# Supporting Information

# Tunable Piezochromic Luminescence via Isomer Control in N,N'-Azotriazole Energetic molecules

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**Sample preparation :**

4,4'-azoAzo-1,2,4-triazole: Acetic acid was added to a solution of sodium dichloroisocyanurate (SDIC) in water with vigorous stirring at 30 °C for 1 h. After this time, 4-amino-1,2,4-triazole dissolved in water was added at 7 °C. The reaction was continued at 15 °C for 1 h. The mixture was cooled, and the precipitate filtered off, product was obtained.[1]

1,1'-azoAzo-1,2,3-triazole : 1-aminoAmino-1,2,3-triazole was dissolved in 40 ml $CH_3CN$. The solution was cooled at -2~0 °C and a solution of sodium dichloroisocyanurate in water and $CH_3COOH$ was added dropwise. The reaction was continued at 0 °C for 30 min. The solution was neutralised with $NaHCO_3$, then filtrated to remove insoluble solids. The product isolated as a little yellow solid was obtained after recrystallization from acetone.[2]

**Methods :**

*diamond Diamond anvil cell (DAC):* High-pressure experiments were performed using a diamond anvil cell (DAC). The sample was loaded into a hole (diameter: 150 μm) of a T301 steel gasket, which is pre-pressed to a thickness of 45 μm. A ruby sphere was placed in the sample chamber for in situ pressure calibration by the R1 fluorescence method.

*in In situ high-pressure PL and UV-Vis:* In the in situ high-pressure PL and luminescence photographs experiments, we used a 355 nm laser as the excitation source. UV-Vis absorption spectra were measured using a deuterium-halogen light source. Excitation spectra were performed with Shimadzu RF-5301PC.

*in In situ high-pressure Raman and FT-IR:* Raman spectra were collected on a Horiba high-resolution Raman spectrometer, the laser wavelength is 532 nm, the laser power was 20 mW, and the spectral resolution was 1.8 $cm^{-1}$. The pressure transition medium (PTM) is silicone oil (Aldrich). KBr is used as PTM in IR experiments. The microscope model used for sample processing was Nikon SMZ745. The whole experiment was performed at room temperature.

Calculations: Calculations of geometrical optimization of 1,1'-azo-1,2,3-triazole and 4,4'-azo-1,2,4-triazole at different pressures according to first-principles plane-wave pseudopotential density functional theory (DFT) implemented in the Vienna ab initio simulation package based on the single-crystal data the packing models reported previously.[1,2] A geometric optimization (VASP) based plane wave basis set and projector augmented wave method were developed. A van der Waals correction of Grimme's DFT-D3 model was also employed. The energy cutoff was set to 500 eV. The Brillouin zone integration is sampled using a Monkhorst-Pack grid centered on Γ, 2 × 3 × 2 for 1,2,3-triazole and 3 × 2 × 2 for 1,2,4-triazole. The bulk structure is fully relaxed until the maximum force on each atom is less than 0.01 eV/Å, with an energy convergence criterion of $10^{-6}$ eV. The Crystal Explorer program version 8 was used to To visualize and analyze the intermolecular interactions in the crystal structures.

