Supporting information

Mechanical Properties of a Copper Dietary Supplement, Copper Glycinate Hydrate

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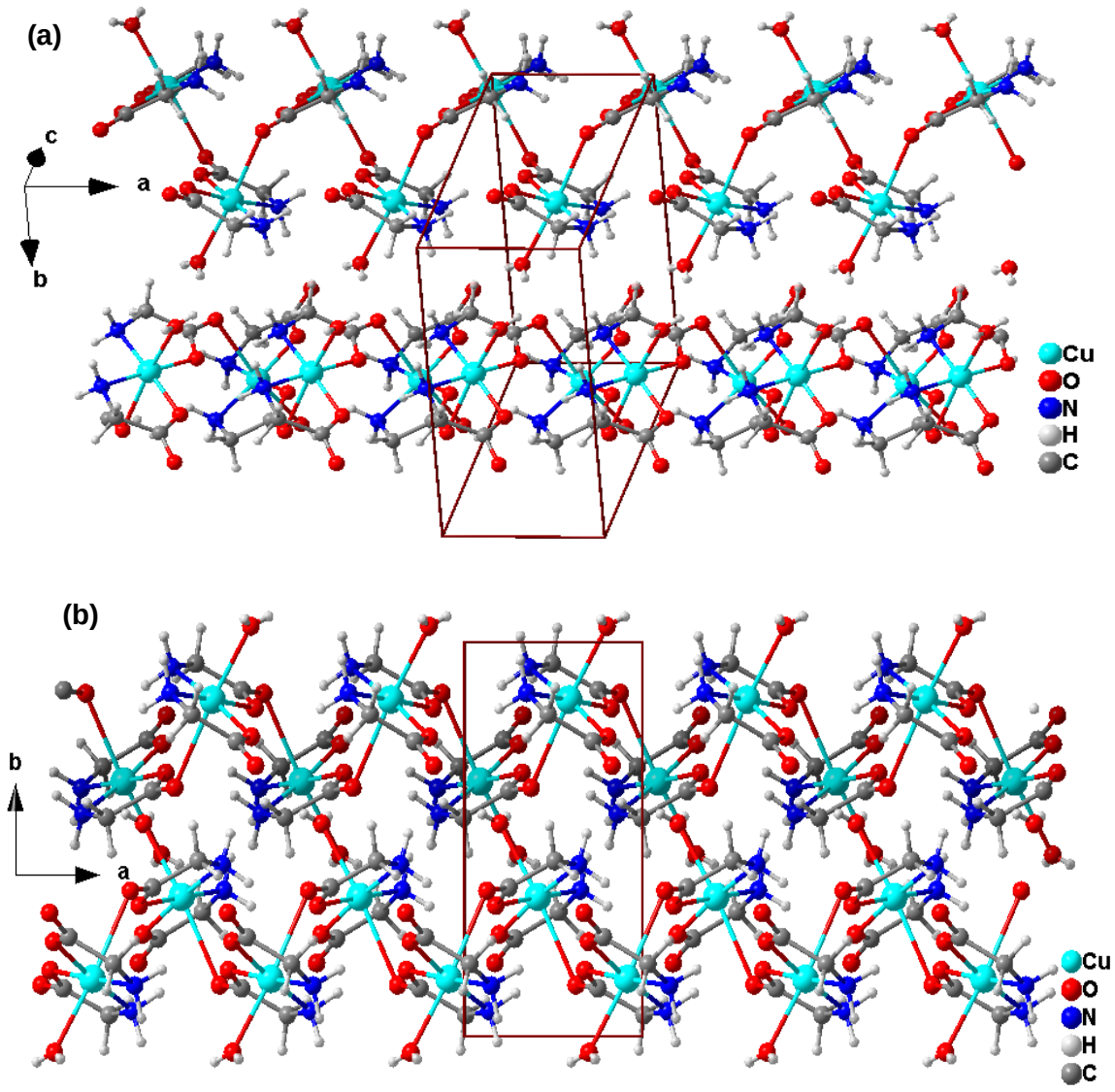

Fig. S1. Crystal structure of Cu-Gly. (a) The chains view in *abc*-plane while chains extending to *a*-axis. (b) The chains view in *ab*-plane while chains extending to *a*-axis. Color scheme: Cu, Turquoise; O, red; C, gray-40%; N, blue and H, gray-25%

