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Electron-density and electrostatic-potential features of orthorhombic chlorine trifluoride

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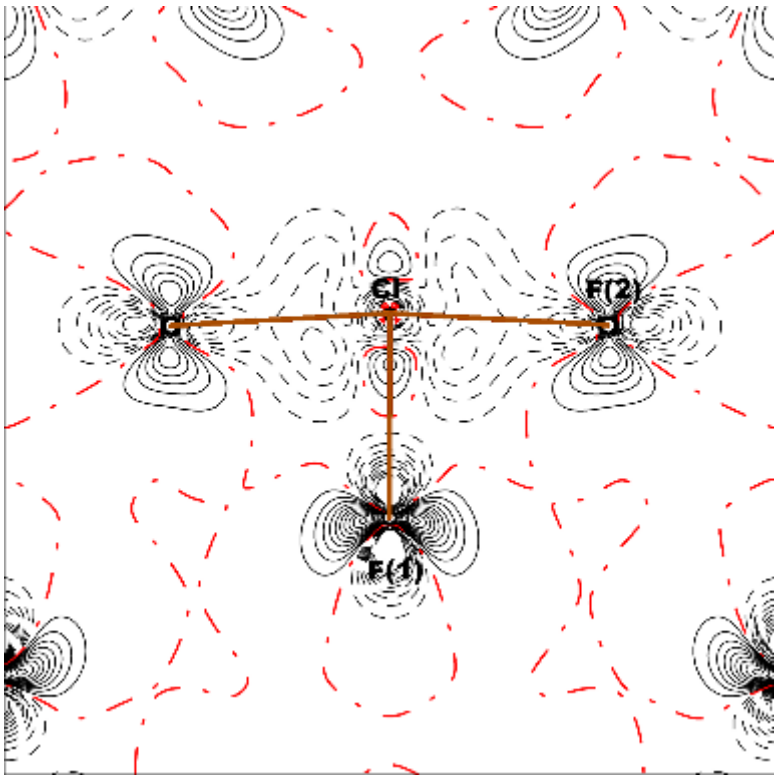

Figure 1S The experimental (multipole) deformation electron density in the crystalline ClF_3. Contour lines are 0.1 e/Å^3. Solid lines show the values of excessive (positive) density.

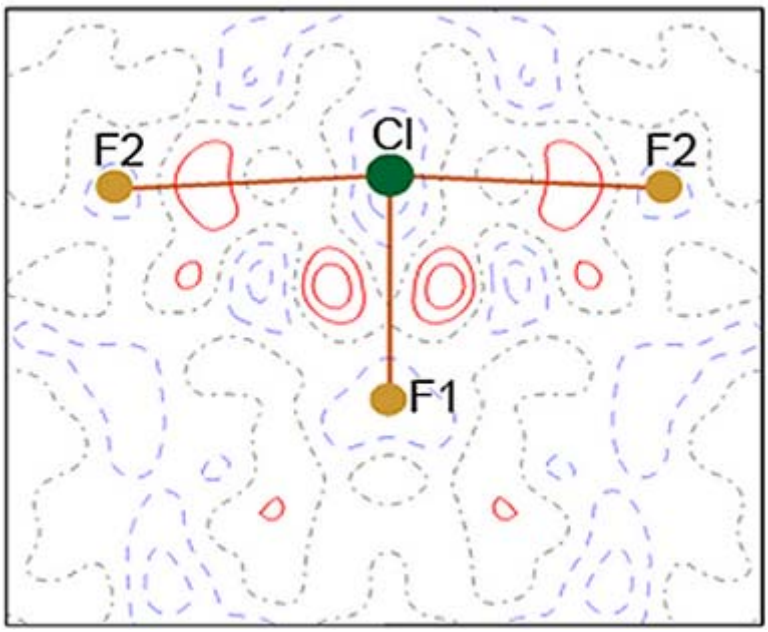

Figure 2S The residual Fourier electron-density map in the crystalline ClF_3. Contour lines are 0.1 e/Å^3. Solid lines show the values of excessive (positive) density.

