

Enhanced Cool White Light Emission in Organic-inorganic Metal Halides through Pressure-Treated Molecular Configurations Regulation

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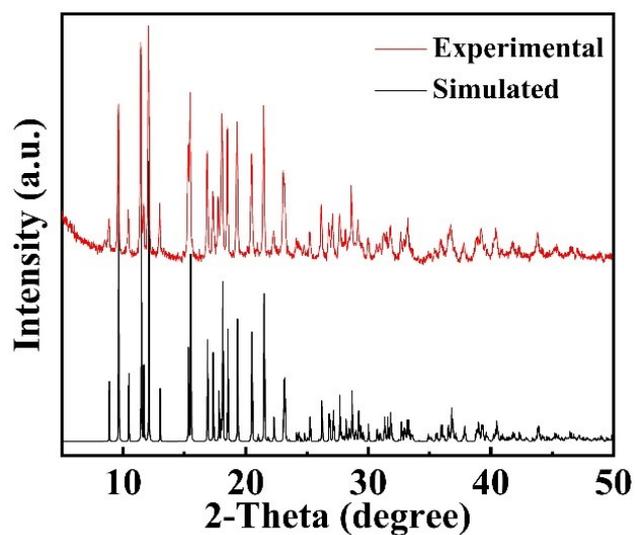


Figure S1. Experimental and simulated XRD patterns of $(\text{ETPP})_2\text{ZrCl}_6$.

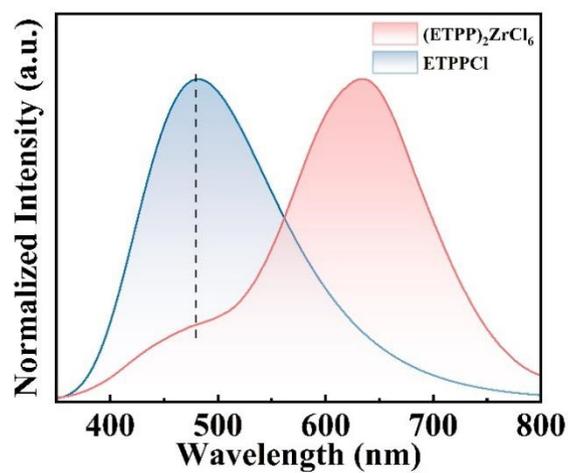


Figure S2. The PL spectra of $(\text{ETPP})_2\text{ZrCl}_6$ and ETPPCl.

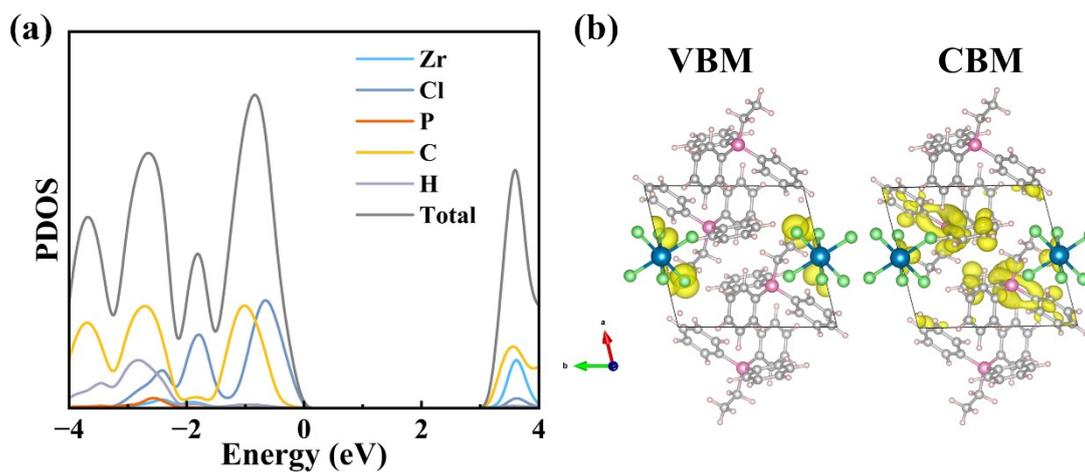


Figure S3. (a) DOS of $(\text{ETPP})_2\text{ZrCl}_6$. (b) The VBM and CBM charge density distribution for $(\text{ETPP})_2\text{ZrCl}_6$.

