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Negative hyperconjugation of some fluorine containing groups

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Supplementary information

Table S 1 DFT calculated energies of compounds with substituents containing fluorine [a]

	CF_3[b]	SF_5	SCF_3
C_6H_5X	–569.4608204	–1129.1621944	–967.6630100
4-$NH_2C_6H_4X$	–624.8398135	–1184.5421382	–1023.0421839
4-NH^--C_6H_4X	–624.2657683	–1183.9810869	–1022.4702712
(*E*)-CH_2=CH–CH=CHX	–493.1878610	–1052.8891357	–891.3905014
(*E,E*)-NH_2CH_2=CHCH=CHX	–548.5715177	–1108.2749347	–946.7728901
4-X-C_8H_{12}-1-COOH	–839.1579047	–1398.8600202	–1237.3551799
4-X-C_8H_{12}-1-COO^-	–838.6101006	–1398.3234754	–1236.8095678
3-X-C_6H_4COOH	–758.0958098	–1317.7960668[c]	–1156.2980510[c]
3-X-$C_6H_4COO^-$	–757.5567767	–1317.266148	–1155.7596246
4-X-C_6H_4COOH	–758.0954459	–1317.7958700	–1156.2949649
4-X-$C_6H_4COO^-$	–757.5576837	–1317.2662598	–1155.7602751

[a] In a. u.; calculated at the level B3LYP/6-311+G(d,p)//B3LYP/6-311+G(d,p) [b] Some of these values were already published, usually only the energies, not the geometrical parameters, ref. 31,32,42,45. [c] Weighted average from two near values for the two coplanar conformations of the COOH group.