**SI Figures :**

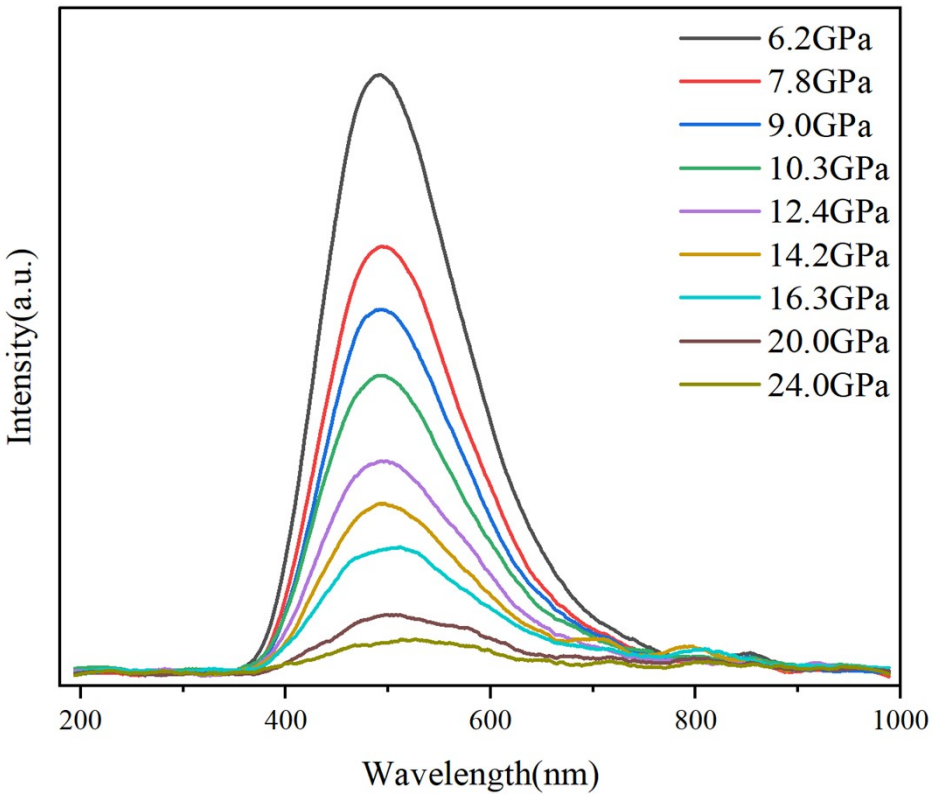


Figure S1. PL spectra of 4,4'-azo-1,2,4-triazole at the pressure of 6.2 GPa-24.0GPa d by a 355 nm laser.

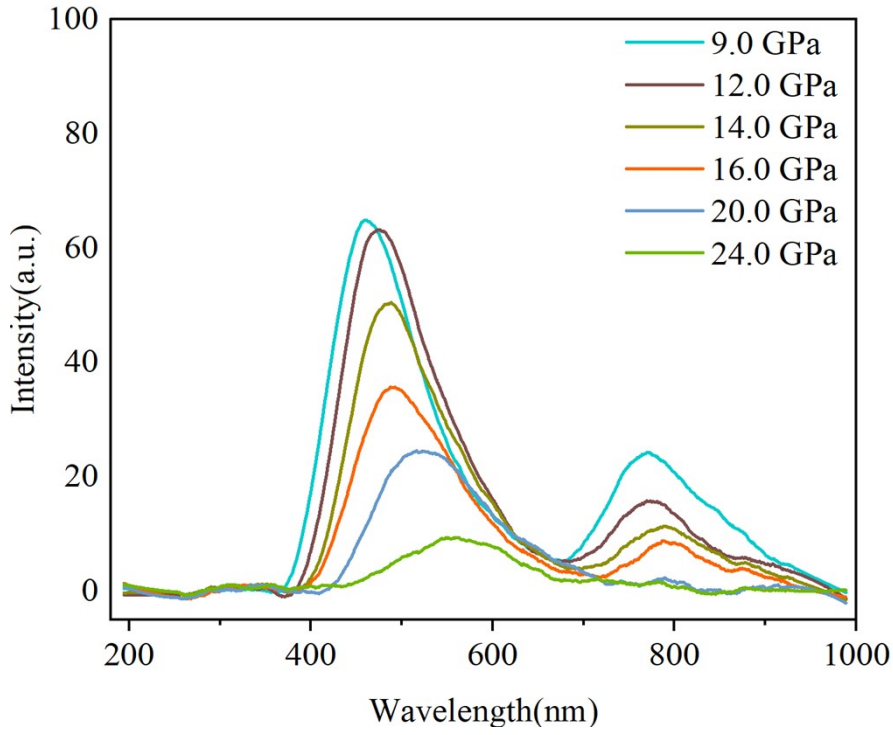

Figure S2. PL spectra of 1,1'-azo-1,2,3-triazole at the pressure of 9.0 GPa-24.0GPa d by a 355 nm laser.

