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Energy Decomposition Analysis of *Gauche* Preference in 2-Haloethanol, 2-Haloethylamine (Halogen = F, Cl), Their Protonated Forms and *Anti* Preference in 1-Chloro-2-Fluoroethane

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Supplementary Information

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Table S1. Theoretically calculated (MP2/6-311++G**) and experimentally determined bond lengths (d/Å), bond angles (τ/°) and torsional angles (θ/°) of *anti* and *gauche* conformers of 1,2-difluoroethane.

Conformation		d_{CC}	d_{CF}	d_{CH}[a]	d_{CH}[b]	τ_{CCF}	τ_{CCH}[a]	τ_{CCH}[b]	θ_{FCCF}
anti	calc	1.5163	1.3917	1.0918		107.93	110.93		180
	exp[c]	1.501(4)	1.401(6)	1.094(2)		107.4(5)	111.4(2)		
gauche	calc	1.5039	1.3887	1.0926	1.0946	110.30	110.65	109.54	69.98
	exp[d]	1.493(8)	1.390(3)	1.099(2)	1.093(5)	110.6(5)	108.4(6)	111.3(6)	710(3)

[a] *Gauche* to the CF bond on the other carbon. [b] *Anti* to the CF bond on the other carbon. [c] From ref. 36 in the manuscript (infrared spectroscopy). [d] From ref. 37 in the manuscript (microwave spectroscopy).

Table S2. Theoretically calculated (MP2/6-311++G**) and experimentally determined bond lengths (d/Å), bond angles (τ/°) and torsional angles (θ/°) of *anti* and *gauche* conformers of 1-chloro-2-fluoroethane.

Conformation		d_{CC}	d_{CF} d_{CCl}	d_{CH}[a] d_{CH}[b]	d_{CH}[c] d_{CH}[d]	τ_{CCF} τ_{CCCl}	τ_{CCH}[a] τ_{CCH}[b]	τ_{CCH}[c] τ_{CCH}[d]	θ_{FCCF}
anti	calc	1.5150	1.3925	1.0895		108.33	110.68		180
			1.7793	1.0919		108.71	111.08		
	exp[e]	1.504(6)	1.391(3)	1.107(7)		108.5(11)	110.6(19)		
			1.784(3)	1.107(7)		109.3(11)	110.6(19)		
gauche	calc	1.5089	1.3874	1.0903	1.0918	110.16	110.07	109.33	67.24
			1.7781	1.0921	1.0948	111.50	111.30	110.07	
	exp[e]	1.504(6)	1.391(3)	1.107(7)	1.107(7)	111.1(4)	110.6(19)	110.6(19)	111.9(16)[f]
			1.784(3)	1.107(7)	1.107(7)	111.5(4)	110.6(19)	110.6(19)	

[a] *Gauche* to the CF bond on the other carbon. [b] *Gauche* to the CCl bond on the other carbon. [c] *Anti* to the CF bond on the other carbon. [d] *Anti* to the CCl bond on the other carbon. [e] From ref. 18a in the manuscript (electron diffraction). [f] Taking *anti* as 0°.

Table S3. Theoretically calculated (MP2/6-311++G**) and experimentally determined (values in parentheses) bond lengths (d/Å), bond angles (τ/°) and torsional angles (θ/°) of the five conformers of 2-fluoroethanol.[a]

Conformation	d_{CC}	d_{CF} d_{CO}	d_{OH}	d_{CH}[b] d_{CH}[c]	d_{CH}[d] d_{CH}[e]	τ_{CCF} τ_{CCO}	τ_{CCH}[b] τ_{CCH}[c]	τ_{CCH}[d] τ_{CCH}[e]	θ_{FCCO}
aa	1.5154	1.3937 1.4233	0.9599	1.0960/1.0962 1.0920/1.0917		108.67 105.89	109.26/109.36 110.90/110.63		177.79
ag	1.5196	1.3934 1.4219	0.9612	1.0960/1.0907 1.0946/1.0919		109.16 110.51	109.71/109.70 111.11/110.63		178.80
ga	1.5070	1.3913 1.4208	0.9597	1.0962 1.0928	1.0992 1.0940	110.29 108.25	110.29 110.22	108.29 110.32	72.12
gg	1.5119	1.3889 1.4170	0.9614	1.0916 1.0957	1.1002 1.0947	110.68 113.47	109.40 111.15	107.84 110.08	64.03
gg′(HB)[f]	1.5097 [1.518(6)]	1.4011 [1.398(24)] 1.4174 [1.432(16)]	0.9623	1.0975 1.0920	1.0931 1.0932	108.46 [108.5(8)] 111.73 [112.3(14)]	109.25 110.96	109.15 111.48	63.52 [64.0(8)]

[a] The first letter refers to the FCCO conformation, the second letter refers to the CCOH conformation. Experimental values are taken from ref. 12a in the manuscript (electron diffraction). [b] *Gauche* to the CF bond on the other carbon. [c] *Gauche* to the CO bond on the other carbon. [d] *Anti* to the CF bond on the other carbon. [e] *Anti* to the CO bond on the other carbon. [f] Structure having the OH hydrogen atom oriented toward the F atom.

