Electronic Supplementary Material (ESI) for RSC Advances.


# Prediction of novel crystal structures and superconductivity of compressed HBr

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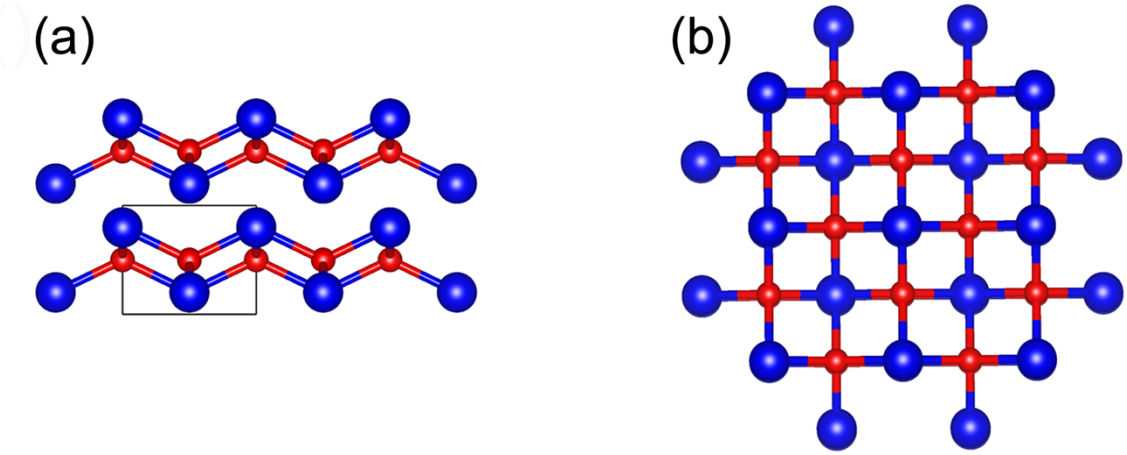