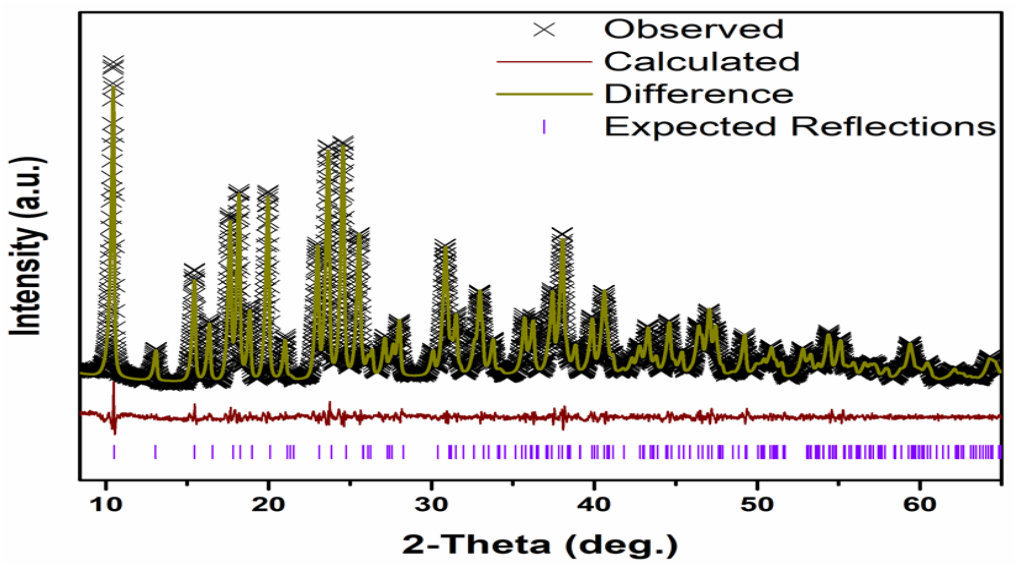

Fig. S2. The patterns of Cu-Gly refined using Le Bail method to indicate its purity at ambient conditions. Black crosses: observed X-ray powder diffraction, Wine line: calculated profile; Greenish yellow line: the difference between observed data and calculated profile. The Purple vertical markers indicate the allowed Bragg reflections. The cell parameters were determined to be a = 5.229(3) Å, b = 10.823(6) Å, c = 13.507(9) Å, V = 764.6(8) $Å^3$.

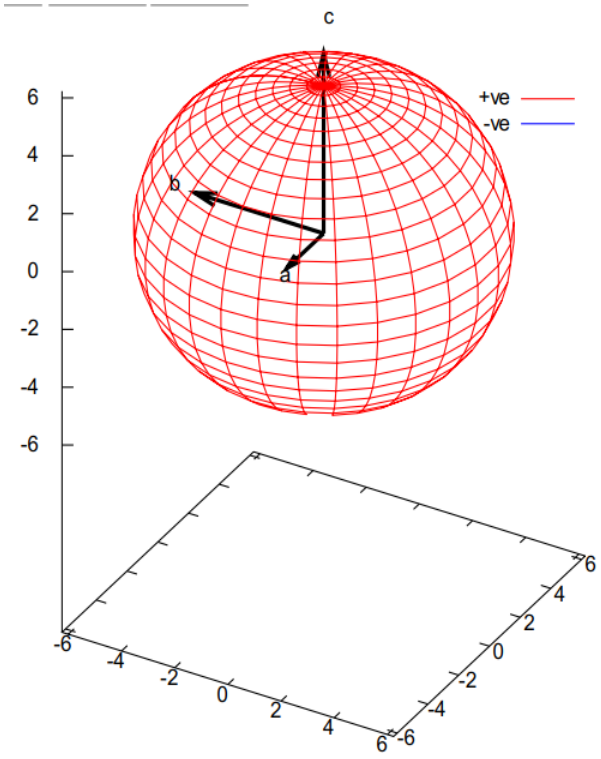

Fig. S3. The compressibility indicatrix for pressure range (0–13.65 GPa), while the magnitudes of corresponding compressibility K_{X1}, K_{X2} and K_{X3} are mentioned. The red values correspond to positive linear compressibility (PLC) and blue shows negative linear compressibility (NLC).

