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SUPPLEMENTARY INFORMATION

The contribution of non-classical CHax···OC hydrogen bonds to the anomeric effect in fluoro and oxa-methoxycyclohexanes

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Computational details

All compounds were optimized at the M06-2X/aug-cc-pVTZ theoretical level and harmonic frequency calculations were carried out at the same level using SuperFine integration grids in order to identify each conformer as true energy minima, showing no imaginary frequencies using the Gaussian16 Rev C.01 program.[1] The same harmonic frequency calculations were used to obtain enthalpies and Gibbs free energies at standard pressure and temperature for gas phase calculations. Single point harmonic frequency calculations using the PCM solvent implicit model were run at standard pressure and temperature. DLPNO-CCSD(T)/def2-TZVP single point calculations were run using ORCA 4.2.1 package of programs.[2] NBO calculations, including NPA, NCE and NSA analysis were done at the M06-2X/aug-cc-pVTZ level using the NBO 7.0 program.[3] QTAIM topological analysis was done on the electron densities obtained from the M06-2X/aug-cc-pVTZ optimized geometries through the AIMALL 19.10.12 program using 10^{-6} au envelope for integrations.[4] The quality of the integral properties were confirmed by the integrated values of the Laplacian of the charge density in each atom (that should be zero for an ideal integration), which were always lower than 10^{-3} au. The NCI calculations were performed on the same M06-2X/aug-cc-pVTZ electron densities using the NCIPLOT 3.0 program.[5]

1 Results and Discussion

Table S1: Gas phase calculated electronic energy (Δ*E*) from DLPNO-CCSD(T)/def2-TZVP and M06-2X/aug-cc-pVTZ for molecule 1-18 and their respective Absolute Error, in kcal mol^{-1}.

Compound	Δ*E* DLPNO-CCSD(T)	Δ*E* M06-2X	Absolute Error
1	-1.23	-1.39	0.16
2	-1.54	-1.36	0.18
3	1.71	0.80	0.91
4	-1.09	-1.08	0.01
5	-2.42	-2.28	0.14
6	-2.80	-2.96	0.16
7	2.59	2.53	0.06
8	-3.61	-3.81	0.20
9	-0.94	-0.79	0.15
10	-0.59	-0.60	0.01
11	-0.43	-0.41	0.02
12	-0.46	-0.47	0.01
13	0.42	0.35	0.07
14	0.23	0.25	0.02
15	-1.11	-1.26	0.15
16	-0.72	-0.90	0.18
17	1.88	1.59	0.29
18	0.20	-0.03	0.23
		MAE:	0.16

Table S2. Gas phase calculated total relative energy (Δ*E*), total relative enthalpy energy (Δ*H*) and total relative Gibbs free energy (Δ*G*) obtained at the M06-2X/aug-cc-pVTZ theoretical level for compounds 1-18, in kcal mol^{-1}. Negative energy values represent axial preference, and the positive ones equatorial preference.

Compound	Δ*E*	Δ*H*	Δ*G*
1	-1.39	-1.21	-1.10
2	-1.36	-1.30	-1.22
3	0.80	0.83	1.42
4	-1.08	-1.00	-0.74
5	-2.28	-2.17	-2.06
6	-2.96	-2.94	-2.56
7	2.53	2.50	3.05
8	-3.81	-3.83	-3.40
9	-0.79	-0.69	-0.59
10	-0.60	-0.43	-0.26
11	-0.41	-0.27	0.25
12	-0.47	-0.40	-0.10
13	0.35	0.39	0.87
14	0.25	0.35	0.36
15	-1.26	-1.04	-1.02
16	-0.90	-0.78	-0.44
17	1.59	1.57	1.81
18	-0.03	0.07	0.36

Table S3. NBO analysis relative energies (in kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ theoretical level for compounds 1-18, where ΔE(T) is the electronic, ΔE(L) the Lewis, ΔE(NL) the non-Lewis, ΔE(NCE) the electrostatic and ΔE(NSA) the steric energies. Negative values represent a preference for the axial conformer and positive ones for the equatorial conformer.

