Supporting Information

Compression behavior and vibrational properties of new energetic material LLM-105 analyzed using the dispersion-corrected density functional theory

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Table S1. Characteristics of vibrational modes in LLM-105 crystal at ambient pressure. dν/dp is slope of pressure-induced Raman shift. Abbreviation: st: stretch, sci: scissor, tw: twist, bre: breathe, def: deformation, sym: symmetric, asym: asymmetric.

Mode	Wavenumber/cm^{-1}			Assignments	dν/dp/cm^{-1} GPa^{-1}	
	A_g	B_g	Expt.[S1]		This work	Expt. [S1]
ν_1	3456	3456	3439	NH_2 asym. st.	-0.31	
ν_2	3414	3416	3403	NH_2 asym. st.	-2.44	
ν_3	3257	3257	3300	NH_2 sym. st.	-6.33	
ν_4	3238	3245	3281	NH_2 sym. st.	-6.13	
ν_5	1614	1620	1650	NH_2 sci., C-NH_2 st.	4.40	5.04
ν_6	1575	1577	1643	NH_2 sci., C-NH_2 st.	3.53	4.86
ν_7	1518	1509	1600	NH_2 sci.	3.39	3.96
ν_8	1495	1495	1566	NH_2 sci.	3.17	3.42
ν_9	1455	1459	1551	NH_2 sci., ring def.	4.24	2.70
ν_{10}	1436	1437	1519	NO_2 st., NH_2 sci., ring def.	3.23	3.78
ν_{11}	1409	1432	1499	NH_2 sci., NO_2 st.	3.02	3.96
ν_{12}	1393	1408	1474	NH_2 sci., NO_2 st.	1.26	3.96
ν_{13}	1350	1354	1456	HN_2 rock, ring st.	4.86	2.52
ν_{14}	1333	1337		HN_2 sci., ring st.	3.79	
ν_{15}	1275	1281	1378	HN_2 rock, ring bre., NO_2 st.	5.41	5.94
ν_{16}	1249	1249	1265	HN_2 sci., ring bre., NO_2 st.	3.13	3.06
ν_{17}	1192	1204	1251	HN_2 sci., ring def., NO_2 st.	2.69	2.34
ν_{18}	1158	1167	1188	NH_2 rock, N-O rock	3.06	3.42
ν_{19}	1078	1081	1089	HN_2 rock, ring bre.	2.58	3.60
ν_{20}	1039	1040	1062	NH_2 rock, ring st.	1.49	2.34
ν_{21}	896	898	921	NH_2 rock, ring st.	1.26	1.71
ν_{22}	869	866	893	NH_2 rock, ring st., NO_2 st.	3.02	
ν_{23}	794	791	817	NH_2 rock, ring st., NO_2 st.	1.46	1.59
ν_{24}	739	739	759	NH_2 rock, ring def., NO_2 st.	3.93	1.10
ν_{25}	732	732	736	NH_2 tw., ring def., NO_2 st.	1.30	2.45
ν_{26}	715	716	715	NH_2 st., ring st.	2.66	1.35
ν_{27}	709	713	703	NH_2 tw.	1.91	1.84
ν_{28}	696	697		NH_2 rock, ring def., NO_2 tw.	2.25	
ν_{29}	686	691		NH_2 tw.	1.84	
ν_{30}	681	681		NH_2 tw.	1.89	
ν_{31}	673	674	637	NH_2 tw., ring def., NO_2 tw.	0.09	0.98
ν_{32}	617	617		NH_2 tw.	2.97	
ν_{33}	574	576	560	NH_2 wag	5.34	3.92
ν_{34}	552	552	544	NH_2 wag	5.30	0.98
ν_{35}	531	533		NH_2 tw., ring def.	1.63	
ν_{36}	530	531		NH_2 wag	0.80	
ν_{37}	472	476	485	NH_2 tw., ring def., NO_2 tw.	3.63	3.92
ν_{38}	426	426	434	NH_2 tw., ring def., NO_2 tw.	1.13	1.75

