Electronic Supplementary Information for

Topology of the magnetically induced current density and proton magnetic shielding in hydrogen bonded systems

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Table 1: Origin dependence of $\xi_{\perp,\mathcal{D}}$ of ClH$\cdots$BF for two arbitrary domains obtained cutting the complex at $z = 0$ and $z = 1$ (in au).

Origin	$-\infty < z < 0$	$0 \leq z < \infty$	Total	$-\infty < z < 1$	$1 \leq z < \infty$	Total
Cl	−2.2609	−4.9759	−7.2368	−2.5859	−4.6509	−7.2368
H	−2.1852	−5.0528	−7.2380	−2.2971	−4.9409	−7.2380
B	−2.0525	−5.1875	−7.2400	−1.7910	−5.4490	−7.2400
F	−1.9789	−5.2622	−7.2411	−1.5101	−5.7311	−7.2412
average	−2.1194	−5.1196	−7.2390	−2.0460	−5.1930	−7.2390
std.dev.	0.1102	0.1119	0.0017	0.4203	0.4220	0.0017

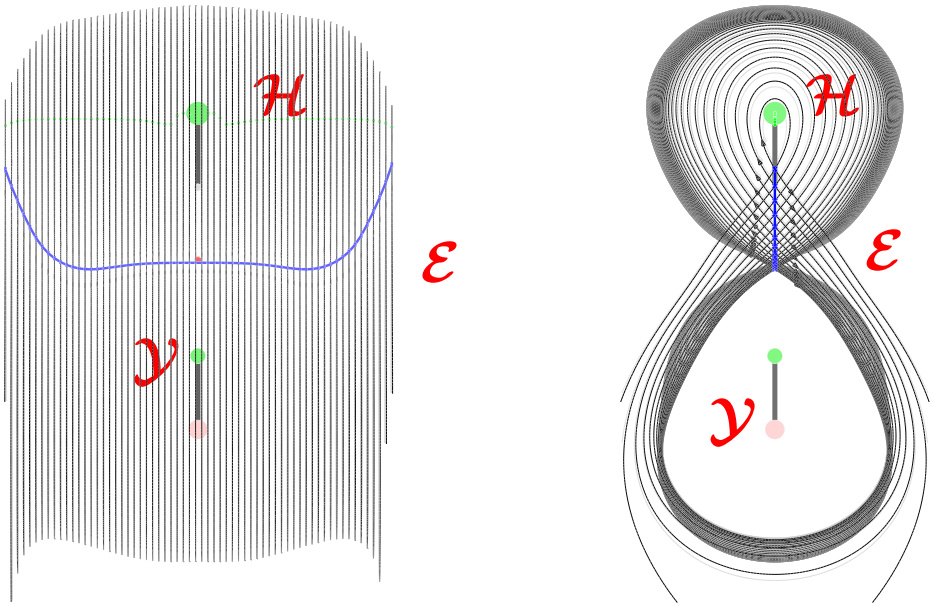

Figure 1: Side and top views of the separatrices formed by all the asymptotic trajectories originating and terminating at saddle points along the saddle line (in blue) of $\mathbf{J}^{\mathbf{B}}$ induced by a static magnetic field perpendicular to the H-bond of the ClH$\cdots$FB linear complex. Chlorine and fluorine are green, boron is pink, and hydrogen is light gray. A line of centers (small green dots) passing through chlorine is also reported. The separatrices divide the molecular space into three distinct regions of current confinement, also referred to as basin of current density, which are here indicated with the letters $\mathcal{H}$, $\mathcal{Y}$, and $\mathcal{E}$, see main text for major details. The bond critical point (BCP) of the electron density is marked by a small red cross.

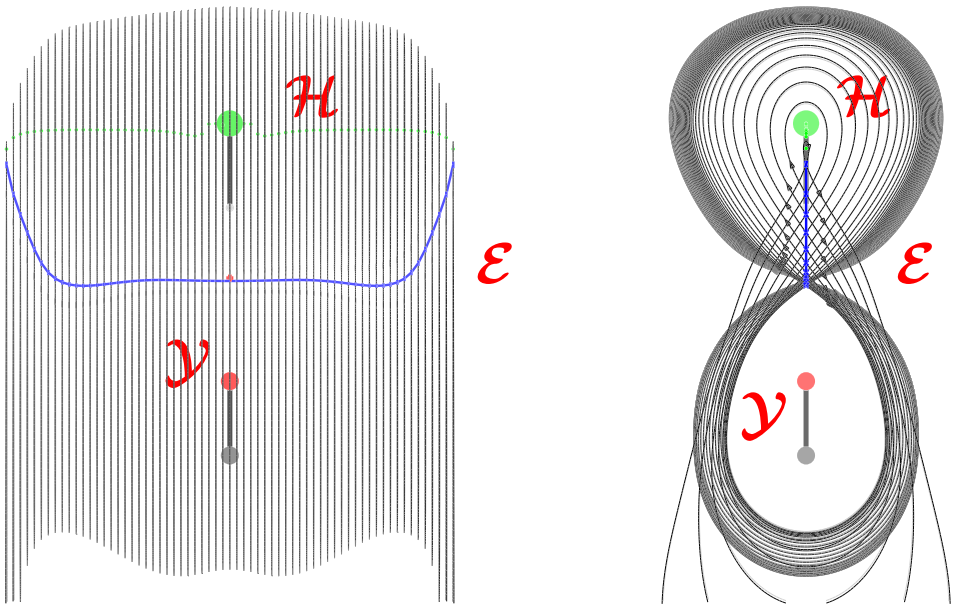

Figure 2: As in Fig. 1 for the ClH$\cdots$OC linear complex. Chlorine is green, oxygen is red, carbon is black and hydrogen is light gray.