Table S4. Theoretically calculated (MP2/6-311++G**) and experimentally determined (values in parentheses) bond lengths (d/Å), bond angles (τ/°) and torsional angles (θ/°) of the five conformers of 2-chloroethanol.[a]

Conformation	d_{CC}	d_{CCl} d_{CO}	d_{OH}	d_{CH}[b] d_{CH}[c]	d_{CH}[d] d_{CH}[e]	τ_{CCCl} τ_{CCO}	τ_{CCH}[b] τ_{CCH}[c]	τ_{CCH}[d] τ_{CCH}[e]	θ_{ClCCO}
aa	1.5158	1.7804 1.4235	0.9607	1.0964 1.0898		109.73 106.04	109.57 110.40		180.00
ag	1.5212	1.7818 1.4208	0.9613	1.0963/1.0909 1.0919/1.0898		109.96 110.80	109.89/109.78 111.05/110.23		177.50
ga	1.5115	1.7808 1.4191	0.9596	1.0959 1.0908	1.0994 1.0911	111.57 108.02	109.62 109.57	108.05 110.20	69.75
gg	1.5180	1.7791 1.4149	0.9615	1.0914 1.0930	1.1002 1.0920	111.82 113.62	109.90 110.75	107.61 109.76	61.84
gg′(HB)[f]	1.5166 [1.519(2)]	1.7887 [1.801(1)] 1.4145 [1.413(2)]	0.9628 [1.033(2)]	1.0973 1.0902 [1.093(2)]	1.0936 1.0910 [1.093(2)]	110.20 [110.7(1)] 112.50 [113.8(3)]	109.57 110.36	108.48 110.89	64.92 [62.4(6)]

[a] The first letter refers to the ClCCO conformation, the second letter refers to the CCOH conformation. Experimental values are taken from ref. 19a in the manuscript (electron diffraction). [b] *Gauche* to the CCl bond on the other carbon. [c] *Gauche* to the CO bond on the other carbon. [d] *Anti* to the CCl bond on the other carbon. [e] *Anti* to the CO bond on the other carbon. [f] Structure having the OH hydrogen atom oriented toward the Cl atom.

Table S5. Theoretically calculated (MP2/6-311++G**) bond lengths (d/Å), bond angles (τ/°) and torsional angles (θ/°) of the five conformers of protonated 2-fluoroethanol.[a]

Conformation	d_{CC}	d_{CF} d_{CO}	d_{OH}	d_{CH}[b] d_{CH}[c]	d_{CH}[d] d_{CH}[e]	τ_{CCF} τ_{CCO}	τ_{CCH}[b] τ_{CCH}[c]	τ_{CCH}[d] τ_{CCH}[e]	θ_{FCCO}
aa	1.5238	1.3714	0.9749	1.0881		104.29	113.33		180.00
		1.5174	0.9749	1.0936		111.15	111.71		
ag	1.5231	1.3724	0.9754	1.0882/1.0890		104.20	113.15/112.65		176.87
		1.5217	0.9753	1.0913/1.0939		107.09	111.63/111.40		
ga(HB)[f]	1.5102	1.3914	0.9814[g]	1.0881	1.0888	105.50	113.06	115.33	49.18
		1.5151	0.9755	1.0923	1.0918	107.70	112.90	109.88	
gg(HB)[f]	1.5097	1.3944	0.9822[g]	1.0892	1.0882	105.39	112.88	114.24	51.76
		1.5143	0.9751	1.0909	1.0910	103.74	112.23	110.07	
gg′	1.5057	1.3715	0.9747	1.0882	1.0901	108.84	112.44	113.46	60.74
		1.5229	0.9747	1.0952	1.0946	107.12	112.15	107.40	

[a] The first letter refers to the FCCO conformation, the second letter refers to the CCO: conformation. [b] *Gauche* to the CF bond on the other carbon. [c] *Gauche* to the CO bond on the other carbon. [d] *Anti* to the CF bond on the other carbon. [e] *Anti* to the CO bond on the other carbon. [f] Structure having an OH_2^+ hydrogen atom oriented toward the F atom. [g] Oriented toward the F atom.

Table S6. Theoretically calculated (MP2/6-311++G**) bond lengths (d/Å), bond angles (τ/°) and torsional angles (θ/°) of the five conformers of protonated 2-chloroethanol.[a]

Conformation	d_{CC}	d_{CCl} d_{CO}	d_{OH}	d_{CH}[b] d_{CH}[c]	d_{CH}[d] d_{CH}[e]	τ_{CCCl} τ_{CCO}	τ_{CCH}[b] τ_{CCH}[c]	τ_{CCH}[d] τ_{CCH}[e]	θ_{ClCCO}
aa	1.5114	1.7663	0.9745	1.0881		104.56	113.82		180.00
		1.5355	0.9745	1.0914		111.64	111.71		
ag	1.5096	1.7669	0.9749	1.0881/1.0890		104.54	112.93/113.85		-178.63
		1.5397	0.9754	1.0898/1.0917		107.60	111.13/111.80		
ga(HB)[f]	1.5129	1.7817	0.9933[g]	1.0877	1.0893	107.64	112.93	114.52	48.68
		1.5085	0.9753	1.0907	1.0909	108.54	112.37	108.97	
gg(HB)[f]	1.5116	1.7838	0.9956[g]	1.0893	1.0886	107.80	112.69	113.53	52.14
		1.5065	0.9751	1.0899	1.0903	104.78	111.62	109.18	
gg′	1.5050	1.7652	0.9751	1.0878	1.0905	111.18	113.25	112.89	57.67
		1.5249	0.9746	1.0932	1.0933	107.80	111.38	106.55	

[a] The first letter refers to the ClCCO conformation, the second letter refers to the CCO: conformation. [b] *Gauche* to the CCl bond on the other carbon. [c] *Gauche* to the CO bond on the other carbon. [d] *Anti* to the CCl bond on the other carbon. [e] *Anti* to the CO bond on the other carbon. [f] Structure having an OH_2^+ hydrogen atom oriented toward the Cl atom. [g] Oriented toward the Cl atom.