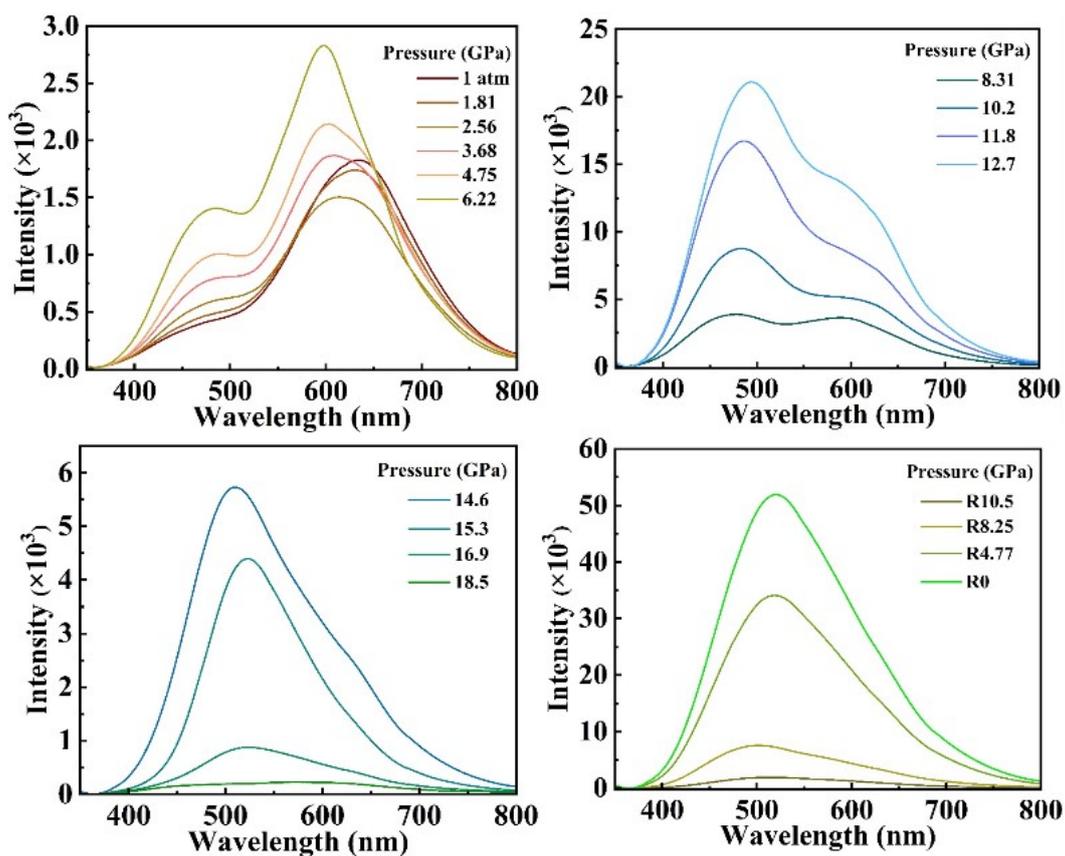


Figure S4. (a-c) PL spectra evolution of $(\text{ETPP})_2\text{ZrCl}_6$ upon compression up to 18.5 GPa. (d) PL spectra of $(\text{ETPP})_2\text{ZrCl}_6$ collected after decompression.