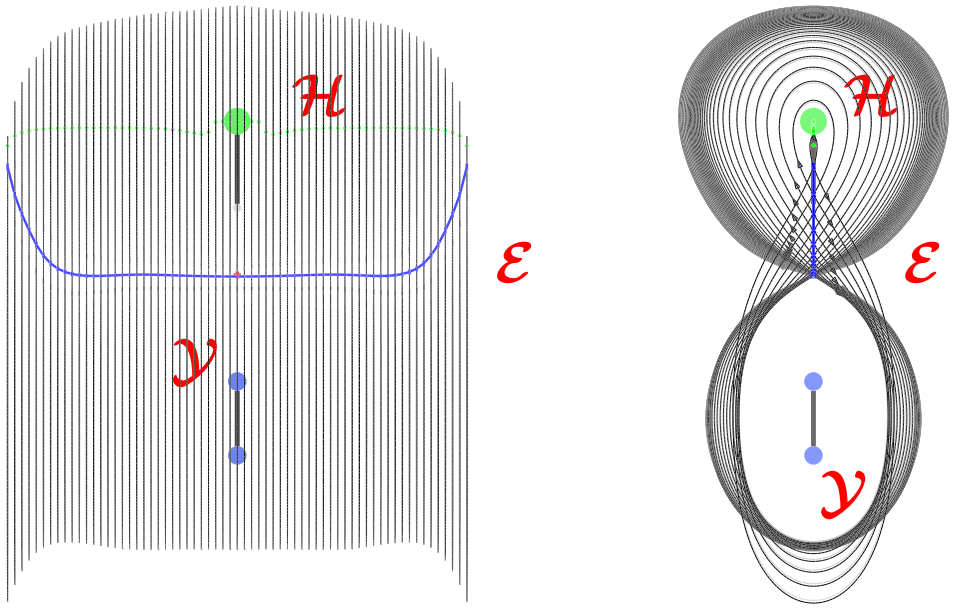

Figure 3: As in Fig. 1 for the ClH$\cdots$N$_2$ linear complex. Chlorine is green, nitrogen is blue and hydrogen is light gray.

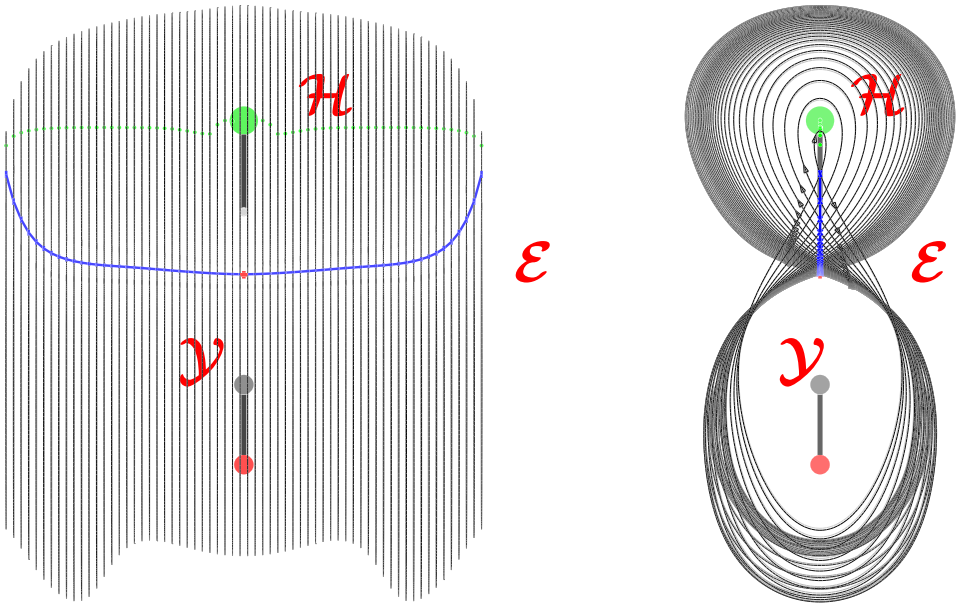

Figure 4: As in Fig. 1 for the ClH$\cdots$CO linear complex. Chlorine is green, oxygen is red, carbon is black and hydrogen is light gray.