ν_{39}	396	401	415	HN_2 rock	1.85	2.96
ν_{40}	370	372	379	HN_2 rock	3.13	2.85
ν_{41}	361	360	354	HN_2 rock, NO_2 sci.	2.48	3.95
ν_{42}	349	346	344	NH_2 st., ring def., NO_2 st.	3.14	3.07
ν_{43}	342	339	336	NH_2 tw., ring def., NO_2 tw.	3.41	
ν_{44}	332	329	272	NH_2 tw., ring def., NO_2 tw.	3.17	
ν_{45}	269	275	267	NH_2 wag, ring def.	2.35	2.74
ν_{46}	191	210	196	NH_2 tw., ring def., NO_2 rock	6.41	
ν_{47}	160	180	179	lattice vibration	9.24	6.36
ν_{48}	157	151	172	lattice vibration	7.78	
ν_{49}	139	130	145	NH_2 tw., ring def., NO_2 tw.	8.20	6.47
ν_{50}	117	126		NO_2 rock	8.36	
ν_{51}	106	111	110	lattice vibration	7.51	7.78
ν_{52}	103	107	100	lattice vibration	6.89	
ν_{53}	84	91	88	lattice vibration	7.69	6.69
ν_{54}	77	86	76	lattice vibration	4.06	7.13
ν_{55}	70	72	60	NH_2 rock, ring rock, NO_2 rock	3.76	4.60
ν_{56}	61	59	51	lattice vibration	1.34	4.28
ν_{57}	37	29		lattice vibration	2.20	

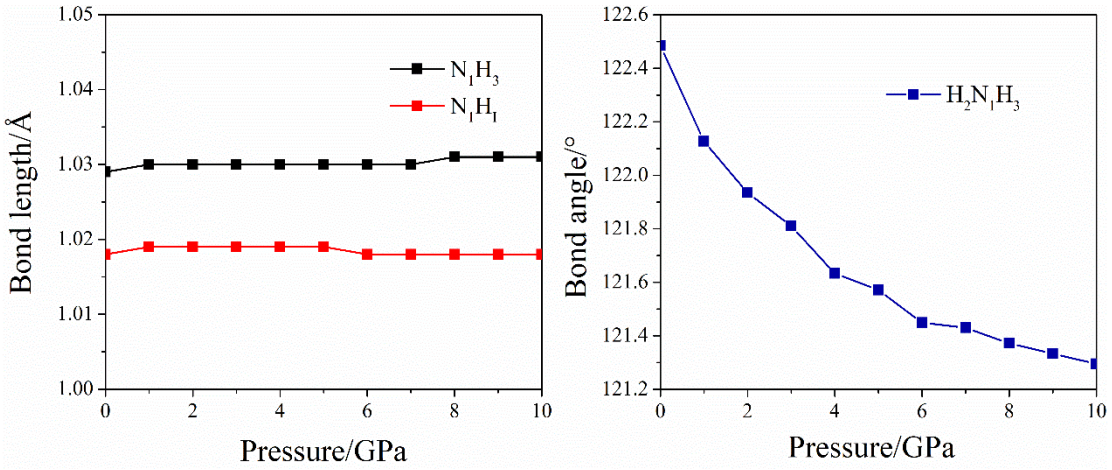

Figure S1. The evolutions of NH_2 bond length and angle of LLM-105 molecular under hydrostatic pressure.