Table S7. Theoretically calculated (MP2/6-311++G**) and experimentally determined (values in parentheses) bond lengths (d/Å), bond angles (τ/°) and torsional angles (θ/°) of the five conformers of 2-fluoroethylamine.[a]

Conformation	d_{CC}	d_{CF} d_{CN}	d_{NH}	d_{CH}[b] d_{CH}[c]	d_{CH}[d] d_{CH}[e]	τ_{CCF} τ_{CCN}	τ_{CCH}[b] τ_{CCH}[c]	τ_{CCH}[d] τ_{CCH}[e]	θ_{FCCN}
aa	1.5217	1.3951 1.4602	1.0149 1.0149	1.0935 1.0947		109.96 113.82	109.05 110.97		180.00
ag	1.5175	1.3955 1.4647	1.0148 1.0135	1.0984/1.0930 1.0943/1.0916		109.54 108.25	108.83/108.76 110.94/110.75		-177.59
ga(HB)[f]	1.5173 [1.516(3)]	1.3985 [1.398(3)] 1.4585 [1.461(3)]	1.0150[g] 1.0155	1.0944 1.0946	1.0960 1.0943	109.25 [109.3(5)] 115.48 [115.5(5)]	108.57 111.34	108.12 111.48	60.96 [60.9(5)]
gg(HB)[f]	1.5098 [1.509(3)]	1.4009 [1.400(3)] 1.4619 [1.466(3)]	1.0154[g] 1.0146	1.1002 1.0922	1.0955 1.0930	108.95 [109.2(5)] 109.57 [109.8(5)]	108.38 110.72	107.81 111.49	65.05 [65.3(5)]
gg′	1.5139	1.3899 1.4607	1.0150 1.0139	1.0937 1.0951	1.1027 1.0943	110.82 111.06	108.20 110.96	107.08 110.32	68.19

[a] The first letter refers to the FCCN conformation, the second letter refers to the CCN: conformation. Experimental values are taken from ref. 13d in the manuscript. [b] *Gauche* to the CF bond on the other carbon. [c] *Gauche* to the CN bond on the other carbon. [d] *Anti* to the CF bond on the other carbon. [e] *Anti* to the CN bond on the other carbon. [f] Structure having an NH_2 hydrogen atom oriented toward the F atom. [g] Oriented toward the F atom.

Table S8. Theoretically calculated (MP2/6-311++G**) bond lengths (d/Å), bond angles (τ/°) and torsional angles (θ/°) of the five conformers of 2-chloroethylamine.[a]

Conformation	d_{CC}	d_{CCl} d_{CN}	d_{NH}	d_{CH}[b] d_{CH}[c]	d_{CH}[d] d_{CH}[e]	τ_{CCCl} τ_{CCN}	τ_{CCH}[b] τ_{CCH}[c]	τ_{CCH}[d] τ_{CCH}[e]	θ_{ClCCN}
aa	1.5260	1.7855 1.4582	1.0147 1.0147	1.0935 1.0920		110.78 114.03	109.16 110.77		180.00
ag	1.5202	1.7840 1.4639	1.0150 1.0142	1.0986/1.0932 1.0917/1.0895		110.50 108.45	109.11/108.88 110.84/110.26		179.92
ga(HB)[f]	1.5256	1.7860 1.4547	1.0150[g] 1.0154	1.0941 1.0923	1.0966 1.0921	111.03 116.45	108.85 110.83	107.30 110.73	62.96
gg(HB)[f]	1.5155	1.7900 1.4604	1.0156[g] 1.0146	1.0999 1.0903	1.0959 1.0904	110.76 110.12	108.83 109.98	107.36 111.06	67.38
gg′	1.5190	1.7809 1.4585	1.0151 1.0138	1.0934 1.0926	1.1027 1.0913	112.16 110.98	109.03 110.38	106.81 110.14	66.72

[a] The first letter refers to the ClCCN conformation, the second letter refers to the CCN: conformation. [b] *Gauche* to the CCl bond on the other carbon. [c] *Gauche* to the CN bond on the other carbon. [d] *Anti* to the CCl bond on the other carbon. [e] *Anti* to the CN bond on the other carbon. [f] Structure having an NH_2 hydrogen atom oriented toward the Cl atom. [g] Oriented toward the Cl atom.

Table S9. Theoretically calculated (MP2/6-311++G**) bond lengths (d/Å), bond angles (τ/°) and torsional angles (θ/°, an experimental value is included, as well) of *anti* and *gauche* conformers of protonated 2-fluoroethylamine.

Conformation		d_{CC}	d_{CF} d_{CN}	d_{NH}	d_{CH}^a d_{CH}^b	d_{CH}^c d_{CH}^d	τ_{CCF} τ_{CCN}	τ_{CCH}^a τ_{CCH}^b	τ_{CCH}^c τ_{CCH}^d	θ_{FCCN}
anti	calc	1.5264	1.3707 1.5107	1.0257 1.0257 1.0254	1.0904 1.0947		106.07 110.39	111.03 111.46		180.00
gauche	calc	1.5169	1.3903 1.5098	1.0276[e] 1.0251 1.0242	1.0905 1.0934	1.0909 1.0906	106.45 108.10	111.07 112.39	112.45 110.30	51.52
	exp[f]									67.83(1)

[a] *Gauche* to the CF bond on the other carbon. [b] *Gauche* to the CN bond on the other carbon. [c] *Anti* to the CF bond on the other carbon. [d] *Anti* to the CN bond on the other carbon. [e] Oriented toward the F atom. [f] From ref. 12e in the manuscript (X-ray data).