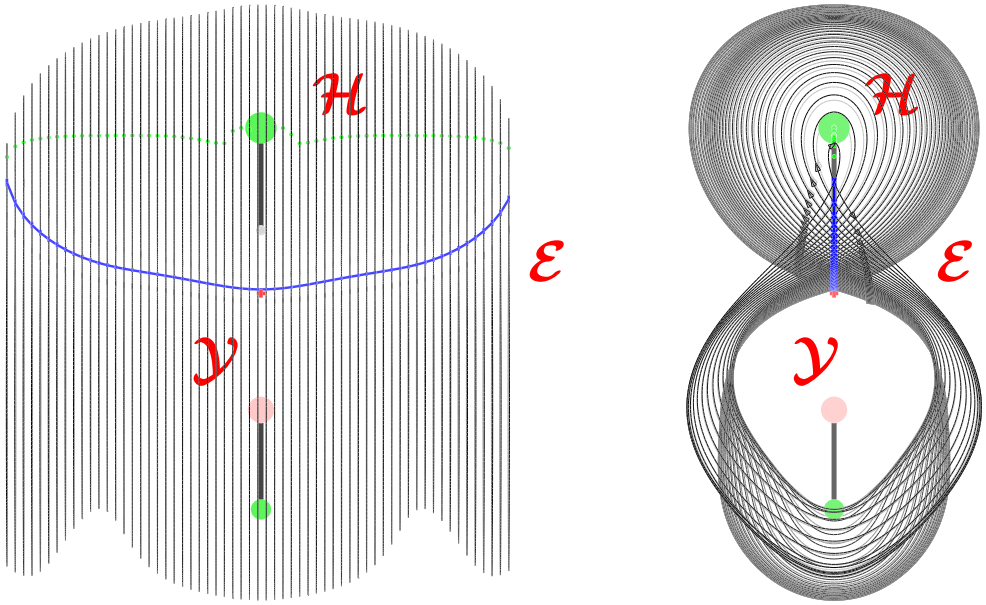

Figure 5: As in Fig. 1 for the ClH···BF linear complex. Chlorine and fluorine are green, boron is pink, and hydrogen is light gray.

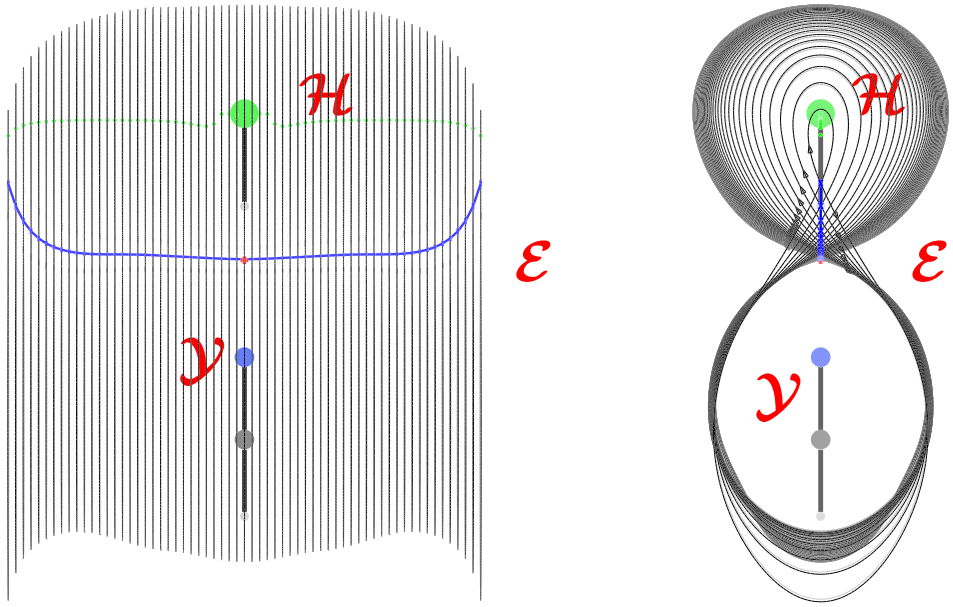

Figure 6: As in Fig. 1 for the ClH···NCH linear complex. Chlorine is green, nitrogen is blue, carbon is black, and hydrogen is light gray.

