPa.

Table S2 Experimental and calculated lattice parameters of CdGF as a function of pressure.

Experimental				**Calculated**			
p (GPa)	*a* (Å)	*c* (Å)	*v* (Å³)	*p* (GPa)	*a* (Å)	*c* (Å)	*v* (Å³)
0	9.2146	19.6072	1441.8	0	9.33848	19.1433	1445.77
0.16461	9.2019	19.4049	1443	0.1	9.34351	18.9978	1436.33
0.32932	9.1945	19.1106	1399.2	0.2	9.34844	18.838	1425.75
0.49412	9.1962	19.0284	1393.6	0.25	9.35118	18.7736	1421.71
0.74151	9.1958	18.848	1380.3	0.3	9.35431	18.682	1415.72
0.90655	9.2002	18.7391	1373.6	0.35	9.35496	18.6271	1411.76
1.15429	9.198	18.5877	1361.9	0.5	9.35948	18.4352	1398.56
1.40224	9.1954	18.4813	1353.3	1	9.36422	17.9358	1362.06
1.65041	9.1855	18.38	1343	2	9.35463	17.2832	1309.81
1.81597	9.1944	18.3477	1343.2	3	9.34078	16.8213	1271.03
2.0645	9.1746	18.2252	1328.6	4	9.31108	16.5053	1239.24
2.31323	9.1427	18.0428	1306.1				
2.86676	9.1277	17.8069	1284.8				
3.4491	9.1228	17.8102	1283.7				
4.11607	9.1109	17.7157	1273.5				

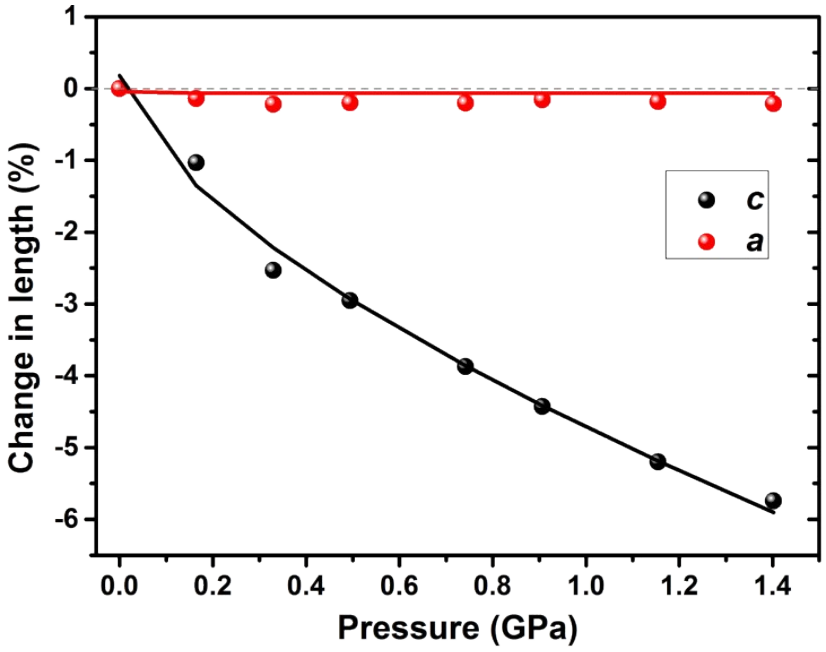

Figure S2 The *ab*-plane showed a near zero area compressibility within the scope of 1.40 Gpa. The solid lines indicate the fits using the second-order Birch– Murnaghan equation of state.

Table S3. Linear compressibility of unit-cell axes over different pressure ranges.

Pressure range	K_a (TPa^{-1})	K_c (TPa^{-1})
Ambient to 1.40GPa	0.0042	32.5834
Ambient to 4.12GPa	2.8199	20.9221

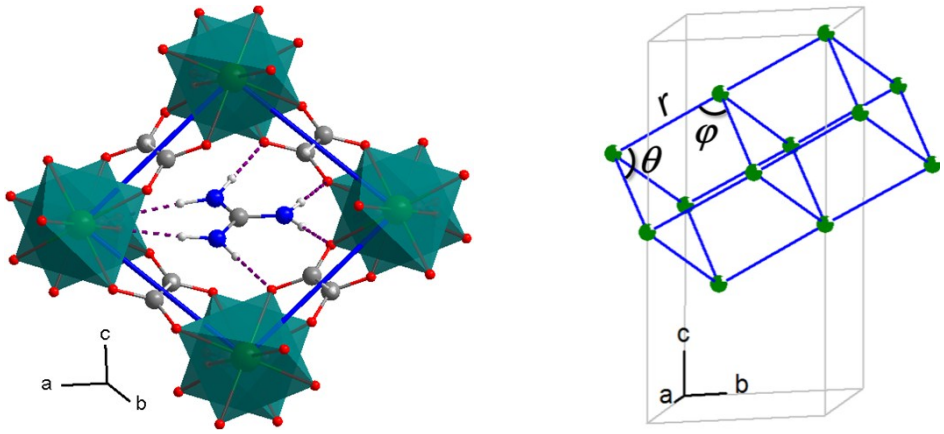

Figure S3 The blue framework frames represent 'hinge-strut' like structure and violet dotted lines represent hydrogen bonds.

