The conformation of 1,2-difluoroethane

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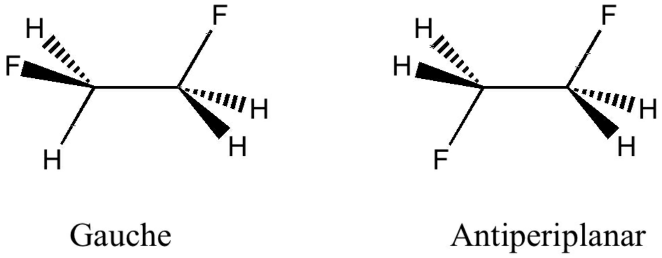
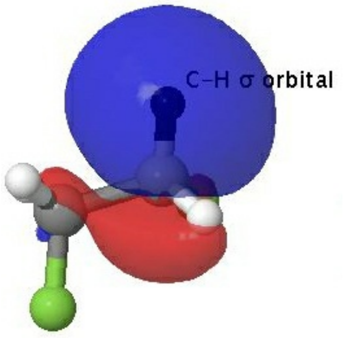
Here I offer another spin-off from writing a lecture course on conformational analysis. This is the famous example of why **1,2-difluoroethane** adopts a *gauche* rather than *antiperiplanar* conformation.

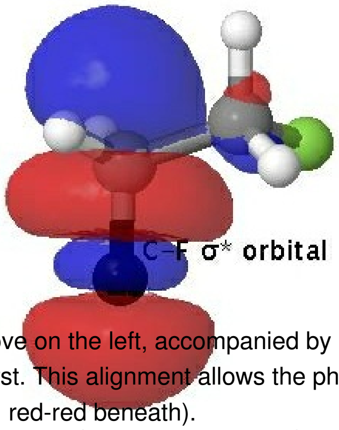


The gauche and antiperiplanar conformations of 1,2-difluoroethane

One major contribution to the greater stability of the gauche is the stereoelectronic interactions, and this is best probed using the NBO (Natural Bond Orbital) approach of Weinhold (DOI: 10.1021/ja00501a009). The process is approximately described as first reducing the wavefunction down to a set of orbitals which have been localized (using appropriate algorithms) down to two or one centres (corresponding to two-centre covalent bonds, or one-centre electron lone pairs). Perturbation theory is then used to evaluate the interaction energy between any filled and any empty combination. For the molecule above, **six** such combinations are inspected, involving any one of the six filled C-H or C-F σ-orbitals, and the best-overlapping σ* orbital which turns out to be located on the C-H or C-F bond anti-periplanar to the filled orbital.



Filled C-H NBO orbital. Click for 3D to superimpose empty C-F anti bonding orbital.



Empty C-F antibonding NBO orbital. Click for 3D

A filled C-H orbital is shown above on the left, accompanied by an empty C-F σ* orbital on the right which is anti-periplanar to the first. This alignment allows the phases of the two orbitals to overlap maximally (blue-blue on the top, red-red beneath).

The interaction energy between this pair is determined not only by the efficacy of the overlap, but by the energy gap between the two. The smaller the gap, the better the interaction energy (referred to as **E2**, in kcal/mol). For the gauche conformation, the six pairs of orbitals have the following interaction energies; two σC-H/σ*C-F interactions (illustrated above), 4.9; two σC-H/σ*C-H 2.6 and two σC-F/σ*C-H 0.8 kcal/mol. For the anti-periplanar conformation, the terms are four σC-H/σ*C-H 2.5 and two σC-F/σ*C-F 1.8 kcal/mol. The two totals (16.6 vs 13.6) indicate that gauche is stabilized more by such interactions.

There is of course a bit more to this story, but I have documented the above here, since I can include an explicit (and rotatable) illustration of the orbitals involved (which I have not seen elsewhere). If you want a recipe for generating these orbitals, go here.