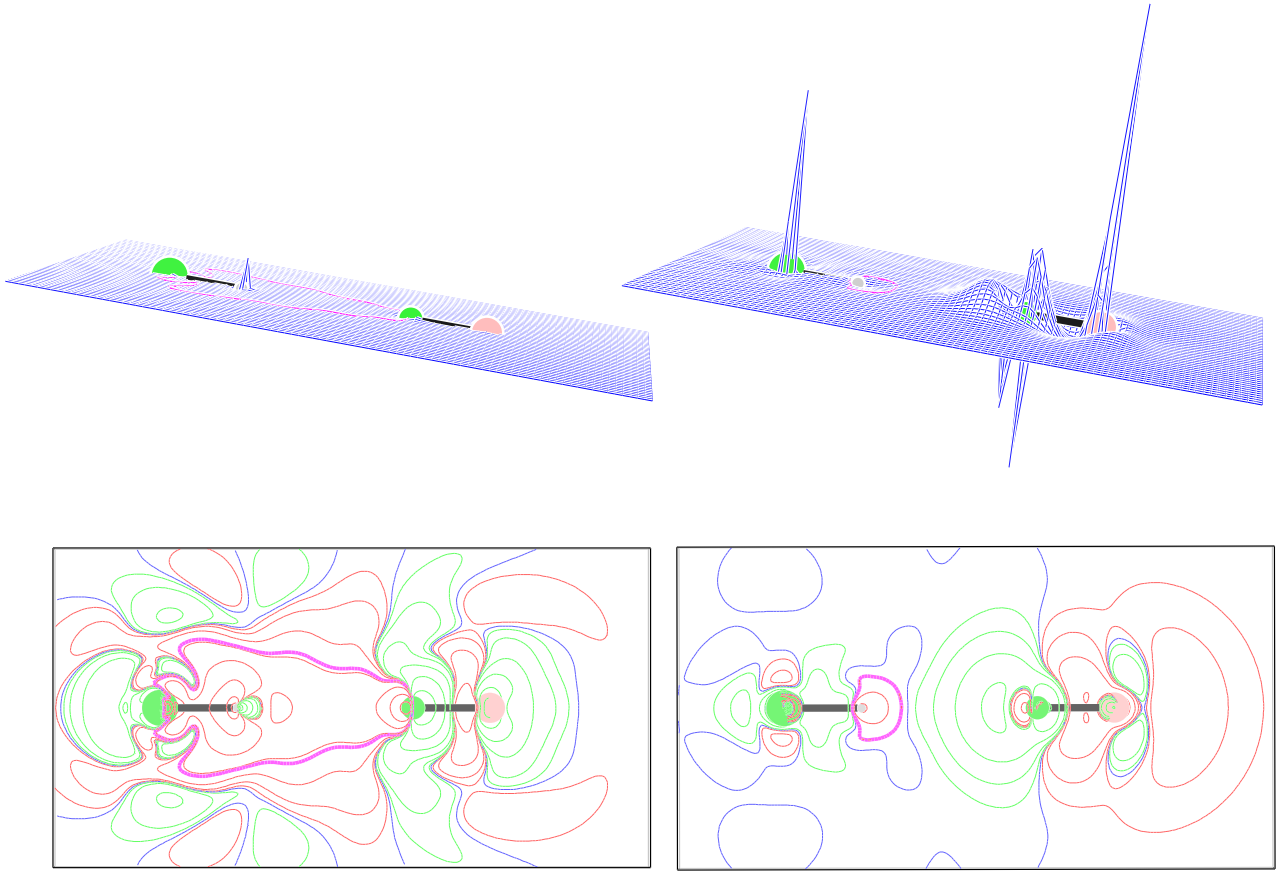

Figure 7: The change in the perpendicular component of the proton shielding density $\Delta\Sigma^{\mathrm{H}}_{\perp,\mathrm{pro}}$ on the left and in the charge density $\Delta\rho_{\mathrm{pro}}$ on the right arising from H-bond formation for the ClH$\cdots$FB complex on a plane containing the supra-molecular axis. Negative/positive contours are red/green, scaled by 4. Minimum values that can be appreciated are -0.164 ppm$/a_0^3$ and -0.16×10^{-3} e/a_0^3. Magenta contours corresponds to -0.5×10^{-3} ppm$/a_0^3$ and -10^{-5} e/a_0^3.