Table S10. Theoretically calculated (MP2/6-311++G**) bond lengths (d/Å), bond angles (τ/°) and torsional angles (θ/°) of *anti* and *gauche* conformers of protonated 2-chloroethylamine.

Conformation	d_{CC}	d_{CCl} d_{CN}	d_{NH}	d_{CH}^a d_{CH}^b	d_{CH}^c d_{CH}^d	τ_{CCCl} τ_{CCN}	τ_{CCH}^a τ_{CCH}^b	τ_{CCH}^c τ_{CCH}^d	θ_{ClCCN}
anti	1.5206	1.7633 1.5158	1.0256 1.0256 1.0258	1.0907 1.0928		107.50 110.50	111.50 111.09		180.00
gauche	1.5176	1.7770 1.5087	1.0290[e] 1.0251 1.0241	1.0904 1.0919	1.0916 1.0900	109.49 109.73	111.13 111.70	111.69 108.85	56.99

[a] *Gauche* to the CCl bond on the other carbon. [b] *Gauche* to the CN bond on the other carbon. [c] *Anti* to the CCl bond on the other carbon. [d] *Anti* to the CN bond on the other carbon. [e] Oriented toward the Cl atom.

Table S11. Comparison of LMOEDA and NBOEDA results.[a,b] Values are in kcal/mol.

	LMOEDA							NBOEDA			
Conformational isomerization	ΔE_{elstat}	ΔE_{ex+rep}	ΔE_{pol}	ΔE_{disp}	ΔE_{int}	ΔE_{prep}	ΔE	$\Delta E_{elstat+struct}$	ΔE_{steric}	ΔE_{deloc}	ΔE
a-DFE → *g*-DFE	-3.38	7.57	-4.53	-0.61	-0.95	0.18	-0.77	-6.38	13.15	-7.57	-0.80
a-CFE → *g*-CFE	-0.82	3.66	-2.13	-0.37	0.34	0.18	0.52	-1.59	5.62	-3.46	-0.57
aa-FE → *ga*-FE	-2.73	7.30	-3.82	-0.42	0.33	-0.48	-0.15	-0.10	5.56	-5.55	-0.09
ag-FE → *gg*-FE	-1.28	3.86	-2.55	-0.69	-0.66	0.75	0.09	-1.72	9.02	-7.15	0.15
ag′-FE → *gg′*-FE	-5.34	5.77	-3.03	-0.51	-3.11	0.57	-2.54	-10.36	11.03	-3.07	-2.41
aa-CE → *ga*-CE	-1.29	5.07	-2.25	-0.39	1.14	-0.62	0.52	-1.41	4.45	-2.27	0.77
ag-CE → *gg*-CE	0.59	1.17	-0.92	-0.64	0.20	0.76	0.96	-0.65	5.69	-3.82	1.22
ag′-CE → *gg′*-CE	-3.45	3.97	-2.01	-0.66	-2.15	0.46	-1.69	-4.14	5.30	-2.64	-1.49
aa-FEH → *ga*-FEH	-12.84	9.60	-5.26	-0.16	-8.66	0.80	-7.86	-23.75	15.35	-0.77	-7.63
ag-FEH → *gg*-FEH	-12.32	9.52	-5.40	-0.84	-9.04	0.81	-8.23	-23.14	15.83	-0.66	-7.98
ag′-FEH → *gg′*-FEH	-6.88	8.41	-5.82	-0.72	-5.01	0.80	-4.21	-5.73	8.52	-6.95	-4.16
aa-CEH → *ga*-CEH	-9.86	9.13	-4.33	-1.86	-6.92	0.96	-5.96	-22.57	26.52	-9.56	-5.61
ag-CEH → *gg*-CEH	-9.48	9.65	-5.04	-2.61	-7.48	0.79	-6.69	-20.20	28.12	-14.05	-6.13
ag′-CEH → *gg′*-CEH	-2.66	1.70	-0.74	-0.81	-2.51	0.72	-1.79	0.40	0.36	-2.00	-1.24
aa-FEA → *ga*-FEA	-2.71	2.43	-1.17	-0.06	-1.51	0.34	-1.17	-9.62	10.15	-1.62	-1.08
ag-FEA → *gg*-FEA	-1.46	1.04	-1.62	-1.28	-3.32	1.93	-1.39	-8.74	9.81	-2.29	-1.22
ag′-FEA → *gg′*-FEA	1.22	1.08	-1.26	-0.69	0.35	0.84	1.19	-0.30	6.51	-5.01	1.20
aa-CEA → *ga*-CEA	-1.21	1.04	-0.39	-0.23	-0.79	0.21	-0.58	-7.88	9.06	-1.48	-0.30
ag-CEA → *gg*-CEA	-0.89	0.96	-1.25	-1.41	-2.59	1.58	-1.01	-0.62	1.74	-1.77	-0.65
ag′-CEA → *gg′*-CEA	1.94	-0.09	-0.40	-0.73	0.72	0.72	1.44	0.47	3.51	-2.29	1.69
a-FEAH → *g*- FEAH	-9.45	5.96	-3.55	-0.14	-7.18	0.34	-6.84	-16.35	8.63	1.12	-6.60
a- CEAH → *g*-CEAH	-6.65	4.49	-2.34	-0.93	-5.43	0.19	-5.24	-6.22	4.38	-3.21	-5.06

[a] In the LMOEDA scheme: ΔE_{elstat} = 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 energy change upon isomerization. In the NBOEDA scheme: $\Delta E_{elstat+struct}$ = electrostatic and structural energy, ΔE_{steric} = exchange repulsion energy, ΔE_{deloc} = delocalization energy, ΔE = total energy change upon isomerization. [b] LMOEDA was performed at the MP2/6-311++G(d,p)//MP2/6-311++G(d,p) level, NBOEDA was performed at the B3LYP/6-311++G(d,p)//MP2/6-311++G(d,p) level.