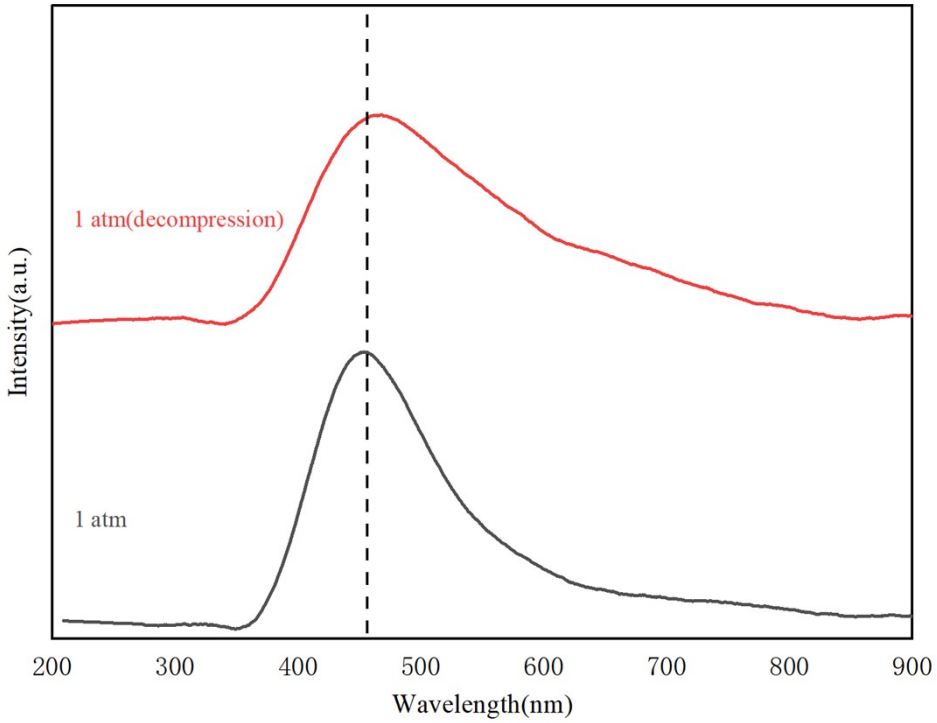


Figure S3. PL spectra of 1,1'-azo-1,2,3-triazole at the pressure of 0 GPa and release pressure of 20 GPa released by a 355 nm laser.