**Fig. S1** predicted *Pmmn* structure at 300GPa.

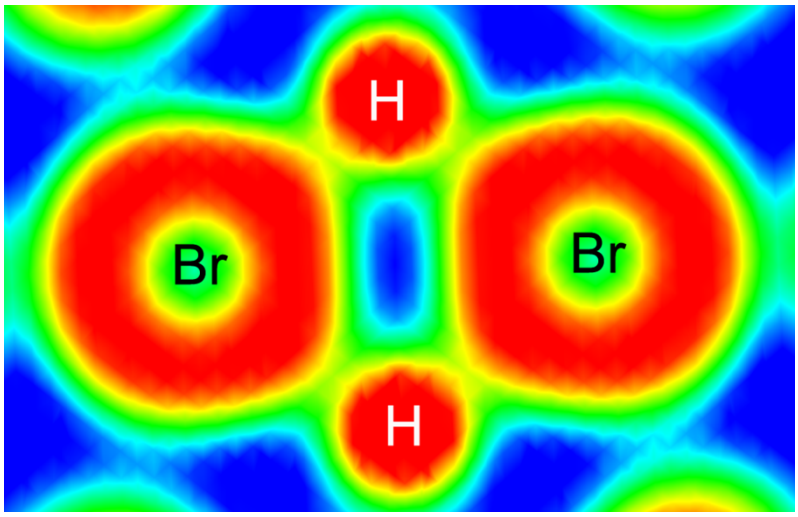


**Fig. S2.** Calculated ELF of *Pmmn* structure at 300GPa.

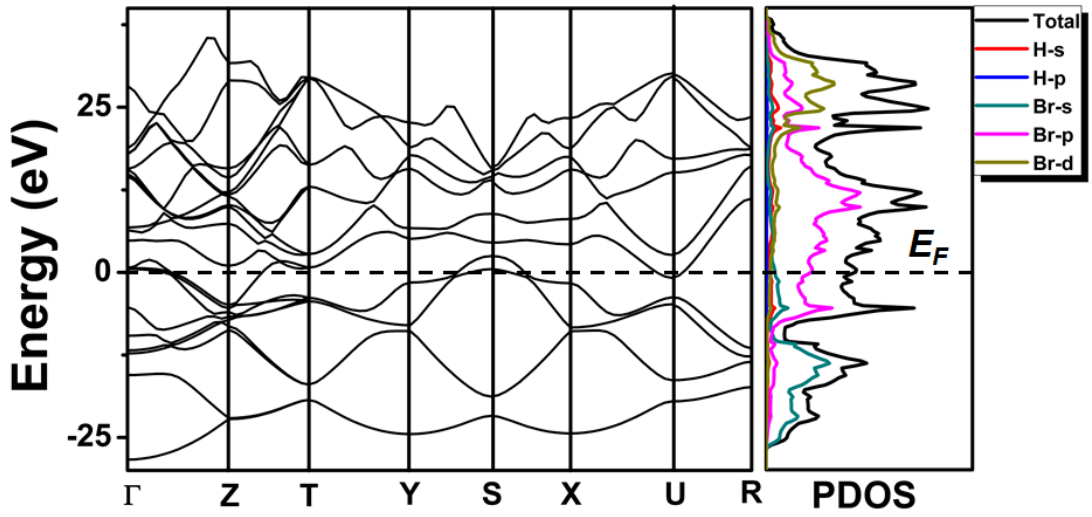


**Fig. S3** Calculated the electron properties of predicted *Pmmn* structure.

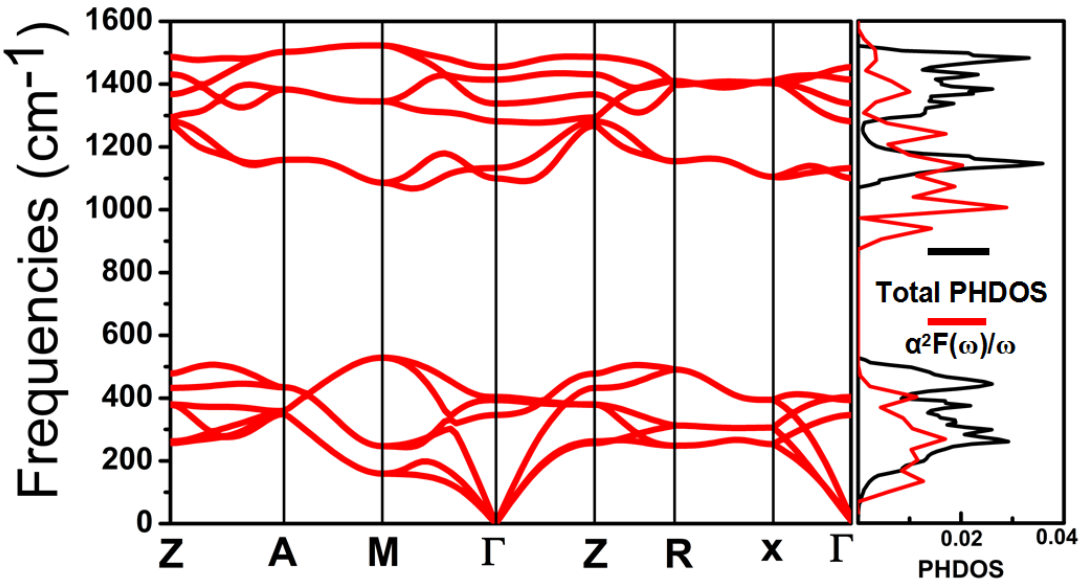


**Fig. S4** The phonon spectrum, phonon density of states and Eliashberg phonons spectral function for *Pmmn* structure.

Table I. optimized structure lattice and atomic positions of *I*-42*d*, *C*2/*m* and *Pmmn* structures.

| structures | Lattice (Å, degree) | Atomic positions | | | |
|---|---|---|---|---|---|
| *I*-42*d* | a=b=c=5.6644, | Br | 1.13093 | 2.33831 | 1.75524 |
| | α=β=118.3354 | H | -0.11601 | 0.88399 | 0 |
| | γ=92.9081 | H | -0.125 | 0.83099 | 0.45599 |
| *C*2/*m* | a=b=2.5919, c=4.0851, | Br | 0.15547 | 0.15547 | 0.10262 |
| | α=β=100.7282, | H | 0.30147 | 0.30147 | 0.72946 |
| | γ=72.9573 | | | | |
| *Pmmn* | a=b=3.0338,c=2.4565 | Br | 0 | 0 | 0.49831 |
| | α=β=γ=90 | H | 0 | 0 | 0.79935 |