Quantum Electronic Pressure in Crystals with Cl…Cl, Br…Br, I…I Halogen Bonds under the External Hydrostatic Pressure

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The electron density and the energy characteristics determined by it are the main objects of analysis to establish the characteristics of chemical bonds and the principles of spatial organization of molecular crystals. As a characteristic of electron density in real space of crystals under pressure, the quantum electron pressure function QEP(**r**) [1,2] was used. Physically QEP(**r**) characterizes the variation of the internal energy under a local deformation that changes the volume of a small element of the electron continuum without changing its shape.

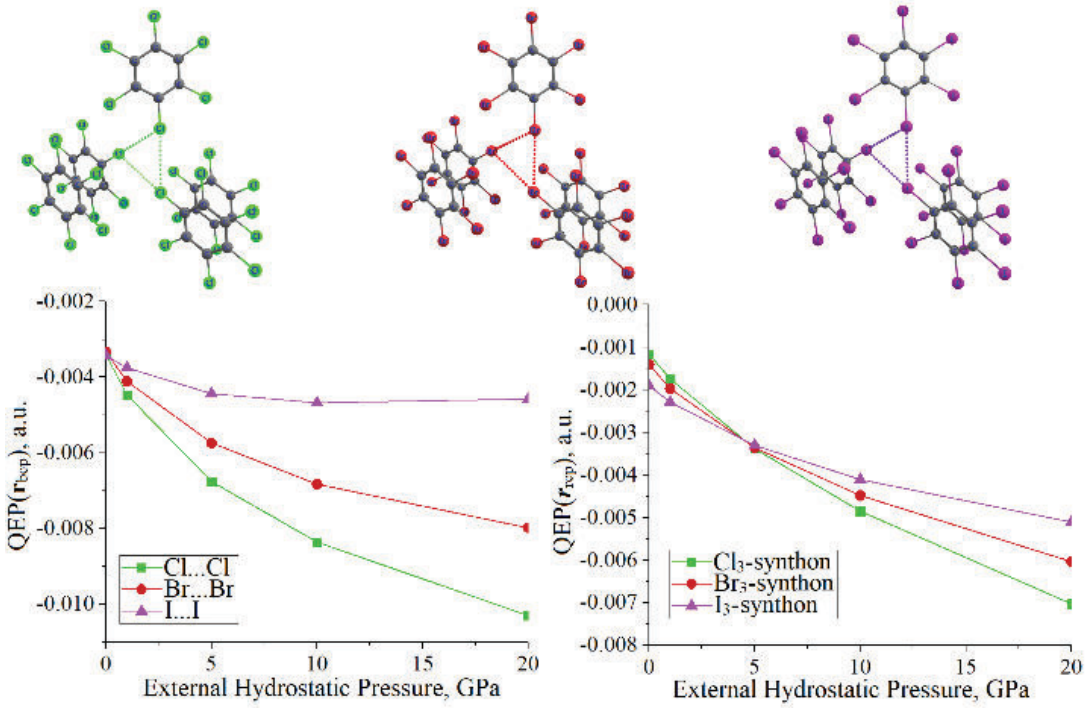

Figure 1: Change in the values of QEP(**r**) at the bond and ring critical points of a) the halogen bonds and b) the centers of Hal_3-synthons with external hydrostatic pressure increasing

A comparison of the QEP(r) function at the critical points of electron density for Hal_3-synthons and interlayer Hal…Hal interactions, of the C_6Cl_6, C_6Br_6, and C_6I_6 crystals at an external hydrostatic pressure of 1, 5, 10, 20 GPa were carried out. The anisotropy of QEP(**r**) in Hal_3-synthons increases in C_6Cl_6 and C_6Br_6 crystals, nevertheless, it decreases for C_6I_6 crystal.

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References

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