Supporting Information

"Conformational preference analysis in C_2H_6 using Orbital Forces and Non-Covalent Interactions; comparison with related systems"

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NCI analysis

a) s(ρ) diagram

Conformational differences are very subtle. Nonetheless, they can be identified by comparison of the s(ρ) diagram among the various conformers. This is shown in Figure S1 for ethane (left) and C_2F_6 (right).

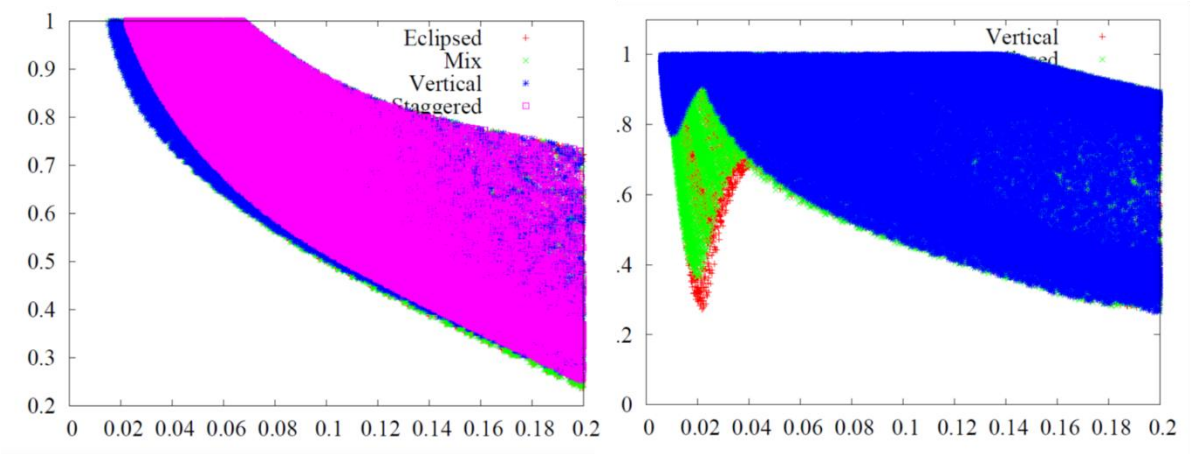


Figure S1. Reduced density gradient vs density plot enabling to see deformations for the different conformations. Left: ethane. Right: C_2F_6.

It can be seen that differences are very subtle in ethane. Setting ρmax=0.037 and s=0.8, we can isolate the small differences and highlight the differential interactions as done in Scheme 1. This value is chosen so as to avoid including the baseline, which would show the atomic features.

Differences are much more visible in fluoroethane. In this case, setting ρmax=0.04 and s=0.6 allows to visualize F···F interactions between the CF3 fragments (Scheme 2). If a higher isosurface is plotted (ρmax=0.04, s=0.9), the F···F interactions within each fragment also appear (Figure S2).

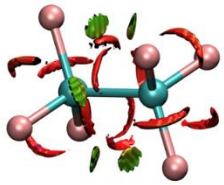
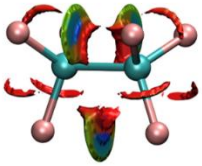
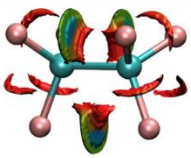
	Staggered	Vertical	Eclipsed
s=0.9			

Figure S2. Evolution of NCI surfaces for the different C_2F_6 states for ρmax=0.04, s=0.9.

Optimized geometry coordinates (H-F/aug-cc-pvQZ)

C_2H_6 (Staggered)

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.524135
3	1	0	1.010147	0.000000	-0.391992
4	1	0	-0.505073	0.874813	-0.391992
5	1	0	-0.505073	-0.874813	-0.391992
6	1	0	0.505073	0.874813	1.916127
7	1	0	0.505073	-0.874813	1.916127
8	1	0	-1.010147	0.000000	1.916127

C_2H_6 (Eclipsed)