Compound	Δ*E*(T)	Δ*E*(L)	Δ*E*(NL)	Δ*E*(NCE)	Δ*E*(NSA)
1	-1.39	-4.11	2.72	-0.41	1.39
2	-1.36	-9.16	7.80	-8.84	1.61
3	0.80	1.01	-0.21	1.37	2.43
4	-1.08	-3.73	2.65	-3.50	3.38
5	-2.28	-10.61	8.33	-14.71	1.66
6	-2.96	-13.34	10.38	-22.18	0.31
7	2.53	5.84	-3.31	5.54	0.62
8	-3.81	-14.50	10.69	-28.34	0.81
9	-0.79	-5.19	4.40	-4.71	-0.01
10	-0.60	3.11	-3.71	0.75	1.79
11	-0.41	2.41	-2.83	2.01	1.57
12	-0.47	2.33	-2.80	0.31	1.50
13	0.35	3.26	-2.91	9.16	2.51
14	0.25	-5.51	5.76	0.04	2.84
15	-1.26	-7.38	6.12	-5.03	1.71
16	-0.90	-2.88	1.98	-0.25	1.27
17	1.59	4.16	-2.57	-0.82	4.29
18	-0.03	-5.90	5.87	-2.18	0.83

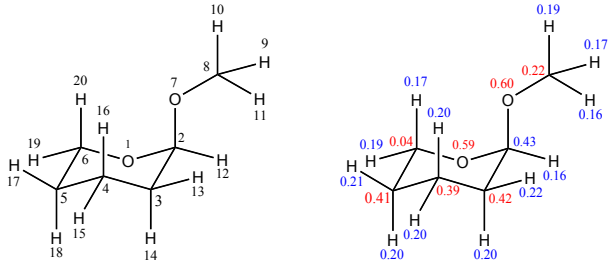


Table S4. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 1_{ax}.

	O1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20
O1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-60.19	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	34.45	-39.94	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	26.87	-22.36	36.20	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	33.79	-20.78	23.60	35.59	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	6.04	-2.63	2.15	2.28	3.98	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	50.48	-60.77	35.62	26.41	23.69	3.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	15.65	-13.56	8.59	6.83	6.88	0.94	31.28	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-13.37	9.24	-6.01	-5.08	-5.57	-0.83	-16.54	-11.77	-	-	-	-	-	-	-	-	-	-	-	-
H10	-9.64	8.17	-6.01	-5.04	-4.97	-0.64	-18.27	-12.70	6.03	-	-	-	-	-	-	-	-	-	-	-
H11	-10.29	9.02	-5.82	-4.38	-4.41	-0.58	-15.68	-11.09	5.32	5.70	-	-	-	-	-	-	-	-	-	-
H12	-15.43	20.31	-10.09	-5.85	-5.63	-0.69	-15.05	-4.48	2.98	2.73	3.63	-	-	-	-	-	-	-	-	-
H13	-12.65	14.39	-27.83	-12.86	-8.63	-0.81	-16.70	-4.11	2.74	3.02	2.85	4.38	-	-	-	-	-	-	-	-
H14	-14.77	13.67	-26.21	-12.24	-10.13	-0.90	-12.23	-3.38	2.45	2.38	2.41	4.34	8.20	-	-	-	-	-	-	-
H15	-10.40	8.43	-13.29	-24.32	-13.01	-0.86	-10.27	-2.86	2.12	2.17	1.89	2.45	5.72	5.55	-	-	-	-	-	-
H16	-12.25	10.45	-13.41	-24.37	-13.16	-1.07	-15.16	-3.84	2.80	2.95	2.35	2.76	5.91	4.51	7.86	-	-	-	-	-
H17	-12.08	7.65	-8.42	-12.36	-26.21	-1.39	-9.63	-2.94	2.41	2.22	1.88	2.19	3.42	3.67	5.49	5.66	-	-	-	-
H18	-14.23	8.55	-9.94	-11.81	-24.83	-1.33	-9.21	-2.79	2.26	2.02	1.87	2.51	3.69	5.05	5.34	4.35	7.61	-	-	-
H19	-18.27	8.16	-6.86	-7.03	-11.90	-2.48	-9.72	-3.34	3.09	2.34	2.14	2.41	2.74	3.09	2.93	3.34	5.06	4.93	-	-
H20	-15.73	8.88	-7.12	-7.76	-10.62	-2.19	-12.81	-4.07	3.74	2.87	2.31	2.36	2.91	2.81	2.95	4.31	4.60	3.52	5.77	-