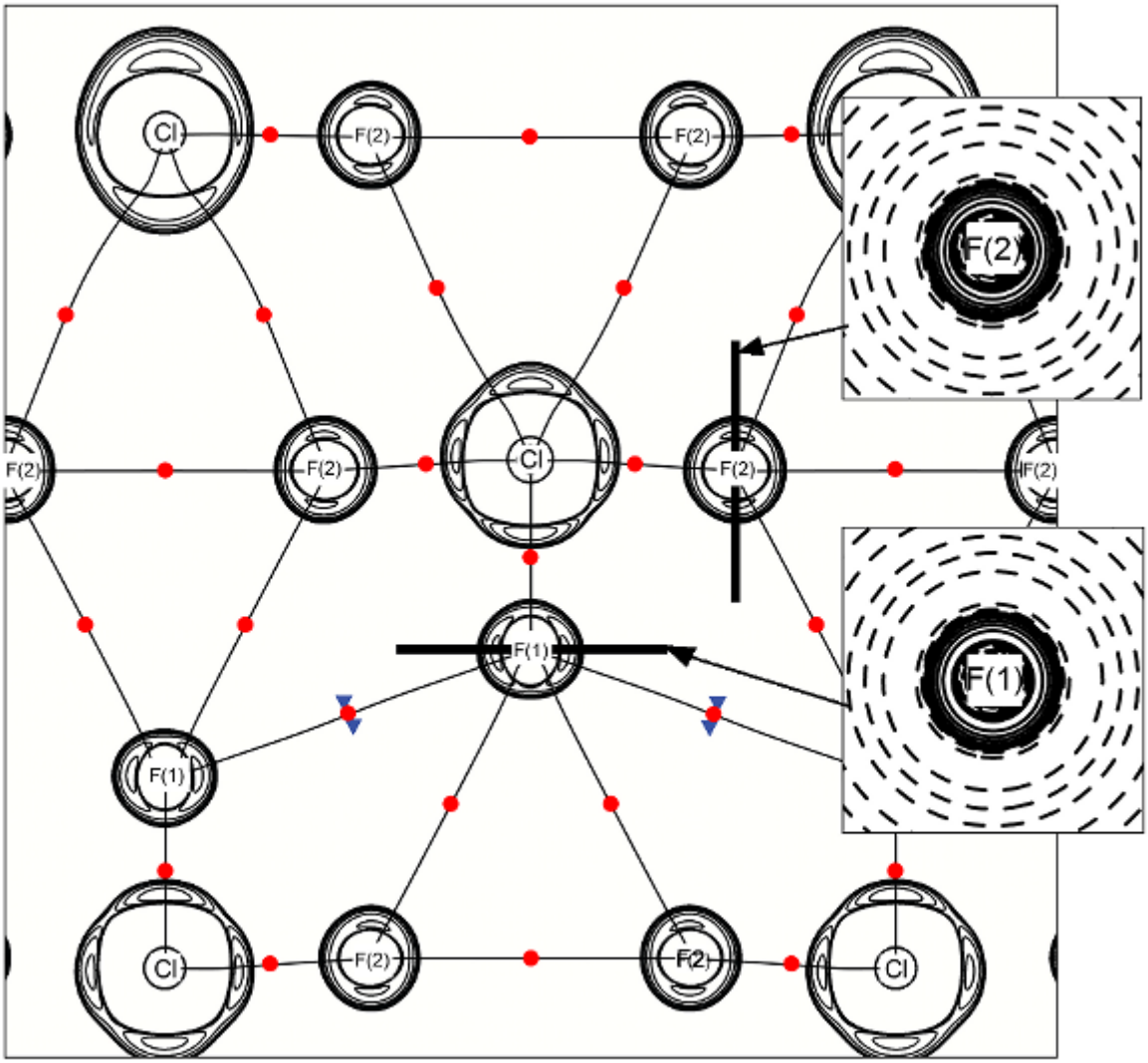

Figure 3S The distribution of Laplacian of the electron density was derived from the B3LYP/QZV2P/model calculation. Here and below, only positive Laplacian values are shown; the line intervals are 2 x 10^n, 4 x 10^n and 8 x 10^n e Å^{-5} ($-2 \leq n \leq 2$). The sections of Laplacian in the planes going through F1 and F2 atoms perpendicular to the Cl-F1 and Cl-F2 lines are also given as the inserts. The critical points (3,-1) and (3,+1) in electron density are marked by the red points and blue triangles.

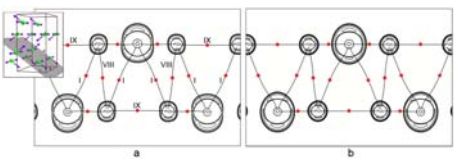

Figure 4S The distribution of Laplacian of electron density in the specified plane: (a) model electron-density derived from the X-ray diffraction experiment; (b) B3LYP/QZV2P/model calculation.

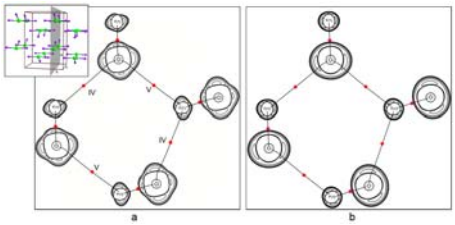

Figure 5S The distribution of positive Laplacian of electron density in the specified plane: (a) model electron-density was derived from the X-ray diffraction experiment; (b) B3LYP/QZV2P/model calculation.

Table 1S Experimental (the first line), the theoretical B3LYP/QZV2P/model (the second line) of the intra- and intermolecular at the bond critical points in the electron density of ClF_3. The intermolecular contacts are enumerated by the Roman numerals.

Contact	R, Å	$\rho(r)$, e·Å^{-3}	$\nabla^2\rho(r)$, e·Å^{-5}
Cl-F1	1.593(1) 1.631	1.64(3) 1.40	7.09(84) 7.47
Cl-F2	1.709(1) 1.757	0.56(3) 0.39	13.59(89) 9.30
Cl-F2 **I**	3.257(1) 3.228	0.03(1) 0.04	0.63(2) 0.68
Cl-F2 **II**	3.169(1) 3.187	0.05(1) 0.04	0.80(2) 0.72
Cl-F1 **III**	3.409(1) 3.381	0.02(1) 0.03	0.39(2) 0.43
Cl-F1 **IV**	3.421(1) 3.366	0.02(1) 0.03	0.36(2) 0.43
F1-F2 **V**	3.041(1) 2.960	0.02(1) 0.03	0.48(2) 0.60
F2-F2 **VI**	2.966(1) 2.931	0.03(1) 0.04	0.70(2) 0.747
F2-F2 **VII**	2.687(1) 2.734	0.04(1) 0.05	0.96(2) 1.08
F1-F1 **VIII**	3.288(1) 3.304	0.01(1) 0.01	0.29(2) 0.27
Cl-F2 **IX**	3.064(1) 3.090	0.05(1) 0.05	0.87(2) 0.80

Table 2S Atomic charges, Q_i, integrated within the atomic ρ-basins and values of atomic basin volumes, Ω_i. Experimental values are given in the first line, and theoretical values obtained from the multipole model calculations are listed in the second line .

	Q_i, e	Ω_i, Å^3
Cl	1.09 1.01	17.508 18.204
F1	-0.29 -0.27	15.130 15.077
F2	-0.40 -0.37	13.982 14.102