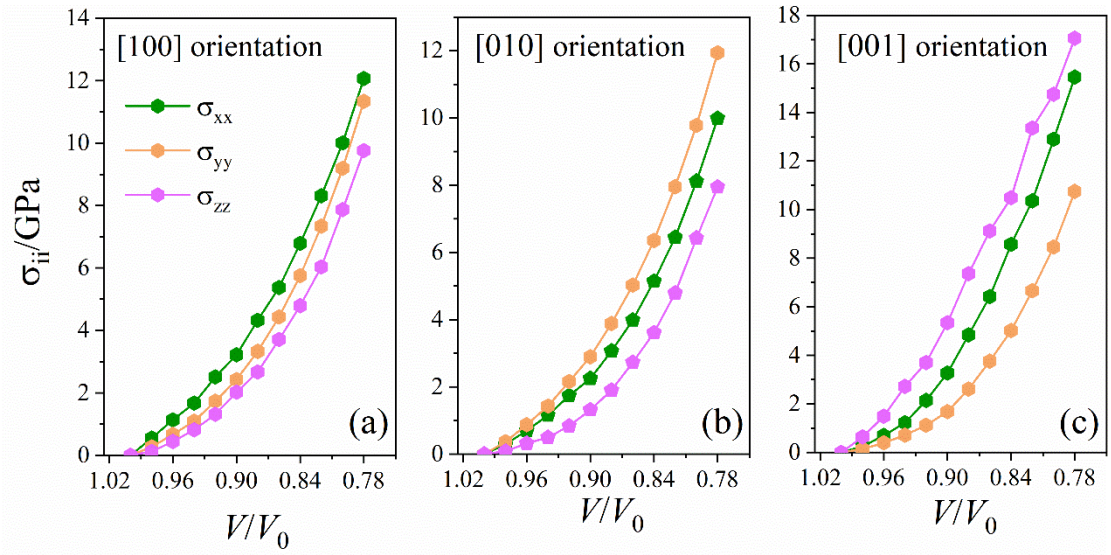

Figure S2. Three principal stresses σ_{xx}, σ_{yy} and σ_{zz} as function of compression ratio V/V_0 under uniaxial loading.

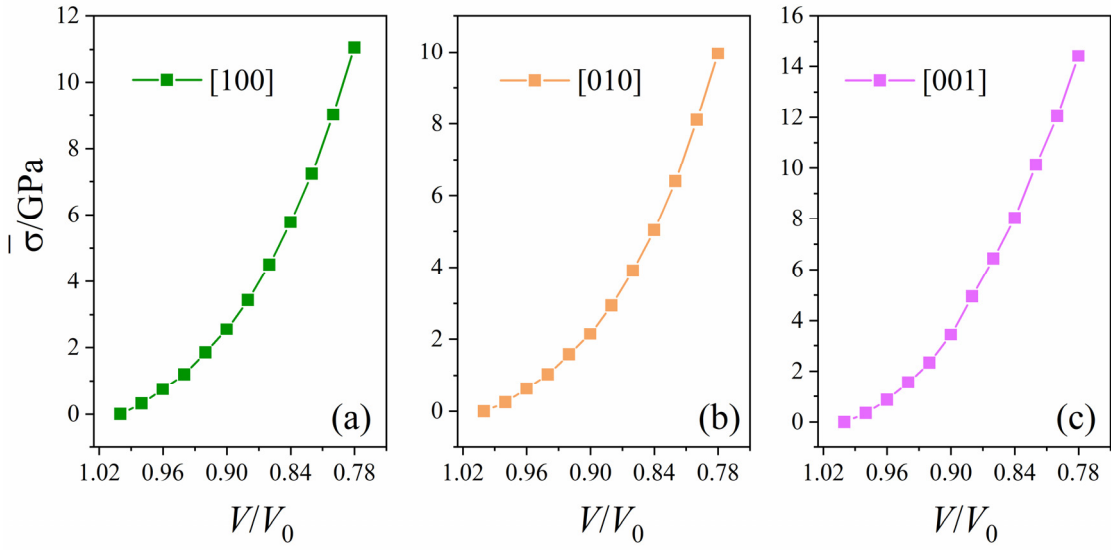

Figure S3. The average principal stress $\bar{\sigma}$ as function of compression ratio V/V_0 under different uniaxial loading.

References

S1. Xu, Z., et al., Pressure- and Temperature-Dependent Structural Stability of LLM-105 Crystal. *The Journal of Physical Chemistry C* **2018**, *123*, 1110-1119.