Electronic Supplementary Material (ESI) for RSC Advances.

Gauche Preference in 1,2-Difluoroethane Originates from both Orbital and Electrostatic Stabilization Interactions

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Supplementary Information

Table S1. Contribution of various energy terms to the total bonding energy between two CH_2F radicals.[a] Values are in kcal/mol.

Molecule and effects	ΔE_{es}	ΔE_{ex+rep}	ΔE_{pol}	ΔE_{disp}	ΔE_{int}	ΔE_{prep}	ΔE
anti-DFE	-158.00	258.97	-180.02	-22.96	-102.01	11.70	-90.31
gauche-DFE(a)[b]	-157.54	258.82	-180.67	-23.10	-102.49	11.70	-90.79
gauche-DFE(a)[b] C–C bond relaxed	-162.87	268.56	-184.84	-23.37	-102.51	11.70	-90.81
gauche-DFE(a)[b] all bonds relaxed	-163.15	269.08	-184.91	-23.36	-102.34	11.54	-90.80
gauche-DFE(a)[b] all bonds and CCF bond angles relaxed	-161.07	265.09	-185.24	-23.09	-104.31	13.24	-91.07
gauche-DFE	-162.09	267.63	-185.67	-23.14	-103.27	12.06	-91.21

[a] ΔE_{es} = electrostatic energy, ΔE_{ex+rep} = exchange repulsion energy, ΔE_{pol} = polarization energy, ΔE_{disp} = dispersion energy, ΔE_{int} = interaction energy, ΔE_{prep} = preparation energy, ΔE = total bonding energy. [b] *Gauche* conformer obtained by change of only the θ_{FCCF} torsional angle.

Absolute energies (atomic units) and x, y, z coordinates (Å) of the optimized structures

anti-1,2-Difluoroethane

E = -278.2596253435 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.427670	0.627310	0.000000
2	1	0	-1.053642	0.679336	0.893506
3	1	0	-1.053642	0.679336	-0.893506
4	6	0	0.427670	-0.627310	0.000000
5	1	0	1.053642	-0.679336	-0.893506
6	1	0	1.053642	-0.679336	0.893506
7	9	0	0.427670	1.734905	0.000000
8	9	0	-0.427670	-1.734905	0.000000

gauche-1,2-Difluoroethane

E = -278.2610891014 a.u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.268888	0.702578	0.510506
2	1	0	1.356305	0.705352	0.400012
3	1	0	-0.009537	1.202855	1.443889
4	6	0	-0.268888	-0.702578	0.510506
5	1	0	0.009537	-1.202855	1.443889
6	1	0	-1.356305	-0.705352	0.400012
7	9	0	-0.268888	1.441961	-0.545215
8	9	0	0.268888	-1.441961	-0.545215