Supplementary information: The Rotational Barrier of Ethane and Some of its Hexasubstituted Derivatives in Terms of the Forces acting on the Electron Distribution

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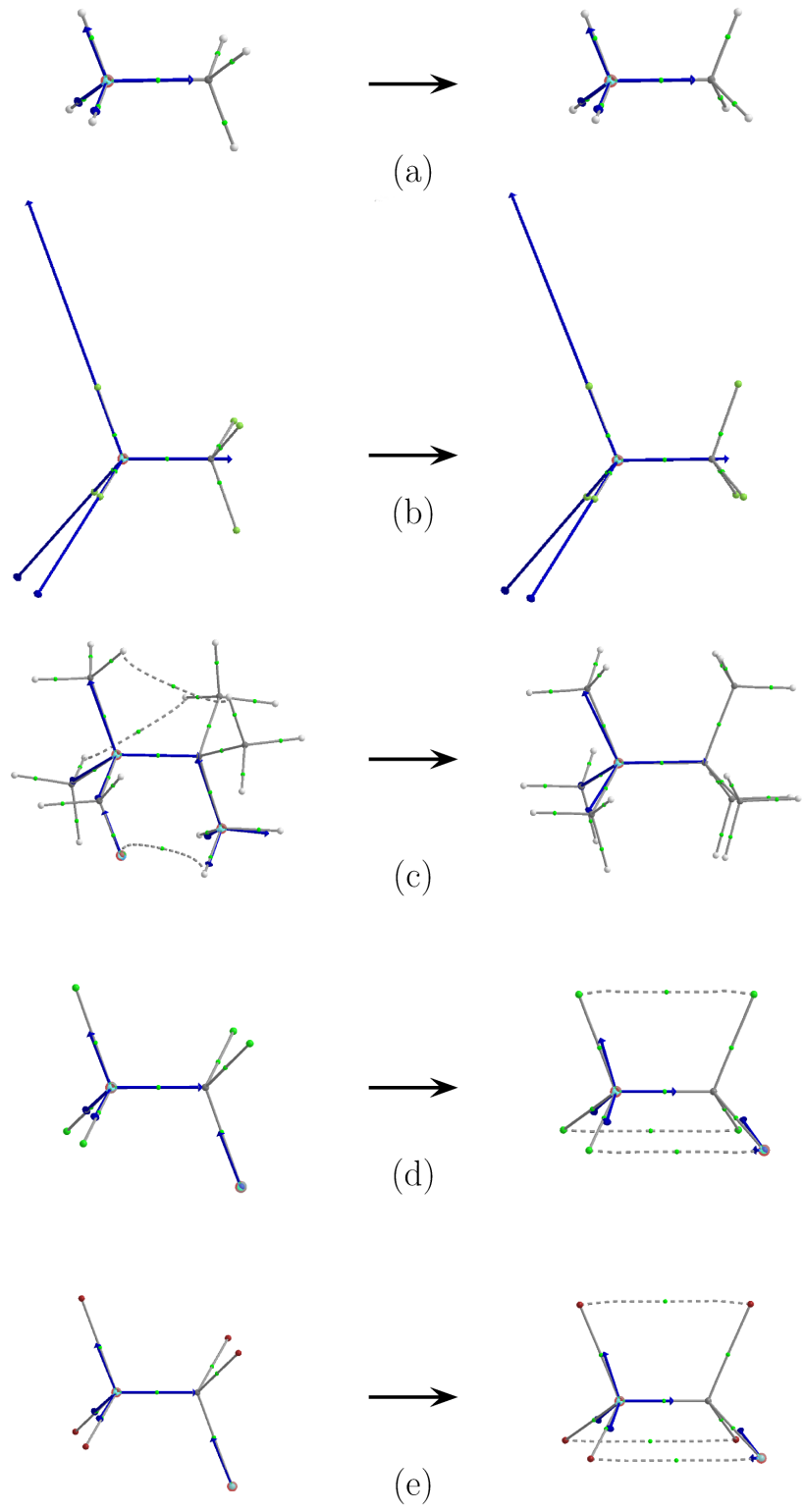

Figure S1. $F_e(C|X)$ contributions to $F_e(C)$ of the molecules CX_3CX_3 (X = H, F, CH_3, Cl and Br.

Table S1. Selected properties and their changes from the staggered to the eclipsed conformations for the molecules CX_3CX_3, with X = H, F, CH_3, Cl, Br.

X	angle	$-\gamma$	R_{cc}	$\lvert\boldsymbol{F_e}(\mathrm{X})\rvert$	$\lvert\boldsymbol{F_e}(\mathrm{C}\lvert\mathrm{C})\rvert$	$\lvert\boldsymbol{F_e}(\mathrm{C}\lvert\mathrm{X})\rvert$	$\nabla^2\rho_b$(C,C)	G_b(C,C)	λ(C)	λ(X)	δ(C,X)
F	60	1.999985	1.544	37.024	14.337	37.023	-0.766	0.054	2.821	9.140	0.595
	0	1.999981	1.577	36.959	13.943	36.958	-0.675	0.050	2.829	9.134	0.597
Δ			0.033	-1.251	-0.349	-0.065	0.091	-0.004	0.007	-0.007	0.002
CH_3	60	2.000946	1.575	3.272	12.028	11.167	-0.497	0.057	4.118	8.374	0.894
	0	2.000930	1.616	3.219	12.486	11.419	-0.425	0.051	4.135	8.368	0.897
Δ			0.041	-0.053	0.458	0.252	0.072	-0.006	0.017	-0.008	0.003
Cl	60	1.999779	1.581	7.299	11.387	7.299	-0.521	0.057	3.957	16.449	0.859
	0	1.999777	1.667	7.275	5.763	6.734	-0.363	0.046	3.994	16.438	0.865
Δ			0.086	-0.024	-5.624	-0.565	0.158	-0.011	0.037	-0.011	0.006
Br	60	1.999915	1.578	7.525	11.602	7.525	-0.493	0.059	4.378	34.298	0.852
	0	1.999914	1.661	7.522	5.229	6.844	-0.344	0.048	4.415	34.289	0.856
Δ			0.083	-0.003	-6.373	-0.681	0.149	-0.011	0.037	-0.009	0.004