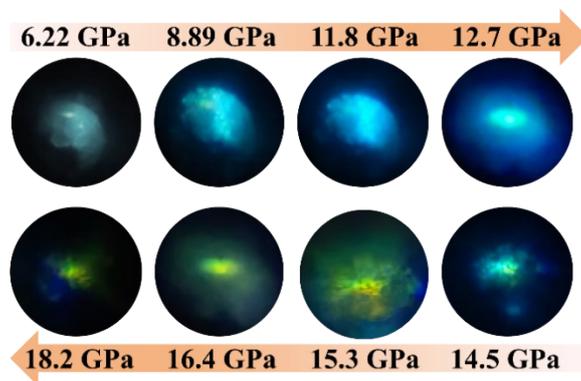


Figure S5. The PL micrographs of the $(\text{ETPP})_2\text{ZrCl}_6$ crystal at selected pressures.

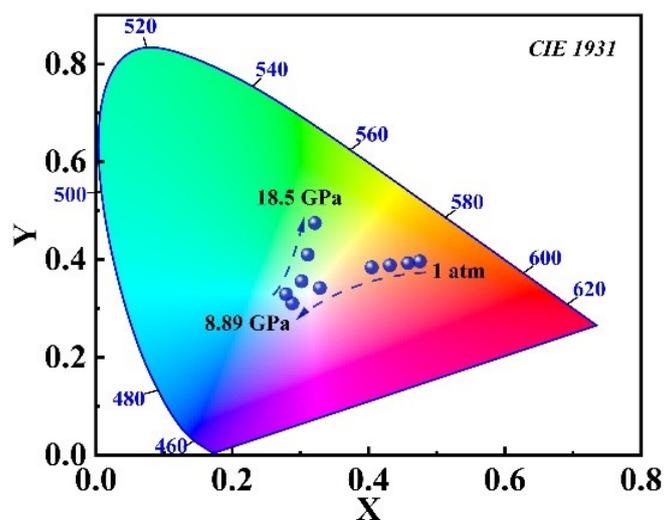


Figure S6. Pressure-dependent chromaticity coordinates of the emissions.

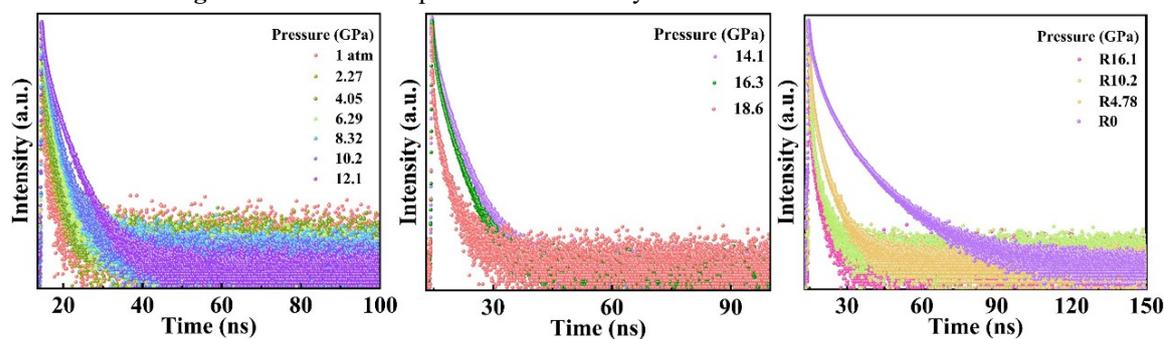
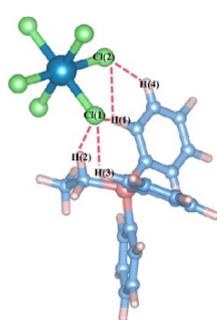


Figure S7. Normalized PL decay curves at different pressures.



$d(\text{H-Cl})$ (Å)	0 GPa	8 GPa	12 GPa	16 GPa
H(1)-Cl(1)	2.8482	2.4975	2.4469	2.3942
H(2)-Cl(1)	2.7440	2.2807	2.2248	2.1821
H(3)-Cl(1)	3.3570	2.6108	2.7008	2.7869
H(1)-Cl(2)	3.1504	2.6556	2.4623	2.3536
H(4)-Cl(2)	3.0200	2.4923	2.4110	2.3427

Figure S8. The distances between different Cl and H atoms under pressure.