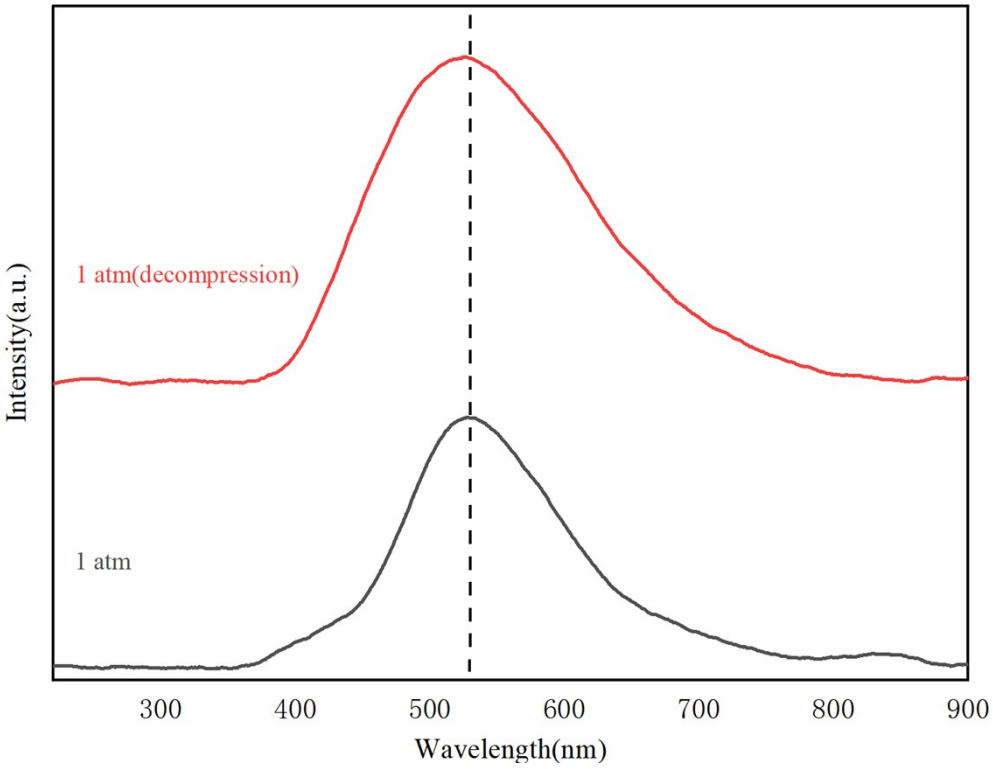

Figure S4. IR of 4,4'-azo-1,2,4-triazole at the pressure of 0 GPa and release pressure of 20 GPa released.

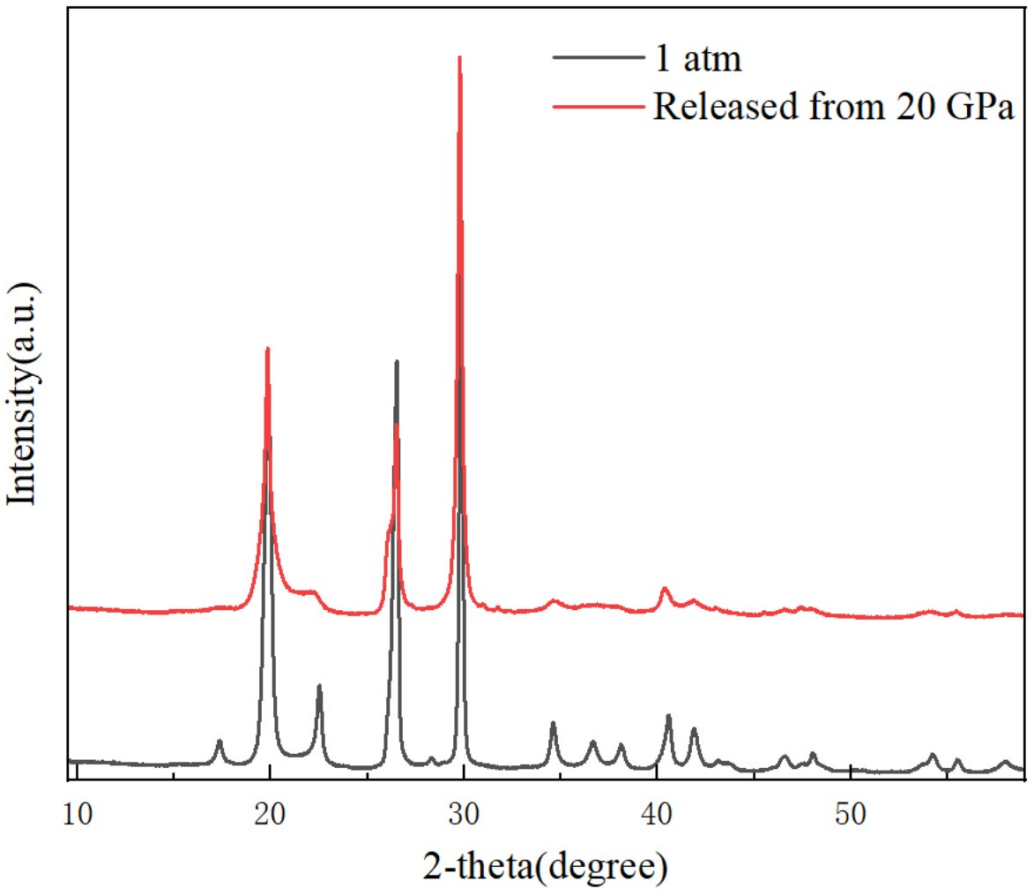


Figure S5. PXRD of 4,4'-azo-1,2,4-triazole at the pressure of 0 GPa and release pressure of 20 GPa released.