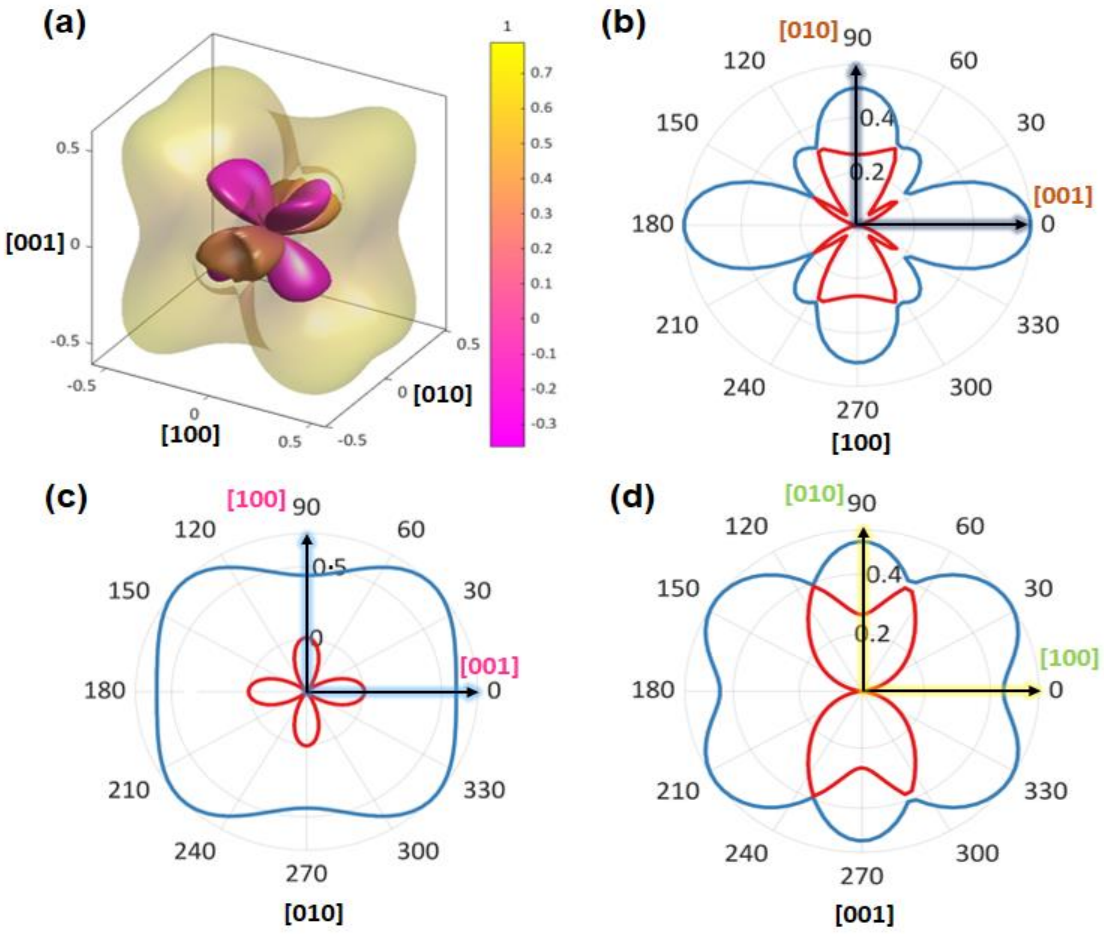

Fig. S4. Surface contours of direction depended Poisson's ratios: (a) 3D view; (b) 2D view projected normal to the (100) plane. (c) 2D view projected normal to the (010) plane. (d) 2D view projected normal to the (001) plane.

Table S1. The elastic moduli (E) and Poisson's ratios (v) extracted from the DFT calculation results.

Elastic modulus		**Shear modulus**			**Poisson's ratios**			
***E* (GPa)**		***G* (GPa)**			***v***			
direction	**value**	**direction**	**max. value**	**min. value**	**direction**	**value**	**direction**	**value**
x	26.28	[100]	23.30	4.54	xy	0.44	xz	0.01
y	15.86	[010]	16.75	4.54	yx	0.27	yz	0.51
z	18.52	[001]	23.30	16.75	zx	0.007	zy	0.59

Table S2. Principal compressibilities and corresponding principal axes were determined using the PASCal software for Cu-Gly.

Principal axis, *i*	**K_{xi} (TPa^{-1})**	**Component of Xi along the crystallographic axes**			**Approximate axis**
		a	***b***	***c***	
1	6.23	0.0000	-1.0000	0.0000	[010]
2	6.13	-1.0000	0.0000	0.0000	[100]
3	5.10	0.0000	0.0000	1.0000	[001]

Table S3. The experimental results of compressibility K_{X1}, K_{X2} and K_{X3} as a function of pressure.

Pressure (GPa)	Compressibility (TPa^{-1})		
	K_{X1}	K_{X2}	K_{X3}
0.00	----	----	----
0.30	27.90	14.54	12.93
0.43	22.76	12.93	11.39
0.58	19.09	11.68	10.21
0.85	15.28	10.28	8.90
1.36	11.64	8.79	7.52
2.09	9.11	7.63	6.45
3.15	7.19	6.65	5.57
4.03	6.23	6.13	5.10
5.03	5.49	5.69	4.71
6.92	4.57	5.12	4.21
7.99	4.20	4.88	4.00
9.37	3.83	4.63	3.77
13.25	3.14	4.13	3.33

Table S4. The lattice parameters of Cu-Gly under different pressures extracted from HP-PXRD experiments.

P (GPa)	***a* (Å)**	***b* (Å)**	***c* (Å)**	***V* (Å^3)**
0.00	5.229(4)	10.823(10)	13.507(23)	764.4(6)
0.30	5.204(5)	10.723(13)	13.477(23)	752.2(7)
0.43	5.196(4)	10.673(13)	13.467(24)	747.0(7)
0.58	5.187(4)	10.632(12)	13.436(24)	741.1(7)
0.85	5.159(5)	10.510(11)	13.424(26)	727.9(7)
1.36	5.144(5)	10.429(14)	13.351(29)	716.3(10)
2.09	5.126(4)	10.354(11)	13.311(33)	706.5(10)
3.15	5.089(6)	10.252(17)	13.208(43)	689.3(17)
4.03	5.050(5)	10.180(17)	13.093(52)	673.2(20)
5.03	5.028(7)	10.123(18)	12.955(54)	659.5(21)
6.92	4.998(7)	10.072(21)	12.789(43)	643.9(17)
7.99	4.980(8)	10.033(23)	12.718(46)	635.6(19)
9.37	4.949(10)	9.976(33)	12.602(48)	622.3(24)
13.25	4.900(17)	9.862(62)	12.470(50)	602.6(40)