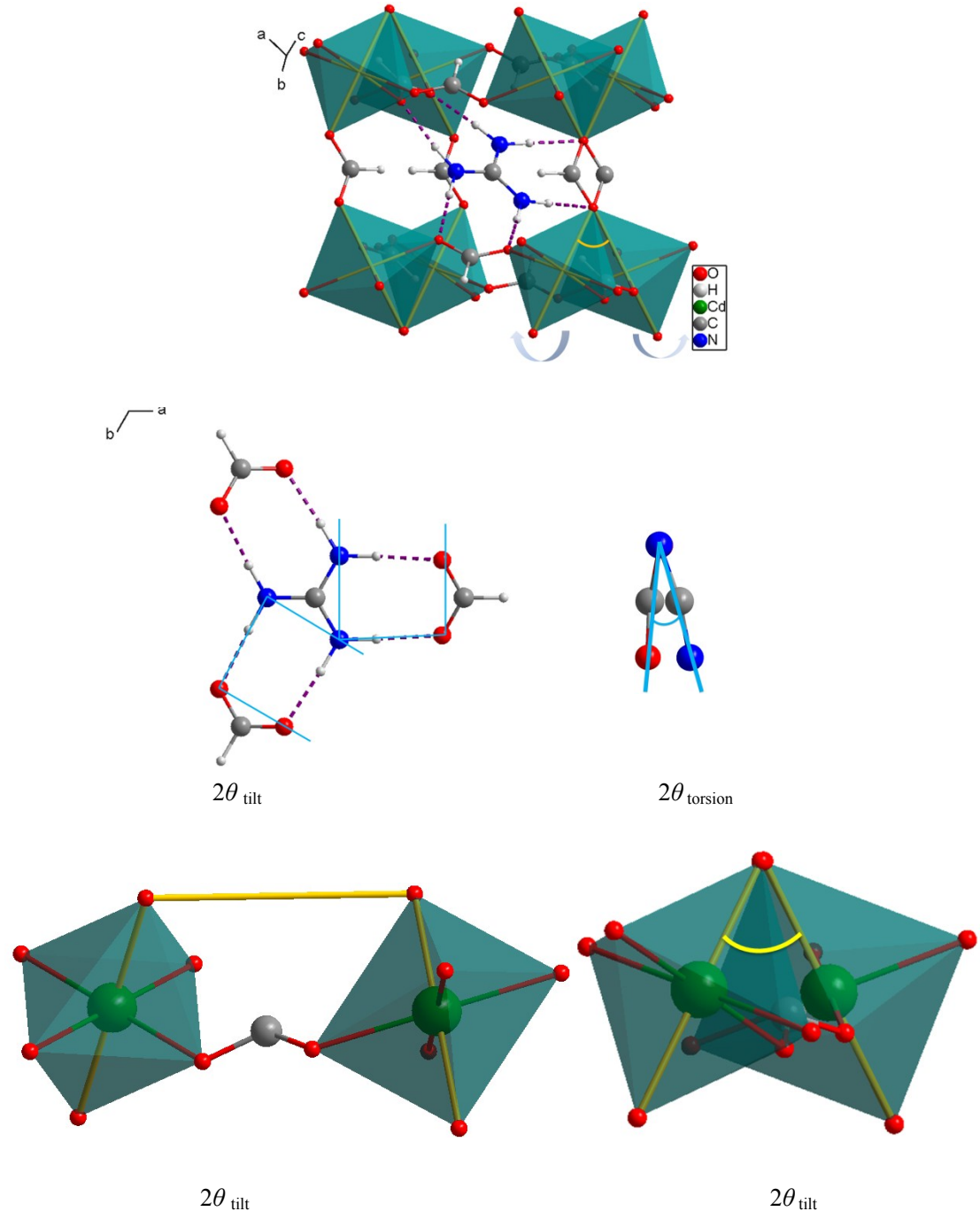

Figure S4. Schematic diagrams of the variation in the formate-guanidinium and octahedral torsion angles.