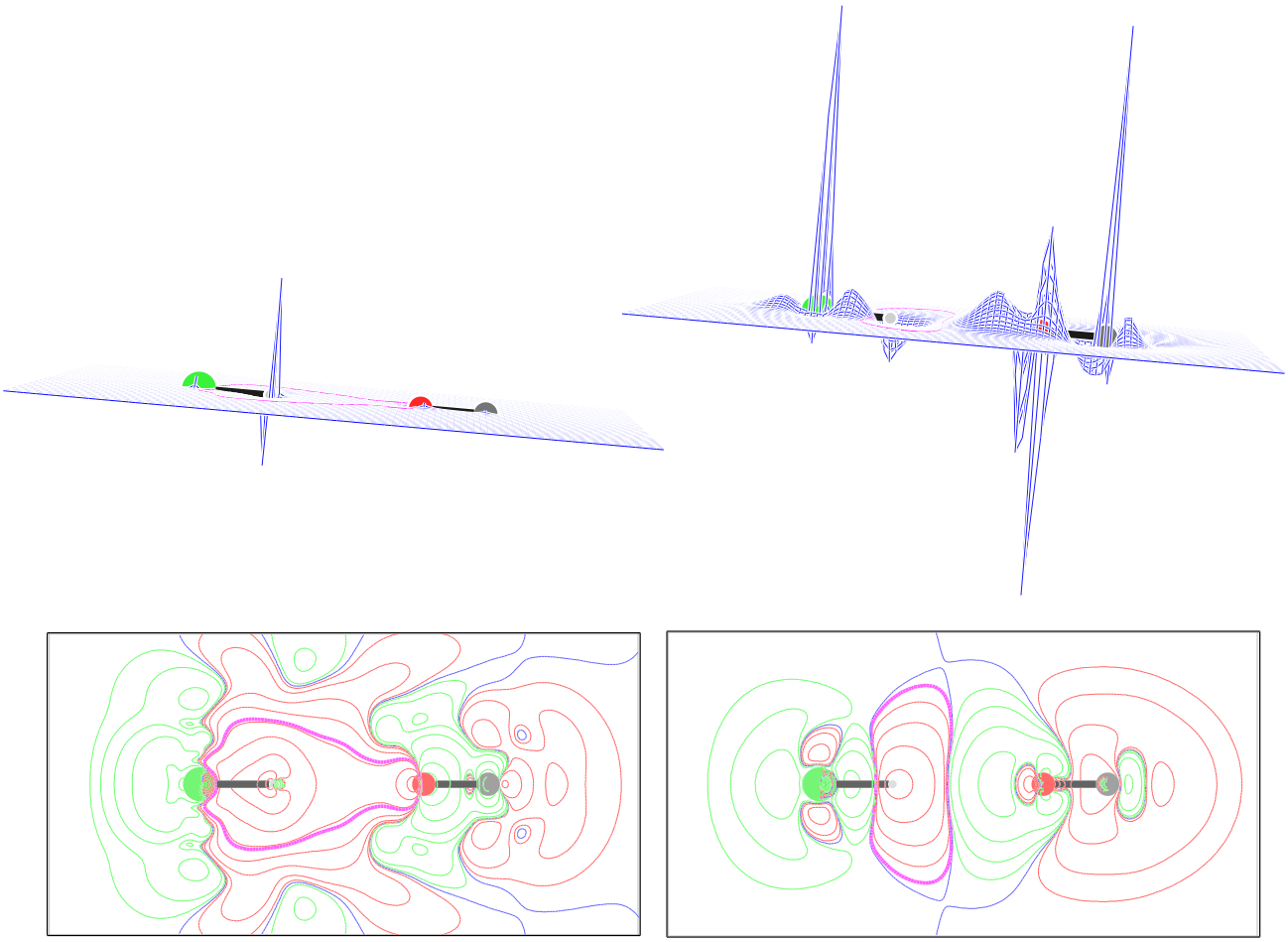

Figure 8: The change in the perpendicular component of the proton shielding density $\Delta\Sigma^{\mathrm{H}}_{\perp,\mathrm{pro}}$ on the left and in the charge density $\Delta\rho_{\mathrm{pro}}$ on the right arising from H-bond formation for the ClH$\cdots$OC complex on a plane containing the supra-molecular axis. Negative/positive contours are red/green, scaled by 4. Minimum values that can be appreciated are -0.655 ppm$/a_0^3$ and -0.64×10^{-3} e/a_0^3. Magenta contours corresponds to -0.002 ppm$/a_0^3$ and -0.2×10^{-5} e/a_0^3.