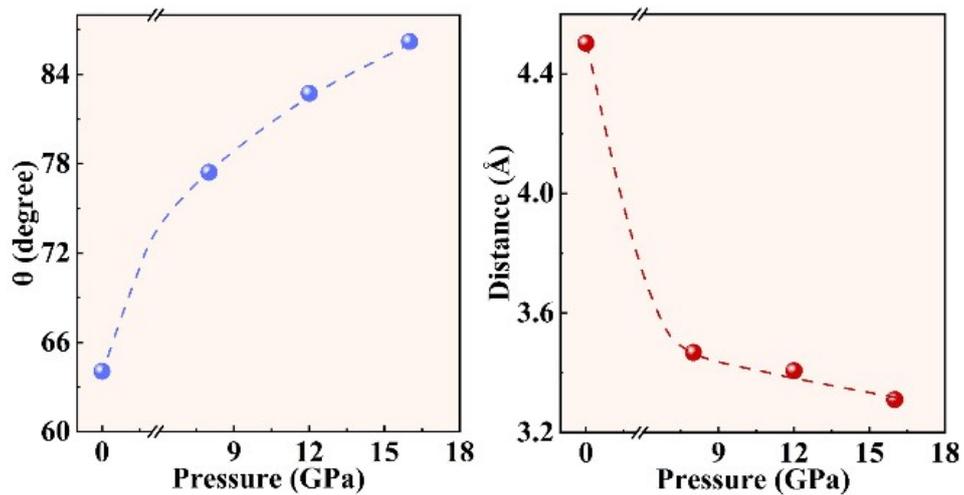


Figure S9. The dislocation angle (a) and interplanar spacing (b) of benzene rings under pressure.

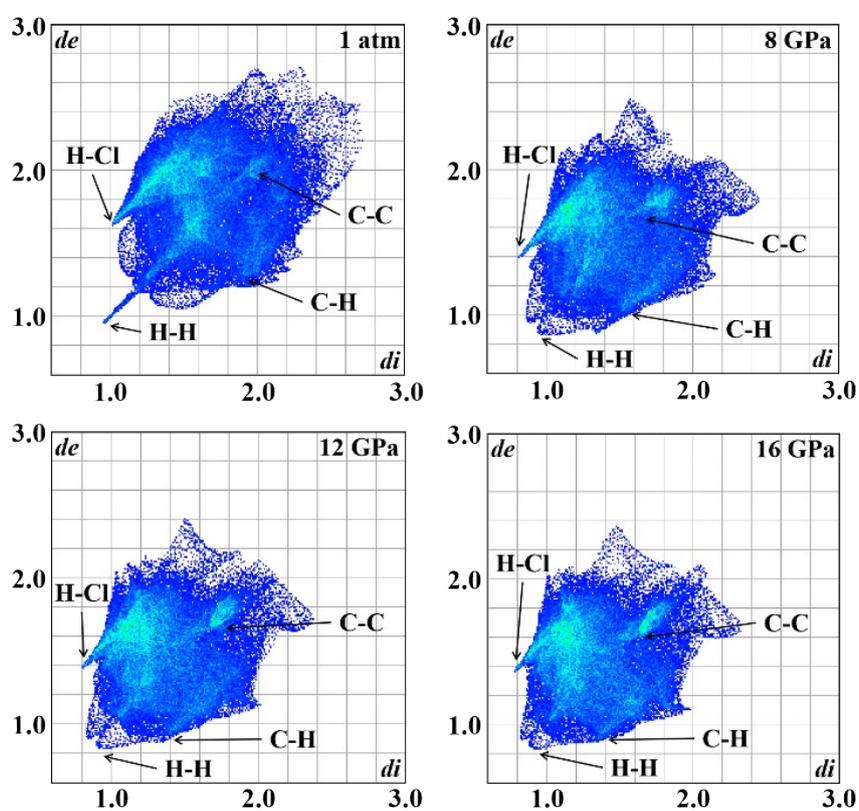


Figure S10. Fingerprint plot for the calculated structure at (a) 1 atm, (b) 8 GPa, (c) 12 GPa and (d) 16 GPa.