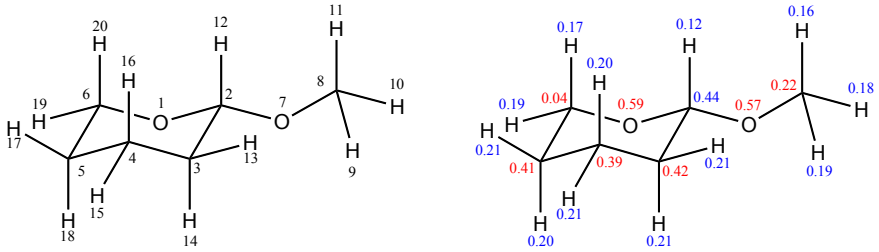


Table S5. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 1_{eq}.

	O1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20
O1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-61.61	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	34.83	-41.25	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	26.94	-22.98	36.18	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	34.12	-21.44	23.68	35.57	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	5.28	-2.36	1.87	1.97	3.46	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	49.50	-60.42	34.13	19.95	19.22	2.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	15.86	-13.96	8.62	5.98	6.17	0.69	29.83	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-9.77	8.41	-6.02	-4.24	-4.33	-0.46	-17.43	-12.67	-	-	-	-	-	-	-	-	-	-	-	-
H10	-14.20	9.91	-6.30	-4.63	-5.11	-0.60	-16.55	-12.32	6.29	-	-	-	-	-	-	-	-	-	-	-
H11	-10.04	9.05	-5.70	-4.17	-4.24	-0.48	-14.60	-10.80	5.55	5.41	-	-	-	-	-	-	-	-	-	-
H12	-11.49	15.76	-7.77	-5.58	-5.11	-0.58	-11.00	-3.43	2.08	2.38	2.71	-	-	-	-	-	-	-	-	-
H13	-12.56	14.61	-27.63	-12.66	-8.55	-0.70	-15.37	-4.02	2.94	2.80	2.75	3.39	-	-	-	-	-	-	-	-
H14	-15.61	14.64	-27.34	-12.61	-10.48	-0.81	-15.64	-3.99	2.91	3.01	2.50	2.74	8.44	-	-	-	-	-	-	-
H15	-10.71	8.87	-13.62	-24.78	-13.34	-0.76	-8.73	-2.68	1.97	2.08	1.86	2.18	5.78	5.85	-	-	-	-	-	-
H16	-11.42	10.05	-12.54	-22.61	-12.34	-0.86	-8.91	-2.81	1.99	2.15	2.06	2.89	5.45	4.36	7.52	-	-	-	-	-
H17	-12.12	7.87	-8.43	-12.29	-26.25	-1.20	-7.57	-2.55	1.82	2.12	1.79	2.02	3.38	3.78	5.59	5.30	-	-	-	-
H18	-14.70	8.96	-10.16	-12.07	-25.57	-1.18	-8.78	-2.81	2.02	2.36	1.87	2.01	3.72	5.31	5.60	4.17	7.79	-	-	-
H19	-18.58	8.52	-6.98	-7.11	-12.12	-2.19	-8.37	-3.04	2.08	2.79	2.09	2.12	2.75	3.26	3.04	3.17	5.13	5.13	-	-
H20	-14.69	8.62	-6.67	-7.18	-9.89	-1.75	-7.52	-2.70	1.79	2.28	2.01	2.58	2.68	2.73	2.80	3.72	4.26	3.36	5.45	-