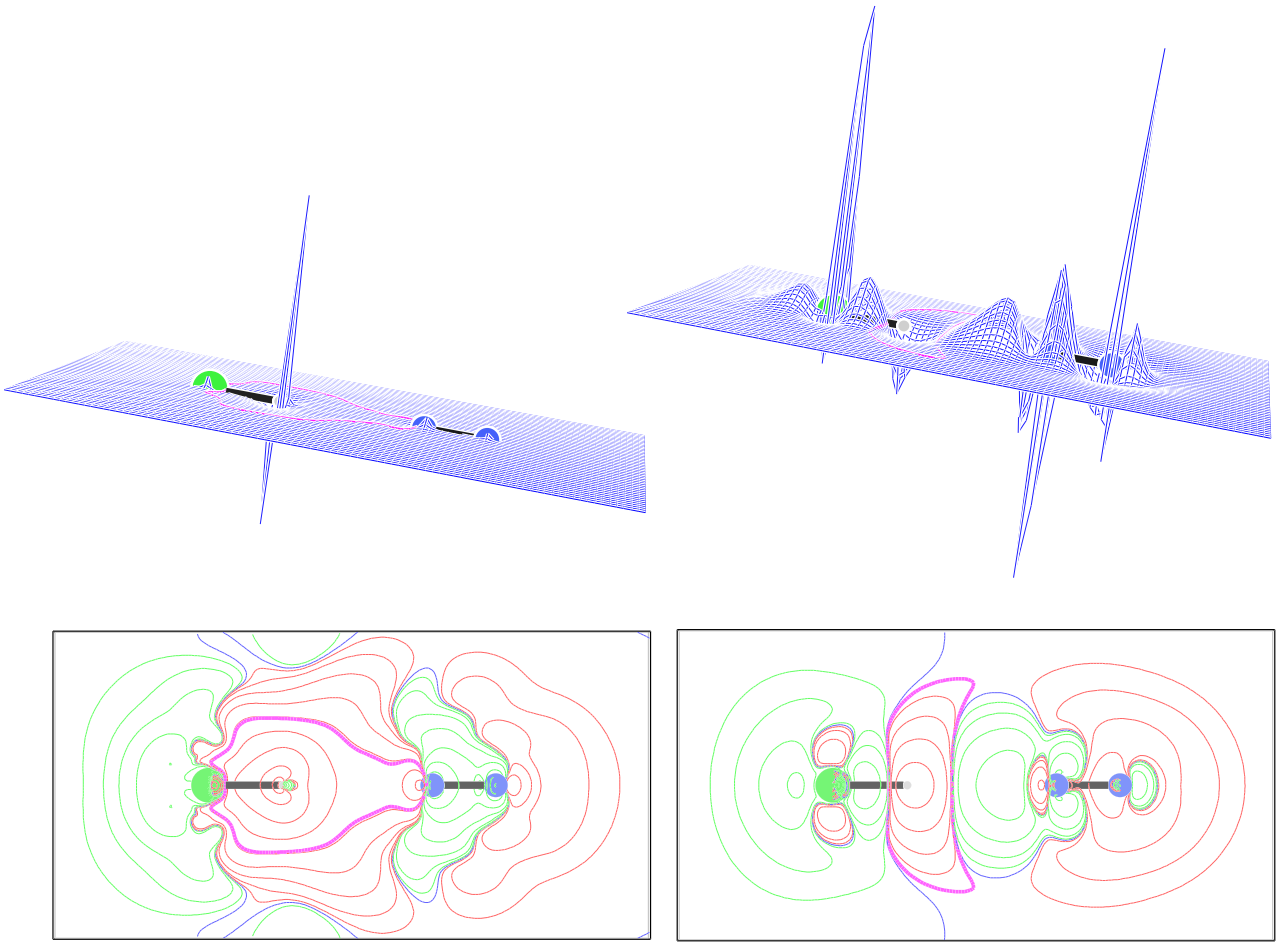

Figure 9: The change in the perpendicular component of the proton shielding density $\Delta\Sigma^{\mathrm{H}}_{\perp,\mathrm{pro}}$ on the left and in the charge density $\Delta\rho_{\mathrm{pro}}$ on the right arising from H-bond formation for the $\mathrm{ClH}\cdots\mathrm{N_2}$ complex on a plane containing the supra-molecular axis. Negative/positive contours are red/green, scaled by 4. Minimum values that can be appreciated are -2.62 ppm$/a_0^3$ and -0.64×10^{-3} e/a_0^3. Magenta contours corresponds to -0.003 ppm$/a_0^3$ and -0.3×10^{-5} e/a_0^3.

