On the conformational preference of chlorothioformate species: molecular structure of ethyl chlorothioformate, ClC(O)SCH$_2$CH$_3$, in the solid phase and NBO analysis

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Supplementary Material

Content:

Table S1: Properties of the intramolecular bond critical points (electrons and Å). First row: crystal, second row: free molecule. R: internuclear distance; $b_{1\,(2)}$: bond path length from the first (second) attractor to the bond critical point; λ_3: positive eigenvalue of the Hessian of ρ; ε: ellipticity.

		R	b_1	b_2	ρ	$\nabla^2\rho$	λ_3	ε
S	C(1)	1.733	0.812	0.922	1.42	-10.76	3.00	0.327
			0.828	0.906	1.43	-10.72	3.42	0.305
C(2)	S	1.813	0.824	0.991	1.23	-7.08	5.90	0.047
			0.834	0.981	1.23	-7.24	5.79	0.057
C(1)	Cl	1.783	0.777	1.007	1.25	-4.97	9.16	0.045
			0.778	1.006	1.25	-4.94	9.17	0.048
C(3)	C(2)	1.513	0.738	0.776	1.70	-14.59	8.03	0.009
			0.737	0.777	1.71	-14.62	8.02	0.008
$H_{(et,out)}$	C(2)	1.091	0.374	0.696	1.92	-24.75	11.51	0.014
			0.384	0.686	1.91	-24.15	11.32	0.008
$H_{(et,in)}$	C(2)	1.092	0.376	0.695	1.88	-24.55	11.50	0.016
			0.377	0.694	1.91	-24.51	11.45	0.014
$H_{(me,out)}$	C(3)	1.093	0.391	0.682	1.88	-23.15	11.18	0.010
			0.391	0.681	1.88	-23.34	11.08	0.001
$H_{(me,in)}$	C(3)	1.093	0.391	0.682	1.88	-23.18	11.14	0.010
			0.388	0.685	1.88	-23.43	11.15	0.010
$H_{(me,trans)}$	C(3)	1.094	0.387	0.686	1.87	-23.19	11.20	0.008
			0.392	0.682	1.87	-23.01	11.06	0.009
C(1)	O	1.181	0.390	0.792	2.91	17.67	72.22	0.071
			0.389	0.792	2.92	18.50	72.61	0.076

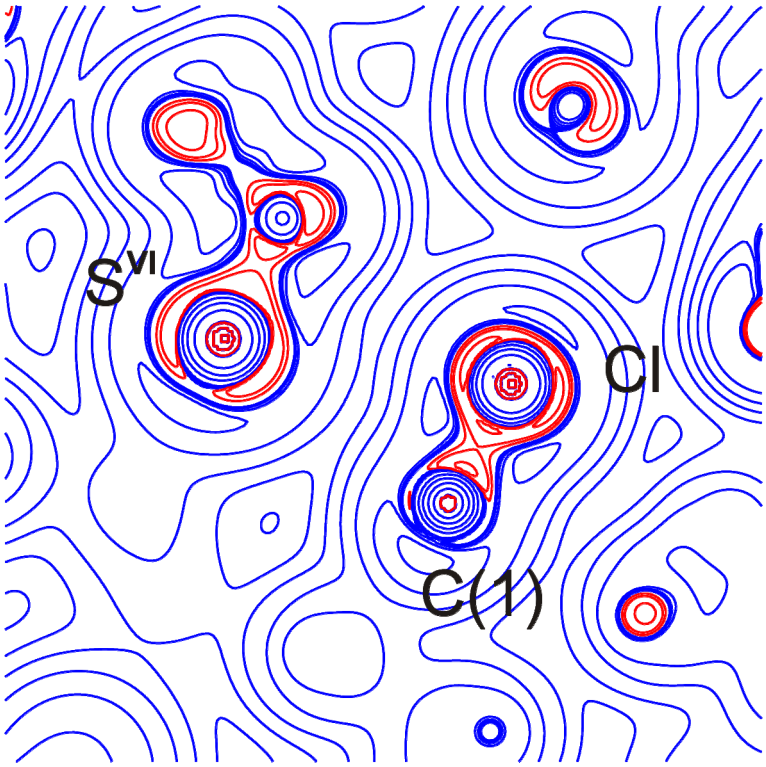

Figure S1

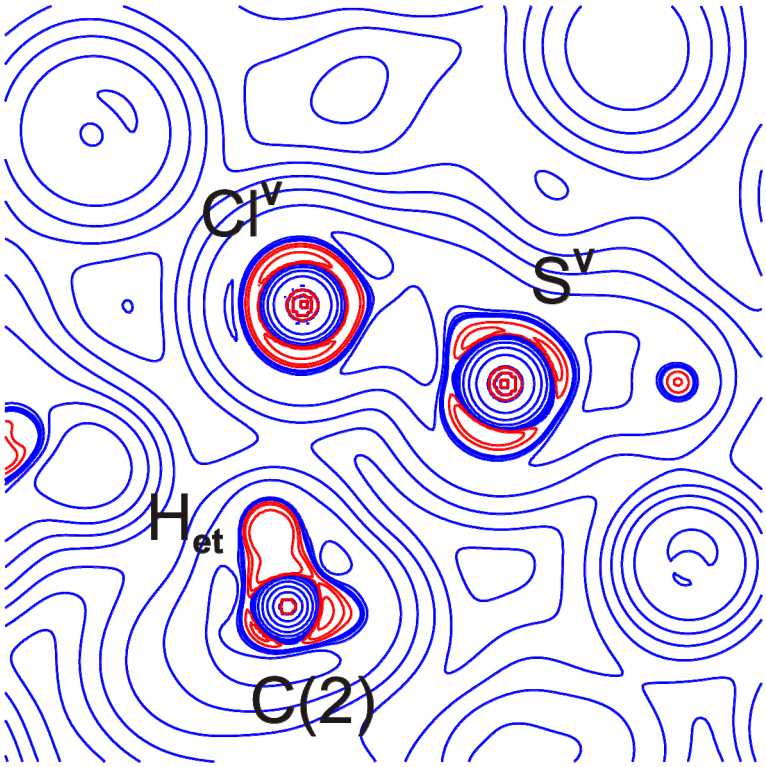

Figure S2