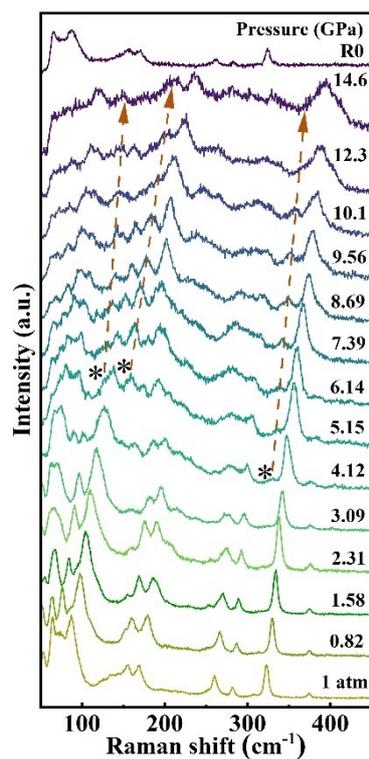


Figure S11. Raman spectra of inorganic octahedra in $(\text{ETPP})_2\text{ZrCl}_6$ during compression.

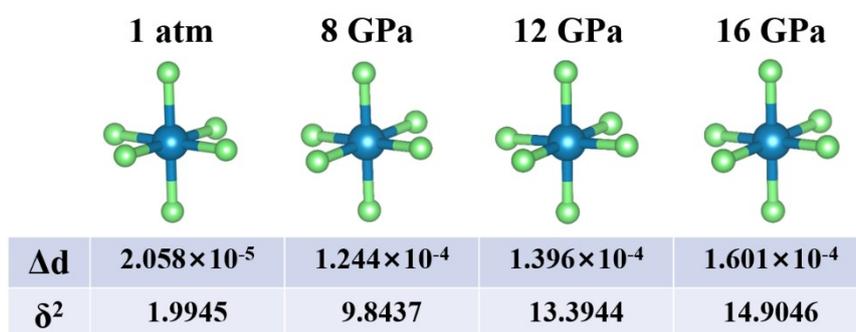


Figure S12. Pressure-dependent bond length distortion (Δd) and bond angle distortion (δ^2) in $(\text{ETPP})_2\text{ZrCl}_6$.