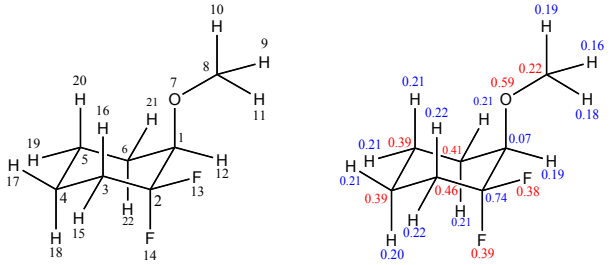


Table S6. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 2_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	H17	H18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	11.72	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-4.33	-75.13	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-3.17	-38.78	38.91	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-3.76	-33.47	23.78	33.46	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-6.40	-40.34	20.96	20.95	34.72	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-10.08	-60.74	30.20	21.73	26.47	33.46	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-2.18	-16.74	8.22	5.81	6.54	8.06	30.07	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	1.47	10.83	-5.19	-3.86	-4.42	-5.79	-15.36	-10.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	1.37	11.34	-6.15	-4.50	-5.09	-5.84	-18.24	-12.39	5.68	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	1.59	14.75	-7.05	-4.68	-4.90	-5.84	-17.03	-11.92	5.46	6.33	-	-	-	-	-	-	-	-	-	-	-	-
H12	4.11	21.74	-8.25	-6.20	-7.05	-11.64	-17.80	-5.46	4.40	3.34	4.10	-	-	-	-	-	-	-	-	-	-	-
F13	-3.89	-69.41	24.80	13.48	12.05	14.01	26.94	9.24	-5.82	-6.19	-9.74	-9.16	-	-	-	-	-	-	-	-	-	-
F14	-3.99	-70.18	25.12	17.37	14.66	18.26	21.37	6.50	-4.59	-4.58	-5.68	-9.60	22.75	-	-	-	-	-	-	-	-	-
H15	1.55	26.05	-31.11	-13.24	-8.38	-7.66	-11.07	-3.32	2.15	2.54	2.97	3.28	-11.01	-11.19	-	-	-	-	-	-	-	-
H16	1.93	26.37	-31.29	-13.45	-10.49	-9.03	-16.50	-4.47	2.67	3.48	3.82	3.71	-11.14	-8.87	9.38	-	-	-	-	-	-	-
H17	1.27	15.01	-14.74	-24.86	-12.58	-8.11	-9.55	-2.68	1.78	2.16	2.17	2.62	-5.91	-6.91	6.09	6.25	-	-	-	-	-	-
H18	1.44	17.93	-14.24	-23.93	-12.21	-9.75	-9.28	-2.62	1.81	2.02	2.14	3.02	-6.37	-9.85	6.01	4.90	7.94	-	-	-	-	-
H19	1.44	13.12	-9.09	-12.44	-24.82	-12.94	-10.43	-2.81	1.97	2.25	2.12	3.00	-5.07	-6.31	3.55	4.07	5.72	5.59	-	-	-	-
H20	1.79	15.47	-11.26	-12.42	-24.68	-12.94	-15.54	-3.73	2.43	3.03	2.71	3.39	-6.05	-6.38	4.02	5.87	5.75	4.51	8.06	-	-	-
H21	2.42	15.47	-8.28	-8.02	-12.89	-26.52	-16.21	-4.18	3.17	3.13	2.89	5.33	-6.09	-7.20	3.20	3.83	3.44	3.79	5.88	5.92	-	-
H22	2.37	18.95	-9.62	-9.85	-12.74	-25.99	-12.46	-3.42	2.54	2.49	2.60	5.36	-6.72	-10.58	3.78	3.92	3.86	5.42	5.82	4.72	8.49	-