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.538668
3	1	0	1.006227	0.000000	-0.398681
4	1	0	-0.503114	-0.871418	-0.398681
5	1	0	-0.503114	0.871418	-0.398681
6	1	0	1.006227	0.000000	1.937348
7	1	0	-0.503114	-0.871418	1.937348
8	1	0	-0.503114	0.871418	1.937348

CH_3SiH_3 (Staggered)

1	14	0	0.000000	0.000000	0.634590
2	6	0	0.000000	0.000000	-1.243005
3	1	0	0.000000	1.384474	1.154178
4	1	0	1.198990	-0.692237	1.154178
5	1	0	-1.198990	-0.692237	1.154178
6	1	0	0.876925	0.506293	-1.629589
7	1	0	-0.876925	0.506293	-1.629589
8	1	0	-0.000000	-1.012585	-1.629589

CH_3SiH_3 (Eclipsed)

1	14	0	0.000000	0.000000	0.637777
2	6	0	0.000000	0.000000	-1.251015
3	1	0	0.000000	1.381345	1.165517
4	1	0	-1.196280	-0.690673	1.165517
5	1	0	1.196280	-0.690673	1.165517
6	1	0	0.000000	1.010795	-1.639780
7	1	0	-0.875374	-0.505398	-1.639780
8	1	0	0.875374	-0.505398	-1.639780

Si_2H_6 (Staggered)

1	14	0	0.000000	0.000000	1.182930
2	14	0	-0.000000	-0.000000	-1.182930
3	1	0	0.000000	1.386577	1.696561
4	1	0	1.200811	-0.693289	1.696561
5	1	0	-1.200811	-0.693289	1.696561
6	1	0	1.200811	0.693289	-1.696561
7	1	0	-1.200811	0.693289	-1.696561
8	1	0	-0.000000	-1.386577	-1.696561

Si_2H_6 (Eclipsed)

1	14	0	0.000000	0.000000	1.188585
2	14	0	0.000000	0.000000	-1.188585
3	1	0	0.000000	1.384785	1.705508
4	1	0	-1.199259	-0.692393	1.705508
5	1	0	1.199259	-0.692393	1.705508
6	1	0	0.000000	1.384785	-1.705508
7	1	0	-1.199259	-0.692393	-1.705508
8	1	0	1.199259	-0.692393	-1.705508

CH_3CF_3 (Staggered)

1	6	0	0.000000	0.000000	-0.033196
2	6	0	0.000000	0.000000	1.466648
3	9	0	0.000000	1.224599	-0.521032
4	9	0	-1.060534	-0.612300	-0.521032
5	9	0	1.060534	-0.612300	-0.521032
6	1	0	-0.882753	0.509658	1.822383
7	1	0	0.882753	0.509658	1.822383
8	1	0	-0.000000	-1.019315	1.822383

CH_3CF_3 (Eclipsed)

1	6	0	0.000000	0.000000	-0.033002
2	6	0	0.000000	0.000000	1.483077
3	9	0	0.000000	1.222571	-0.527378
4	9	0	1.058778	-0.611285	-0.527378
5	9	0	-1.058778	-0.611285	-0.527378
6	1	0	0.000000	1.015507	1.846251
7	1	0	0.879455	-0.507753	1.846251
8	1	0	-0.879455	-0.507753	1.846251

C_2F_6 (Staggered)

1	6	0	0.000000	0.000000	0.769723
2	6	0	-0.000000	-0.000000	-0.769723
3	9	0	0.000000	1.225693	1.211847
4	9	0	1.061481	-0.612846	1.211847
5	9	0	-1.061481	-0.612846	1.211847
6	9	0	1.061481	0.612846	-1.211847
7	9	0	-1.061481	0.612846	-1.211847
8	9	0	-0.000000	-1.225693	-1.211847

C_2F_6 (Eclipsed)

1	6	0	0.000000	0.000000	0.784814
2	6	0	0.000000	0.000000	-0.784814
3	9	0	0.000000	1.221557	1.236349
4	9	0	-1.057900	-0.610779	1.236349
5	9	0	1.057900	-0.610779	1.236349
6	9	0	0.000000	1.221557	-1.236349
7	9	0	-1.057900	-0.610779	-1.236349
8	9	0	1.057900	-0.610779	-1.236349