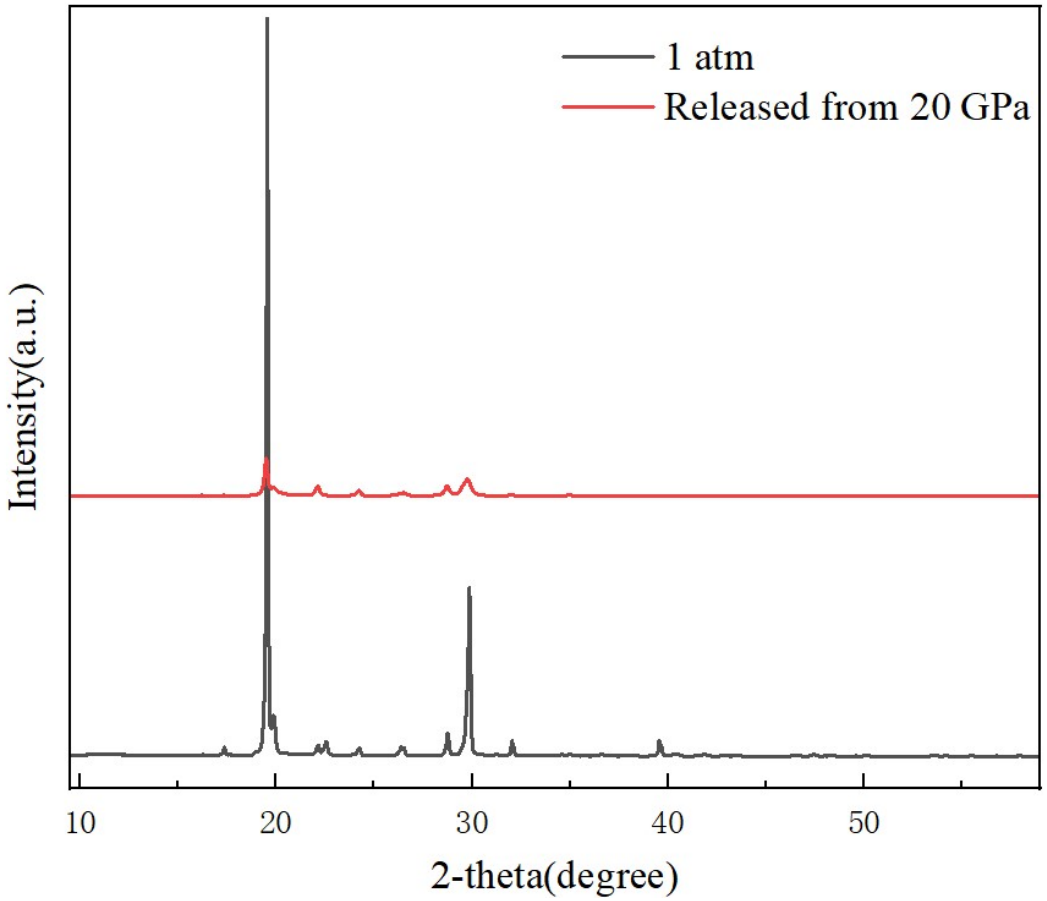


Figure S6. PXRD of 1,1'-azo-1,2,3-triazole at the pressure of 0 GPa and release pressure of 20 GPa released.

## Notes and references

1 C. Qi, S.-H. Li, Y.-C. Li, Y. Wang, X.-K. Chen and S.-P. Pang, J. Mater. Chem, 2011, 21, 3221-3225.

2 Y.-C. Li, C. Qi, S.-H. Li, H.-J. Zhang, C.-H. Sun, Y.-Z. Yu and S.-P. Pang, J. Am. Chem. Soc, 2010, 132, 12172-12173.