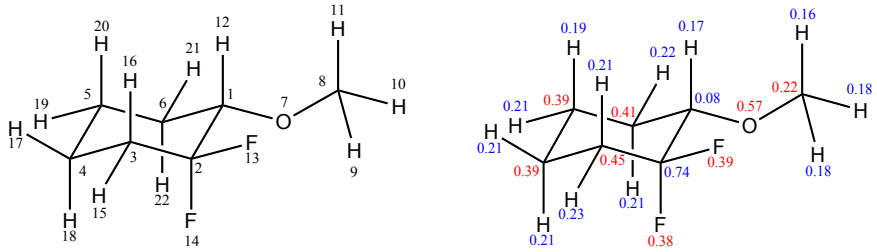


Table S7. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 2_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	H17	H18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	12.69	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-4.69	-73.28	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-3.48	-38.38	38.72	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-4.06	-32.70	23.42	33.34	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-7.01	-39.71	20.78	21.04	34.40	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-10.77	-57.20	22.73	17.67	19.89	32.69	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-2.38	-17.25	7.26	5.36	5.71	7.93	29.07	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	1.66	14.78	-6.09	-4.33	-4.34	-5.71	-16.34	-11.80	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	1.48	11.03	-5.02	-3.88	-4.19	-5.73	-17.33	-12.15	6.15	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	1.65	11.94	-5.38	-3.90	-4.20	-5.53	-14.78	-10.60	5.40	5.54	-	-	-	-	-	-	-	-	-	-	-	-
H12	4.10	19.78	-9.22	-6.63	-7.90	-10.64	-15.79	-4.75	3.22	3.00	4.02	-	-	-	-	-	-	-	-	-	-	-
F13	-4.29	-68.96	24.79	13.64	12.04	14.05	25.32	9.74	-9.52	-6.04	-7.11	-8.59	-	-	-	-	-	-	-	-	-	-
F14	-4.26	-68.37	24.37	16.94	14.03	17.46	26.28	7.87	-7.14	-5.40	-5.02	-6.63	22.44	-	-	-	-	-	-	-	-	-
H15	1.73	26.27	-31.28	-13.53	-8.46	-7.79	-9.47	-3.19	2.79	2.25	2.34	3.43	-11.34	-11.26	-	-	-	-	-	-	-	-
H16	1.99	24.50	-29.15	-12.77	-9.87	-8.55	-9.77	-3.29	2.70	2.27	2.58	4.62	-10.68	-8.21	9.04	-	-	-	-	-	-	-
H17	1.39	14.84	-14.59	-25.01	-12.48	-8.11	-7.53	-2.40	1.95	1.77	1.78	2.83	-5.98	-6.76	6.22	5.91	-	-	-	-	-	-
H18	1.62	18.16	-14.42	-24.61	-12.40	-10.00	-8.94	-2.69	2.21	1.98	1.89	2.91	-6.56	-9.80	6.23	4.74	8.14	-	-	-	-	-
H19	1.60	13.21	-9.20	-12.75	-25.12	-13.20	-8.92	-2.63	2.00	2.00	1.92	3.16	-5.21	-6.22	3.69	3.94	5.85	5.83	-	-	-	-
H20	1.79	14.12	-10.38	-11.58	-22.61	-11.92	-8.91	-2.70	2.03	1.98	2.09	4.12	-5.66	-5.73	3.80	5.18	5.34	4.28	7.64	-	-	-
H21	2.67	15.38	-8.27	-8.11	-12.84	-26.65	-15.92	-4.04	2.79	3.08	2.88	4.96	-6.17	-6.98	3.28	3.66	3.47	3.91	6.04	5.48	-	-
H22	2.65	18.97	-9.68	-10.05	-12.83	-26.36	-16.01	-3.91	2.92	2.92	2.58	3.99	-6.83	-10.20	3.91	3.77	3.93	5.65	6.04	4.43	8.72	-