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

a-1,2-difluoroethane
E = – 277.7327044

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.426695	0.626668	0.000000
2	1	0	-1.051960	0.672765	0.893772
3	1	0	-1.051960	0.672765	-0.893772
4	6	0	0.426695	-0.626668	0.000000
5	1	0	1.051960	-0.672765	-0.893772
6	1	0	1.051960	-0.672765	0.893772
7	9	0	0.426695	1.726036	0.000000
8	9	0	-0.426695	-1.726036	0.000000

g-1,2-difluoroethane
E = – 277.7339398

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.264733	0.703813	0.516113
2	1	0	1.353067	0.706126	0.419196
3	1	0	-0.030304	1.206018	1.442887
4	6	0	-0.264733	-0.703813	0.516113
5	1	0	0.030304	-1.206018	1.442887
6	1	0	-1.353067	-0.706126	0.419196
7	9	0	-0.264733	1.417663	-0.550973
8	9	0	0.264733	-1.417663	-0.550973

a-1-chloro-2-fluoroethane
E = – 637.7138882

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.972281	-0.540694	0.000000
2	1	0	-0.848620	-1.156277	0.893261
3	1	0	-0.848620	-1.156277	-0.893261
4	6	0	0.000000	0.621214	0.000000
5	1	0	-0.132210	1.233440	-0.891473
6	1	0	-0.132210	1.233440	0.891473
7	9	0	-2.267096	-0.028303	0.000000
8	17	0	1.658777	-0.022513	0.000000

g-1-chloro-2-fluoroethane
E = – 637.7130430

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.192865	0.418273	0.362987
2	1	0	1.053077	0.246445	1.432413
3	1	0	1.956223	1.186454	0.202822
4	6	0	-0.095394	0.844903	-0.296654
5	1	0	0.032522	0.881415	-1.378852
6	1	0	-0.381312	1.831458	0.073333
7	9	0	1.652311	-0.761761	-0.203794
8	17	0	-1.418596	-0.286411	0.065084

aa-2-fluoroethanol
E = – 253.7305429

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.581990	-0.502774	-0.016171
2	1	0	-0.534417	-1.147629	0.863763
3	1	0	-0.550748	-1.109066	-0.923533
4	6	0	0.548923	0.505798	-0.000661
5	1	0	0.485153	1.134294	-0.896345
6	1	0	0.455228	1.143282	0.886140
7	9	0	-1.793825	0.185051	0.008986
8	8	0	1.750516	-0.256523	0.025329
9	1	0	2.483480	0.347703	-0.112538

ag-2-fluoroethanol
E = – 253.7301644

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.575162	-0.499600	-0.047645
2	1	0	0.540097	-1.052652	-0.988465
3	1	0	0.520814	-1.200545	0.791265
4	6	0	-0.550288	0.519392	0.016697
5	1	0	-0.465342	1.106358	0.938411
6	1	0	-0.479092	1.199875	-0.832691
7	9	0	1.797977	0.163931	0.029971
8	8	0	-1.813078	-0.125631	-0.088085
9	1	0	-1.942890	-0.642114	0.712113

ga-2-fluoroethanol
E = – 253.7307894

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.717873	0.504284	0.309747
2	1	0	0.641575	0.396185	1.394465
3	1	0	1.273595	1.412531	0.058717
4	6	0	-0.656279	0.544147	-0.307733
5	1	0	-0.556633	0.443883	-1.394802
6	1	0	-1.107442	1.520831	-0.082617
7	9	0	1.435302	-0.582708	-0.179607
8	8	0	-1.424780	-0.513505	0.248540
9	1	0	-2.140140	-0.711610	-0.359701

gg-2-fluoroethanol
E = – 253.7300111

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.714656	0.506653	0.314613
2	1	0	0.662088	0.402359	1.404029
3	1	0	1.268554	1.417497	0.065591
4	6	0	-0.667595	0.556341	-0.295997
5	1	0	-1.134814	1.505943	0.004513
6	1	0	-0.583929	0.543223	-1.384318
7	9	0	1.428516	-0.579409	-0.175312
8	8	0	-1.476248	-0.555794	0.046399
9	1	0	-1.540927	-0.585948	1.005104

gg′-2-fluoroethanol
E = – 253.7342108

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.714525	0.559643	0.285447
2	1	0	0.688960	0.518989	1.376423
3	1	0	1.296490	1.420188	-0.055068
4	6	0	-0.682242	0.575275	-0.287209
5	1	0	-1.190617	1.488719	0.032268
6	1	0	-0.624110	0.573245	-1.383199
7	9	0	1.363116	-0.600213	-0.158428
8	8	0	-1.456887	-0.512005	0.188929
9	1	0	-0.977379	-1.312687	-0.045431

aa-2-fluoroethanol (protonated)
E = – 254.0178528

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.209414	-0.822144	0.000000
2	1	0	0.206388	-1.288214	0.897649
3	1	0	0.206388	-1.288214	-0.897649
4	6	0	0.000000	0.687240	0.000000
5	1	0	-0.377833	1.174667	-0.896471
6	1	0	-0.377833	1.174667	0.896471
7	9	0	-1.572278	-0.974727	0.000000
8	8	0	1.476946	1.035121	0.000000
9	1	0	1.967153	0.764046	0.797849
10	1	0	1.967153	0.764046	-0.797849

