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Pressure-induced hydrogen bond symmetrization in hydrogen halids HX (X=F, Cl, and Br): *ab initio* Study TIAN CUI, DEFANG DUAN, FUBO TIAN, LIANCHENG WANG, XING MENG, YANMING MA, BINGBING LIU, ZHI HE, GUANGTIAN ZOU, State key Laboratory of Superhard Materials, College of Physics, Jilin University, People's Republic of China — Although hydrogen bond symmetrization of HX (X=F, Cl, and Br) have been observed, the symmetric structure is still not direct measured by X-ray or neutron diffraction studies. The changes in hydrogen bonding of HX have been examined by pseudopotential plane-wave method. Our results show that the hydrogen bond symmetrization of HBr and HCl occurred at 25 GPa and 40 GPa, agree well with the experimental data. In the case of HF, symmetric structure happened at 30 GPa, which is higher than the experimental value of 6 GPa. Further calculation show that the hydrogen bond symmetrization is accompanied by a successive change of the potential surface in the X-H$\cdots$X direction from double-well potential to symmetric single-well potential. In addition, the stretching mode A1 of HX decreases with increasing pressure. The hydrogen bond symmetrization process is characterized as a softening of stretching vibration A1.

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