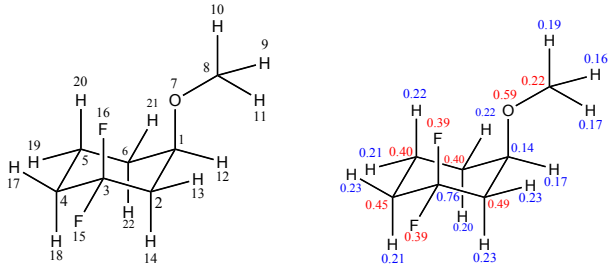


Table S8. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 3_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	F15	F16	H17	H18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-14.57	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	13.75	-82.05	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-6.93	28.89	-75.59	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.23	22.05	-40.37	39.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.01	25.97	-34.78	23.85	34.73	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-19.01	38.81	-48.65	24.64	26.78	33.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-4.24	12.21	-15.22	7.21	6.95	8.04	30.71	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.80	-8.16	9.46	-4.56	-4.33	-5.30	-14.92	-10.61	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.67	-7.80	10.65	-5.35	-5.28	-5.85	-18.51	-12.90	5.65	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.79	-1-	13.19	-5.75	-5.13	-5.52	-16.10	-11.50	5.04	6.13	-	-	-	-	-	-	-	-	-	-	-	-
H12	7.06	-12.89	12.45	-6.45	-6.48	-10.46	-16.19	-4.73	3.78	3.06	3.00	-	-	-	-	-	-	-	-	-	-	-
H13	4.72	-33.81	26.98	-9.81	-7.66	-8.69	-16.14	-6.25	4.34	3.86	5.75	5.04	-	-	-	-	-	-	-	-	-	-
H14	4.79	-33.54	26.98	-11.94	-8.86	-10.78	-13.03	-4.25	3.04	2.88	3.38	5.28	9.63	-	-	-	-	-	-	-	-	-
F15	-4.74	26.71	-71.26	24.52	13.79	12.39	17.39	6.00	-3.92	-4.36	-5.33	-4.86	-11.13	-11.40	-	-	-	-	-	-	-	-
F16	-5.85	26.72	-71.53	24.60	17.23	14.40	26.17	8.73	-5.00	-6.30	-8.21	-5.45	-11.43	-8.85	22.73	-	-	-	-	-	-	-
H17	2.61	-10.65	27.02	-31.01	-13.68	-8.65	-10.23	-3.15	1.98	2.43	2.56	2.57	4.02	4.45	-11.07	-11.47	-	-	-	-	-	-
H18	2.83	-12.08	25.18	-28.71	-12.80	-10.00	-9.53	-2.90	1.91	2.16	2.29	2.84	4.16	5.87	-10.62	-8.25	8.90	-	-	-	-	-
H19	2.74	-8.59	15.32	-14.46	-25.26	-12.81	-10.50	-2.93	1.88	2.30	2.15	2.73	3.16	3.71	-5.93	-6.78	6.17	5.83	-	-	-	-
H20	3.64	-10.81	20.05	-15.30	-26.70	-13.64	-16.64	-4.23	2.50	3.33	3.10	3.29	4.04	4.11	-6.95	-10.42	6.63	5.00	8.65	-	-	-
H21	4.67	-10.32	14.13	-9.44	-13.35	-26.72	-16.86	-4.15	2.77	3.19	2.73	4.95	3.83	4.34	-5.39	-6.43	3.80	4.02	6.04	6.44	-	-
H22	4.19	-11.55	15.17	-10.62	-12.04	-23.97	-11.67	-3.22	2.24	2.37	2.28	4.55	3.91	5.67	-5.89	-5.95	3.89	5.26	5.44	4.71	8.11	-