ag-2-fluoroethanol (protonated)
E = – 254.0186895

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.669533	0.523894	-0.080258
2	1	0	0.594142	1.251498	0.733135
3	1	0	0.646573	1.028785	-1.047457
4	6	0	-0.415260	-0.540796	0.016625
5	1	0	-0.436239	-1.197857	-0.850576
6	1	0	-0.385115	-1.099001	0.951258
7	9	0	1.842121	-0.177372	0.049540
8	8	0	-1.754732	0.179014	-0.041310
9	1	0	-2.505247	-0.393241	-0.287146
10	1	0	-1.980987	0.675459	0.767195

ga-2-fluoroethanol (protonated)
E = – 254.0303603

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.833333	0.553963	0.283211
2	1	0	0.862123	0.555223	1.375141
3	1	0	1.502945	1.318689	-0.115411
4	6	0	-0.558570	0.752059	-0.268098
5	1	0	-0.587355	0.772173	-1.355591
6	1	0	-1.117184	1.580718	0.164121
7	9	0	1.234179	-0.702087	-0.161303
8	8	0	-1.363304	-0.490116	0.055799
9	1	0	-0.822806	-1.288339	-0.128332
10	1	0	-1.687480	-0.534881	0.974732

gg-2-fluoroethanol (protonated)
E = – 254.0317981

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.840016	0.557391	0.263047
2	1	0	0.883958	0.564774	1.353074
3	1	0	1.505952	1.310941	-0.159983
4	6	0	-0.564312	0.758634	-0.253315
5	1	0	-1.094390	1.590592	0.206151
6	1	0	-0.618592	0.766160	-1.341126
7	9	0	1.219206	-0.709224	-0.179963
8	8	0	-1.298176	-0.483384	0.206882
9	1	0	-2.181913	-0.608035	-0.185952
10	1	0	-0.736683	-1.270486	0.034050

gg′-2-fluoroethanol (protonated)
E = – 254.0253935

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.830617	0.483658	0.323353
2	1	0	0.788796	0.388461	1.413565
3	1	0	1.448541	1.349422	0.065108
4	6	0	-0.530896	0.706304	-0.279716
5	1	0	-1.035592	1.593248	0.103509
6	1	0	-0.515533	0.664273	-1.366990
7	9	0	1.369332	-0.659761	-0.209100
8	8	0	-1.385614	-0.500113	0.085222
9	1	0	-1.450458	-0.682809	1.040481
10	1	0	-2.273151	-0.513617	-0.317375

aa-2-chloroethanol
E = – 613.7111264

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.613296	0.000000
2	1	0	-0.148945	1.222303	0.891383
3	1	0	-0.148945	1.222303	-0.891383
4	6	0	-0.953355	-0.565206	0.000000
5	1	0	-0.777361	-1.179892	-0.890682
6	1	0	-0.777361	-1.179892	0.890682
7	17	0	1.681003	0.026587	0.000000
8	8	0	-2.264384	-0.010628	0.000000
9	1	0	-2.889251	-0.740316	0.000000

ag-2-chloroethanol
E = – 613.7111900

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.044875	0.605468	-0.043696
2	1	0	0.054848	1.169636	-0.970740
3	1	0	0.052245	1.283449	0.806668
4	6	0	1.000098	-0.498405	0.015397
5	1	0	0.871446	-1.085145	0.932473
6	1	0	0.879048	-1.167443	-0.837754
7	17	0	-1.679735	-0.100957	0.012459
8	8	0	2.310468	0.041319	-0.086049
9	1	0	2.482823	0.542853	0.715739

ga-2-chloroethanol
E = – 613.7103219

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.127700	0.850795	-0.295958
2	1	0	0.005704	0.874546	-1.378272
3	1	0	-0.449291	1.830977	0.059508
4	6	0	1.172680	0.456323	0.365923
5	1	0	1.879828	1.290350	0.251671
6	1	0	1.003594	0.282159	1.434592
7	17	0	-1.426523	-0.311874	0.067944
8	8	0	1.659523	-0.708443	-0.282307
9	1	0	2.264996	-1.151345	0.316111

gg-2-chloroethanol
E = – 613.7096663

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.123236	0.854162	0.301064
2	1	0	0.014661	0.895972	1.387816
3	1	0	0.435773	1.835996	-0.060566
4	6	0	-1.187107	0.458759	-0.355444
5	1	0	-1.909604	1.267422	-0.169899
6	1	0	-1.047869	0.361104	-1.433469
7	17	0	1.422547	-0.304677	-0.065218
8	8	0	-1.687432	-0.789564	0.084078
9	1	0	-1.793577	-0.742009	1.038485

gg′-2-chloroethanol
E = – 613.7138840

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.104646	0.891709	-0.291114
2	1	0	-0.000037	0.942494	-1.375047
3	1	0	-0.424762	1.856502	0.105226
4	6	0	1.199968	0.451723	0.344849
5	1	0	1.958729	1.212549	0.141254
6	1	0	1.069946	0.370041	1.431365
7	17	0	-1.395905	-0.293692	0.065042
8	8	0	1.692436	-0.753381	-0.208283
9	1	0	1.015092	-1.422371	-0.064657

aa-2-chloroethanol (protonated)
E = – 614.0035081

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.661998	0.000000
2	1	0	-0.221450	1.243292	0.896714
3	1	0	-0.221450	1.243292	-0.896714
4	6	0	-0.725331	-0.664038	0.000000
5	1	0	-0.557872	-1.256609	-0.897115
6	1	0	-0.557872	-1.256609	0.897115
7	17	0	1.712941	0.231024	0.000000
8	8	0	-2.249289	-0.475781	0.000000
9	1	0	-2.607529	-0.041142	0.795249
10	1	0	-2.607529	-0.041142	-0.795249