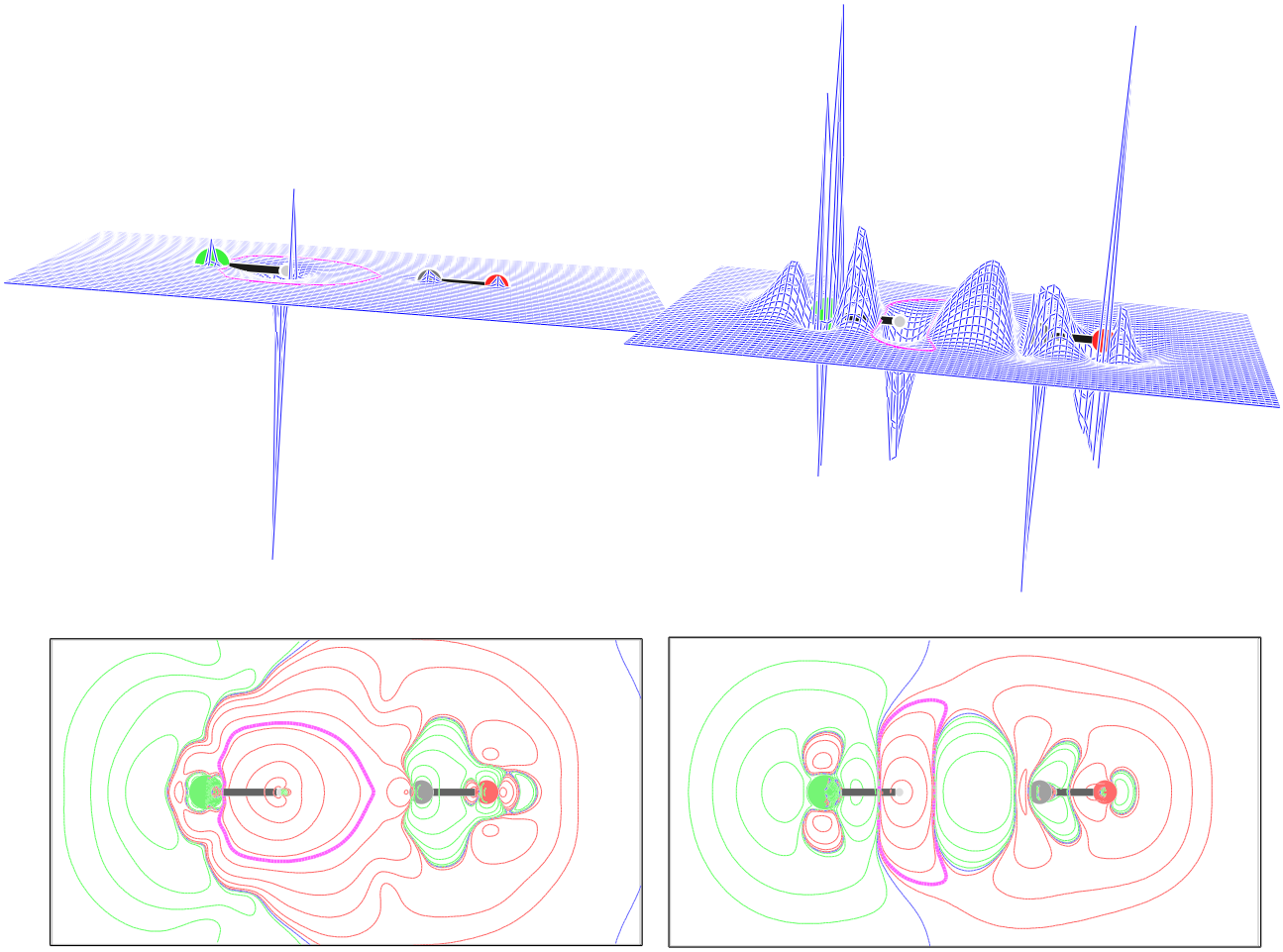

Figure 10: The change in the perpendicular component of the proton shielding density $\Delta\Sigma^{\mathrm{H}}_{\perp,\mathrm{pro}}$ on the left and in the charge density $\Delta\rho_{\mathrm{pro}}$ on the right arising from H-bond formation for the ClH$\cdots$CO complex on a plane containing the supra-molecular axis. Negative/positive contours are red/green, scaled by 4. Minimum values that can be appreciated are -2.62 ppm$/a_0^3$ and -0.256×10^{-2} e/a_0^3. Magenta contours corresponds to -0.0065 ppm$/a_0^3$ and -0.2×10^{-4} e/a_0^3.

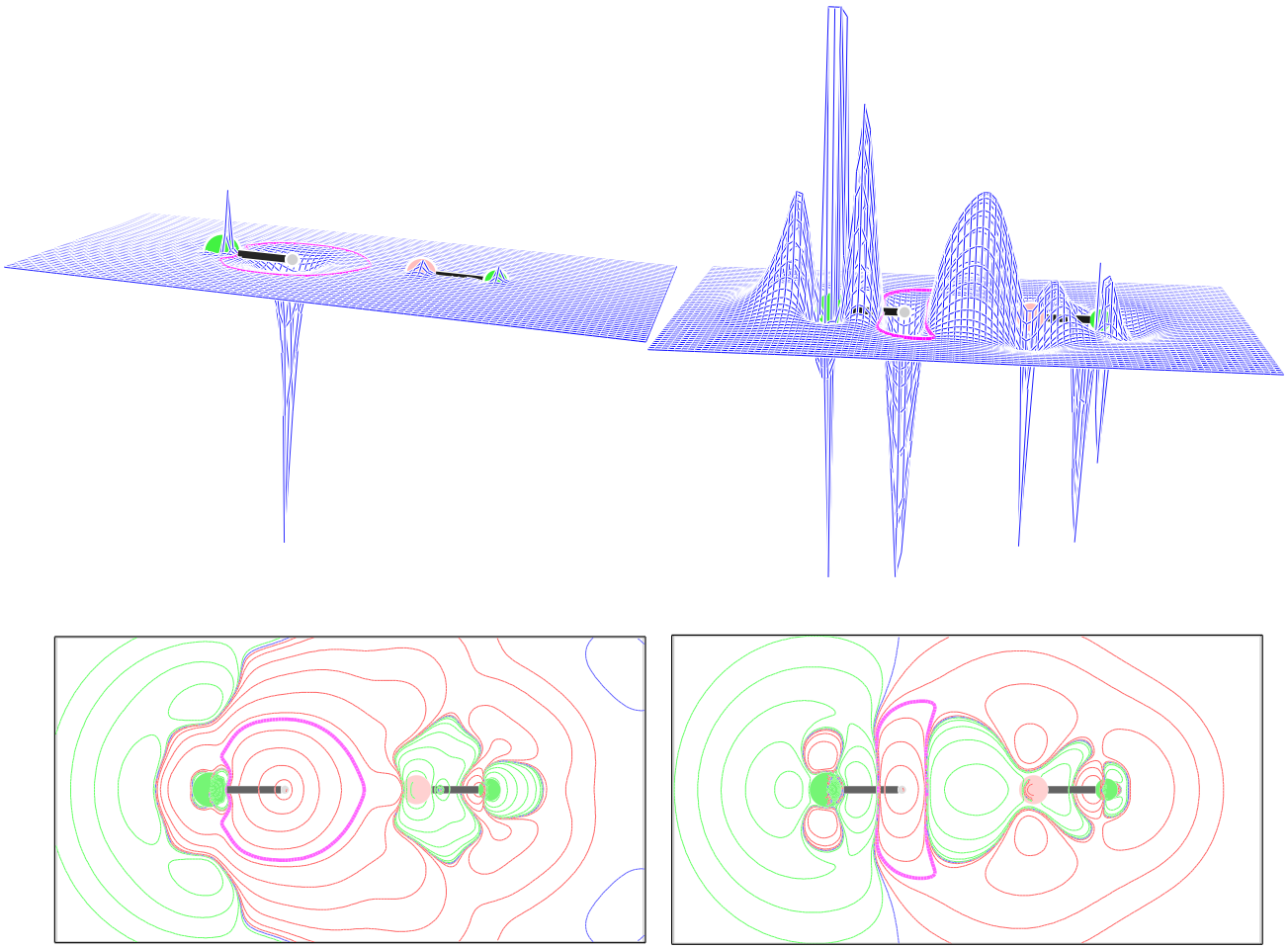

Figure 11: The change in the perpendicular component of the proton shielding density $\Delta\Sigma^{\mathrm{H}}_{\perp,\mathrm{pro}}$ on the left and in the charge density $\Delta\rho_{\mathrm{pro}}$ on the right arising from H-bond formation for the ClH$\cdots$BF complex on a plane containing the supra-molecular axis. Negative/positive contours are red/green, scaled by 4. Minimum values that can be appreciated are -10 ppm$/a_0^3$ and -0.01 e/a_0^3. Magenta contours corresponds to -0.017 ppm$/a_0^3$ and -0.7×10^{-4} e/a_0^3.