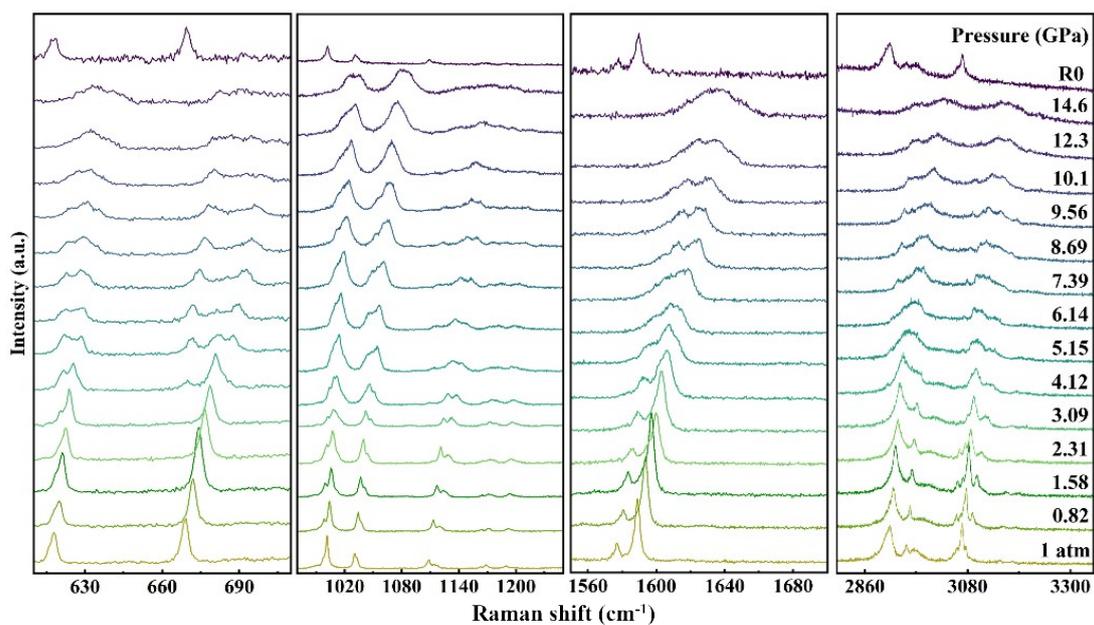


Figure S13. Raman spectra of [ETPP]⁺ cations in (ETPP)₂ZrCl₆ during compression.

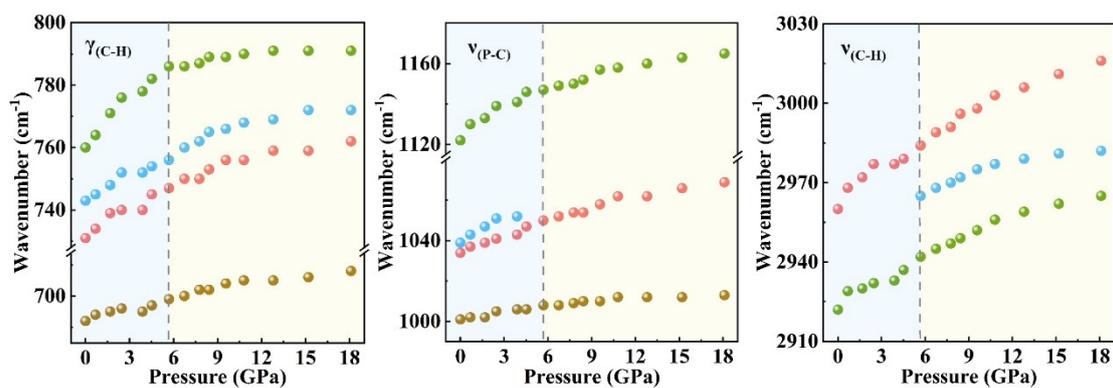


Figure S14. The corresponding wavenumber of IR peaks at different pressures.

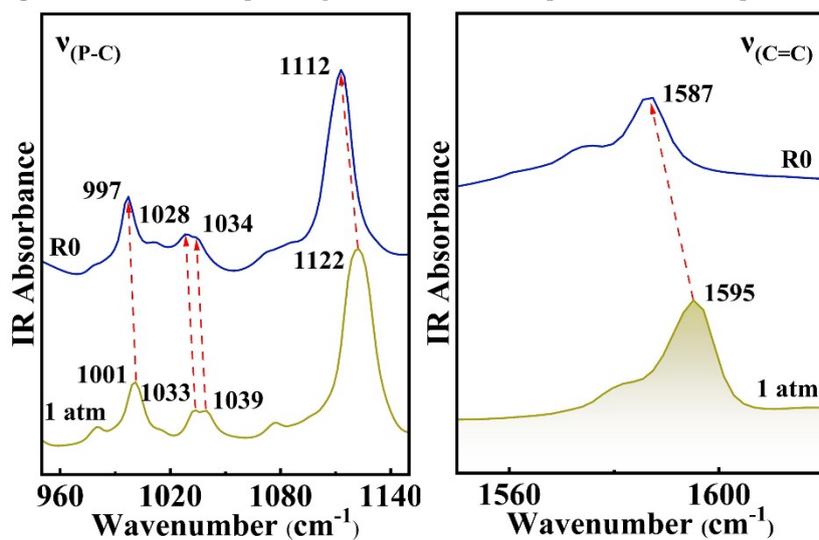


Figure S15. IR spectra of (ETPP)₂ZrCl₆ under ambient pressure and after pressure released.