ag-2-chloroethanol (protonated)
E = – 614.0040151

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.134067	0.648136	-0.057464
2	1	0	0.032747	1.331824	0.787560
3	1	0	0.026665	1.183179	-1.000784
4	6	0	-0.841520	-0.500531	0.030733
5	1	0	-0.800124	-1.159239	-0.834385
6	1	0	-0.791422	-1.049624	0.969865
7	17	0	1.725931	-0.115372	0.012888
8	8	0	-2.261839	0.086965	-0.059680
9	1	0	-2.960719	-0.579213	-0.198255
10	1	0	-2.508539	0.653044	0.694729

ga-2-chloroethanol (protonated)
E = – 614.0130095

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.171186	0.983552	0.292079
2	1	0	0.107054	1.102156	1.374376
3	1	0	0.517945	1.911735	-0.164344
4	6	0	-1.155343	0.597870	-0.324642
5	1	0	-2.002857	1.189483	0.019223
6	1	0	-1.117548	0.541679	-1.410274
7	17	0	1.333004	-0.318331	-0.068323
8	8	0	-1.470734	-0.824537	0.066446
9	1	0	-0.602410	-1.306793	0.065490
10	1	0	-1.892437	-0.918863	0.940834

gg-2-chloroethanol (protonated)
E = – 614.0146769

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.175033	0.990184	-0.271019
2	1	0	-0.117739	1.121405	-1.351449
3	1	0	-0.520783	1.907226	0.206648
4	6	0	1.162769	0.599465	0.314159
5	1	0	1.988565	1.213201	-0.041356
6	1	0	1.136195	0.507840	1.399282
7	17	0	-1.328047	-0.325237	0.078369
8	8	0	1.433577	-0.778054	-0.232298
9	1	0	2.131484	-1.273958	0.234409
10	1	0	0.564050	-1.260140	-0.180263

gg′-2-chloroethanol (protonated)
E = – 614.0068740

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.225733	0.896534	0.324025
2	1	0	0.119134	0.959335	1.410227
3	1	0	0.571340	1.866379	-0.043867
4	6	0	-1.097344	0.631896	-0.342670
5	1	0	-1.872184	1.338175	-0.042775
6	1	0	-1.019377	0.518521	-1.421745
7	17	0	1.406760	-0.349767	-0.085530
8	8	0	-1.572465	-0.749174	0.095661
9	1	0	-1.409307	-0.953108	1.035138
10	1	0	-2.495148	-0.960451	-0.136393

aa-2-fluoroethylamine
E = – 233.8774020

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.070825	-0.769431	0.000000
2	1	0	0.408614	-1.183905	0.892621
3	1	0	0.408614	-1.183905	-0.892621
4	6	0	0.000000	0.750591	0.000000
5	1	0	-0.524292	1.132289	-0.880397
6	1	0	-0.524292	1.132289	0.880397
7	9	0	-1.402850	-1.184191	0.000000
8	7	0	1.361850	1.277417	0.000000
9	1	0	1.874499	0.966035	0.818736
10	1	0	1.874499	0.966035	-0.818736

ag-2-fluoroethylamine
E = – 233.8776015

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.603040	-0.491473	-0.080264
2	1	0	0.585206	-0.998395	-1.046917
3	1	0	0.538945	-1.233026	0.721964
4	6	0	-0.528143	0.515125	0.019962
5	1	0	-0.398158	1.104177	0.937929
6	1	0	-0.463907	1.201816	-0.828003
7	9	0	1.826589	0.167139	0.048380
8	7	0	-1.797287	-0.211658	-0.060304
9	1	0	-2.008176	-0.662196	0.824219
10	1	0	-2.561577	0.423072	-0.260668

ga-2-fluoroethylamine
E = – 233.8792653

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.754074	0.536634	0.294223
2	1	0	0.722808	0.490571	1.387384
3	1	0	1.368507	1.384418	-0.023921
4	6	0	-0.642020	0.610106	-0.295445
5	1	0	-1.094648	1.558151	0.017068
6	1	0	-0.558673	0.634580	-1.386375
7	9	0	1.381445	-0.631551	-0.150246
8	7	0	-1.535558	-0.483353	0.069602
9	1	0	-1.120485	-1.370426	-0.197060
10	1	0	-1.673933	-0.510309	1.075229

gg-2-fluoroethylamine
E = – 233.8798471

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.754144	0.538151	0.292490
2	1	0	0.718850	0.478733	1.382527
3	1	0	1.364630	1.386088	-0.028256
4	6	0	-0.639442	0.610611	-0.283872
5	1	0	-1.087437	1.556258	0.040445
6	1	0	-0.560259	0.633535	-1.380976
7	9	0	1.377423	-0.628336	-0.169420
8	7	0	-1.442936	-0.493927	0.237121
9	1	0	-2.383803	-0.458806	-0.140950
10	1	0	-1.036444	-1.375861	-0.059562

gg′-2-fluoroethylamine
E = – 233.8757129

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.750145	0.485715	0.322449
2	1	0	0.675289	0.359839	1.407700
3	1	0	1.328351	1.387924	0.100849
4	6	0	-0.623239	0.573151	-0.308507
5	1	0	-0.504103	0.521953	-1.394497
6	1	0	-1.028630	1.569315	-0.065216
7	9	0	1.456203	-0.601207	-0.179555
8	7	0	-1.468362	-0.539428	0.117607
9	1	0	-1.738515	-0.430731	1.089990
10	1	0	-2.321122	-0.574633	-0.429726