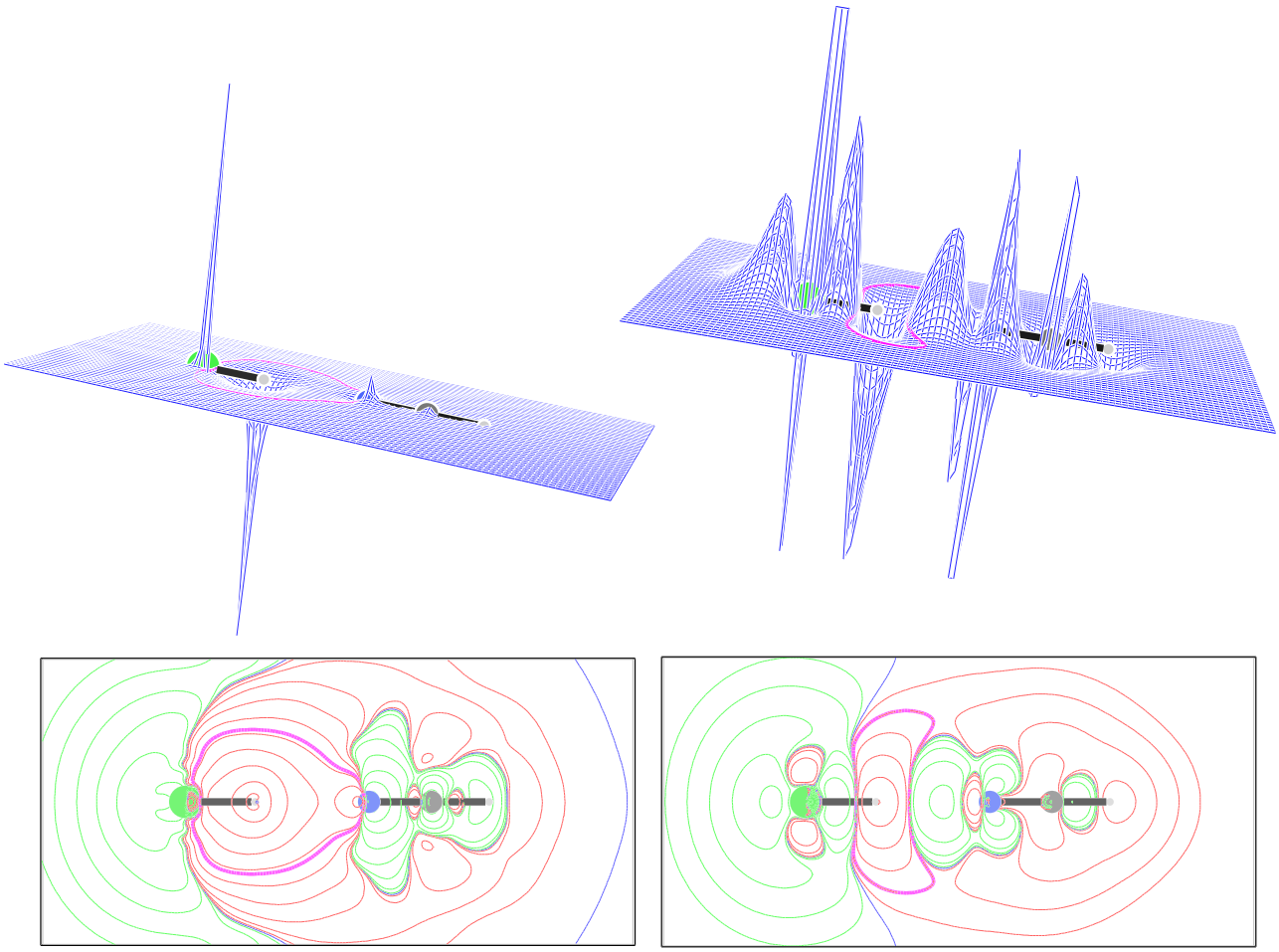

Figure 12: The change in the perpendicular component of the proton shielding density $\Delta\Sigma^{\mathrm{H}}_{\perp,\mathrm{pro}}$ on the left and in the charge density $\Delta\rho_{\mathrm{pro}}$ on the right arising from H-bond formation for the ClH$\cdots$NCH complex on a plane containing the supra-molecular axis. Negative/positive contours are red/green, scaled by 4. Minimum values that can be appreciated are -2.62 ppm$/a_0^3$ and -0.01 e/a_0^3. Magenta contours corresponds to -0.007 ppm$/a_0^3$ and -0.4×10^{-4} e/a_0^3.