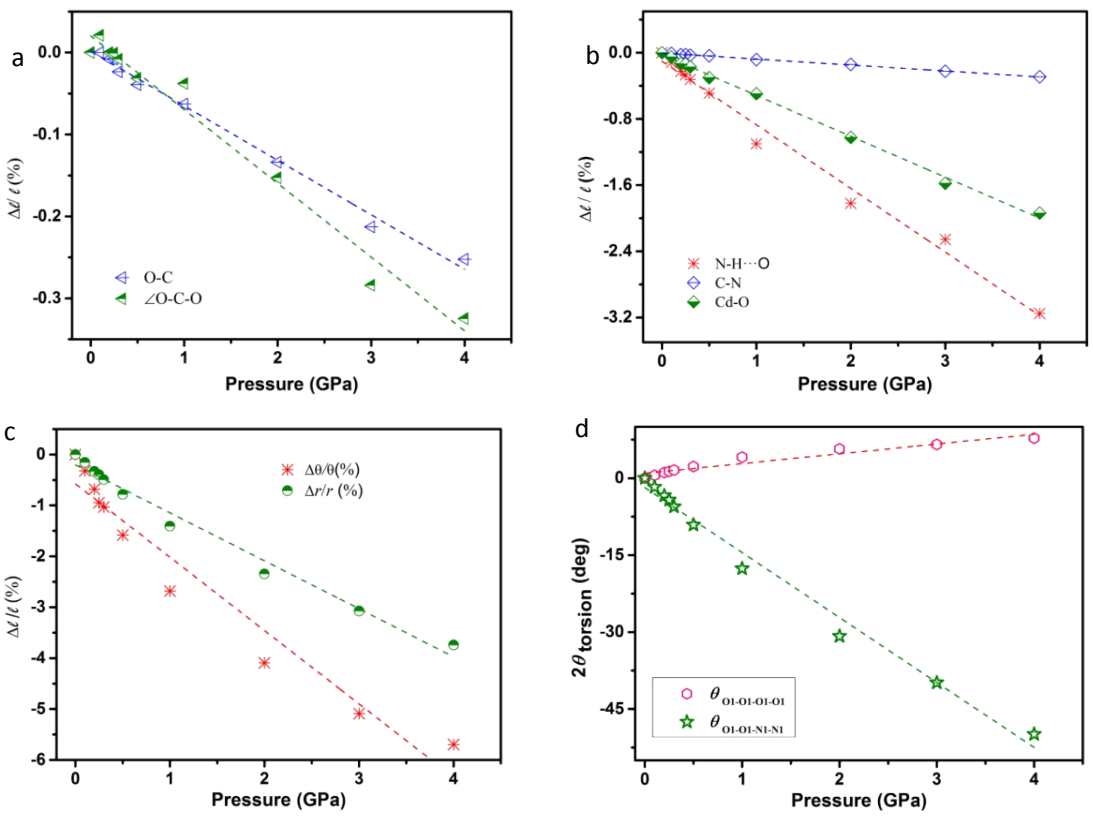

Figure S5. Relative changes of the bond lengths and angles in (a) and (b); Relative changes in the hinging angles (c) and in formate-Gua and octahedral torsion angles (d).

Table S4. Calculated elastic stiffness constant matrix C_{ij} (GPa), compliance constant matrix S_{ij} (GPa^{-1}) and Poisson's ratio v for CdGF.

Elastic Stiffness Constants C_{ij} (GPa)

$$\begin{pmatrix} 76.93731 & 44.28938 & 19.11264 & -5.11143 & 0.00000 & 0.00000 \\ 44.28938 & 76.93731 & 19.11264 & 5.11143 & 0.00000 & 0.00000 \\ 19.11264 & 19.11264 & 15.67069 & 0.00000 & 0.00000 & 0.00000 \\ -5.11143 & 5.11143 & 0.00000 & 11.85205 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 11.85205 & -5.11143 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & -5.11143 & 16.32396 \end{pmatrix}$$

Elastic Compliance Constants S_{ij} (1/GPa)

$$\begin{pmatrix} 24.4079 & -11.0040 & -16.3479 & 15.2721 & 0.0000 & 0.0000 \\ -11.0040 & 24.4079 & -16.3479 & -15.2721 & 0.0000 & 0.0000 \\ -16.3479 & -16.3479 & 103.6906 & 0.0000 & 0.0000 & 0.0000 \\ 15.2721 & -15.2721 & 0.0000 & 97.5464 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 97.5464 & 30.5441 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 30.5441 & 70.8237 \end{pmatrix} \times \mathbf{10^{-3}}$$

The computational C_{ij}'s apparently satisfy the fundamental elastic stability criteria in a trigonal crystal,

$C_{ij} > 0$, i=j;

$C_{11} > |C_{12}|$;

$(C_{11}+C_{12})\, C_{33}-2\, C^2_{13} > 0$;

$(C_{11}-C_{12})\, C_{44}-2\, C^2_{14} > 0$.

Poisson ratios:

$\square v_{ab}=v_{ba}= 0.45$, $\square v_{ca}=v_{cb}= 0.16$, $\square v_{ac}=v_{bc}= 0.67$

Table S5. Summary of the elastic properties of trigonal CdGF. All the elastic constants are obtained from DFT calculations and the unit is GPa. The Young's modulus, shear modulus, and Poisson's ratio were determined using the *ELAM* program. The value of $A_X = X_{max}/X_{min}$ denotes the anisotropy of X.

Elastic constants ($\boldsymbol{C}_{ij}$)		C_{11}	C_{33}	C_{44}	C_{12}	C_{13}	C_{14}			
CdGF	LDA	119.138	19.620	17.736	33.272	25.082	-3.819			
	GGA	76.937	15.671	11.852	44.289	19.111	-5.111			
Elastic properties		E (GPa)		A_E	G (GPa)		A_G	ν		A_ν
		E_{max}	E_{min}		G_{max}	G_{min}		ν_{max}	ν_{min}	
CdGF		54.33	9.64	5.6	19.7	6.1	3.2	0.89	-0.01	89

References

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