a-2-fluoroethylamine (protonated)
E = – 234.2214713

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.213404	-0.827003	0.000000
2	1	0	0.210803	-1.291294	0.896022
3	1	0	0.210803	-1.291294	-0.896022
4	6	0	0.000000	0.684404	0.000000
5	1	0	-0.431080	1.140397	-0.891728
6	1	0	-0.431080	1.140397	0.891728
7	9	0	-1.570611	-1.018616	0.000000
8	7	0	1.475706	1.007575	0.000000
9	1	0	1.946533	0.625563	-0.827296
10	1	0	1.633475	2.020774	0.000000
11	1	0	1.946533	0.625563	0.827296

g-2-fluoroethylamine (protonated)
E = – 234.2323837

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.862879	0.538742	0.272058
2	1	0	0.898689	0.540412	1.364821
3	1	0	1.532716	1.302676	-0.124280
4	6	0	-0.542630	0.743758	-0.260389
5	1	0	-0.546180	0.791297	-1.349819
6	1	0	-1.021219	1.630637	0.157349
7	9	0	1.273453	-0.713221	-0.171862
8	7	0	-1.367571	-0.463541	0.115692
9	1	0	-1.485621	-0.542623	1.130916
10	1	0	-2.300128	-0.439835	-0.307167
11	1	0	-0.887823	-1.313793	-0.204913

aa-2-chloroethylamine
E = – 593.8582034

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.599368	0.000000
2	1	0	-0.158288	1.211883	0.890055
3	1	0	-0.158288	1.211883	-0.890055
4	6	0	-0.934595	-0.606927	0.000000
5	1	0	-0.726165	-1.222486	-0.879429
6	1	0	-0.726165	-1.222486	0.879429
7	17	0	1.707599	0.077691	0.000000
8	7	0	-2.351100	-0.260653	0.000000
9	1	0	-2.597505	0.285191	0.819148
10	1	0	-2.597505	0.285191	-0.819148

ag-2-chloroethylamine
E = – 593.8579236

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.067970	0.598808	-0.072050
2	1	0	0.022464	1.132189	-1.017731
3	1	0	0.031457	1.305913	0.753708
4	6	0	0.986764	-0.492024	0.019962
5	1	0	0.818238	-1.079111	0.933145
6	1	0	0.872167	-1.167546	-0.831841
7	17	0	-1.704672	-0.105219	0.019153
8	7	0	2.307951	0.133126	-0.061277
9	1	0	2.543540	0.589117	0.814423
10	1	0	3.023144	-0.564429	-0.235830

ga-2-chloroethylamine
E = – 593.8591210

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.149432	0.886714	0.298480
2	1	0	0.045312	0.934695	1.384758
3	1	0	0.500473	1.850500	-0.076372
4	6	0	-1.173413	0.501747	-0.356702
5	1	0	-1.027174	0.440597	-1.439243
6	1	0	-1.880690	1.318283	-0.167906
7	17	0	1.416649	-0.320093	-0.058858
8	7	0	-1.780433	-0.742099	0.091190
9	1	0	-1.155060	-1.523042	-0.080091
10	1	0	-1.958985	-0.715524	1.090438

gg-2-chloroethylamine
E = – 593.8595548

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.147362	0.885132	-0.305149
2	1	0	-0.030688	0.907387	-1.388931
3	1	0	-0.504724	1.848117	0.060767
4	6	0	1.166167	0.507293	0.349532
5	1	0	1.873100	1.322658	0.158729
6	1	0	1.014356	0.439454	1.436761
7	17	0	-1.414030	-0.322473	0.070820
8	7	0	1.699332	-0.708556	-0.258926
9	1	0	2.600831	-0.941514	0.144136
10	1	0	1.077471	-1.488726	-0.069223

gg′-2-chloroethylamine
E = – 593.8556452

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.163917	0.844392	0.307816
2	1	0	0.034932	0.859760	1.392644
3	1	0	0.512318	1.824387	-0.022453
4	6	0	-1.147393	0.497778	-0.376026
5	1	0	-0.965546	0.355997	-1.444830
6	1	0	-1.807010	1.374294	-0.263777
7	17	0	1.447290	-0.332779	-0.064608
8	7	0	-1.706055	-0.737617	0.161532
9	1	0	-2.041180	-0.596196	1.109206
10	1	0	-2.494202	-1.050692	-0.393916

a-2-chloroethylamine (protonated)
E = – 594.2048643

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.639920	0.000000
2	1	0	-0.239388	1.221821	0.893512
3	1	0	-0.239388	1.221821	-0.893512
4	6	0	-0.736421	-0.690417	0.000000
5	1	0	-0.504558	-1.275670	-0.890717
6	1	0	-0.504558	-1.275670	0.890717
7	17	0	1.728149	0.289447	0.000000
8	7	0	-2.235646	-0.467233	0.000000
9	1	0	-2.538249	0.058843	-0.826792
10	1	0	-2.746095	-1.356980	0.000000
11	1	0	-2.538249	0.058843	0.826792

g-2-chloroethylamine (protonated)
E = – 594.2132500

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.232582	0.941971	0.296211
2	1	0	0.148058	1.037514	1.380647
3	1	0	0.608321	1.877210	-0.118921
4	6	0	-1.105465	0.623283	-0.345039
5	1	0	-1.012464	0.540854	-1.428345
6	1	0	-1.863574	1.364988	-0.086714
7	17	0	1.390138	-0.355182	-0.071306
8	7	0	-1.596199	-0.718372	0.140178
9	1	0	-1.797984	-0.707623	1.145111
10	1	0	-2.444518	-1.018903	-0.348494
11	1	0	-0.859490	-1.418856	-0.019360