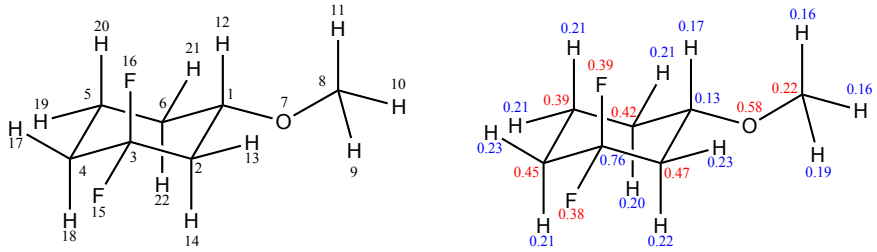


Table S9. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 3_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	F15	F16	H17	H18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-13.72	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	13.65	-78.10	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-6.82	27.52	-75.50	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-7.02	20.74	-40.03	38.60	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.32	25.87	-36.48	24.90	35.92	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-18.43	38.29	-39.70	20.50	20.08	33.01	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-4.13	9.26	-11.36	6.24	6.46	10.06	29.88	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.61	-6.81	8.49	-4.63	-4.58	-6.63	-18.24	-12.70	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.63	-6.02	7.83	-4.58	-4.97	-7.99	-14.92	-10.67	5.76	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.80	-6.43	8.29	-4.49	-4.68	-6.73	-15.14	-10.75	5.79	4.89	-	-	-	-	-	-	-	-	-	-	-	-
H12	6.82	-12.05	15.21	-7.47	-7.90	-10.84	-15.70	-4.73	3.02	2.95	3.93	-	-	-	-	-	-	-	-	-	-	-
H13	4.81	-32.97	27.56	-10.05	-7.76	-9.35	-17.09	-4.34	3.34	2.70	3.12	5.24	-	-	-	-	-	-	-	-	-	-
H14	4.65	-31.51	26.48	-11.82	-8.67	-11.14	-16.75	-4.09	3.13	2.74	2.69	4.05	9.68	-	-	-	-	-	-	-	-	-
F15	-4.60	24.98	-70.30	24.11	13.44	12.72	15.58	4.60	-3.60	-3.18	-3.34	-5.23	-11.21	-10.87	-	-	-	-	-	-	-	-
F16	-6.00	25.88	-72.27	25.04	17.62	15.61	18.06	5.54	-4.14	-3.78	-4.29	-8.20	-11.84	-8.85	22.67	-	-	-	-	-	-	-
H17	2.57	-10.13	26.96	-31.02	-13.54	-9.05	-8.27	-2.63	2.00	1.94	1.94	3.03	4.11	4.40	-10.95	-11.59	-	-	-	-	-	-
H18	2.83	-11.75	25.53	-29.21	-12.87	-10.59	-9.28	-2.80	2.13	2.08	1.95	2.94	4.34	5.94	-10.49	-8.51	9.05	-	-	-	-	-
H19	2.74	-8.33	15.59	-14.70	-25.42	-13.64	-8.88	-3.00	2.19	2.40	2.16	3.13	3.30	3.74	-5.93	-7.08	6.27	6.02	-	-	-	-
H20	3.33	-9.58	18.83	-14.36	-24.70	-13.33	-9.68	-3.27	2.32	2.47	2.52	4.44	3.86	3.80	-6.45	-10.17	6.25	4.77	8.27	-	-	-
H21	4.35	-9.38	13.57	-9.05	-12.71	-26.79	-14.71	-5.47	3.50	4.97	3.73	4.71	3.76	4.10	-5.08	-6.38	3.65	3.91	5.92	5.79	-	-
H22	4.22	-11.27	15.47	-10.78	-12.14	-25.60	-14.62	-4.34	3.06	3.53	2.73	3.67	4.11	5.75	-5.87	-6.24	3.96	5.41	5.65	4.49	7.94	-

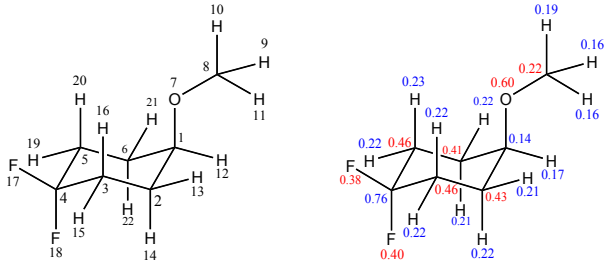


Table S10. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 4_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	F17	F18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.64	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.24	42.43	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	11.89	-43.39	-76.77	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-8.22	21.93	27.36	-76.58	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.07	22.89	20.88	-41.13	40.17	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-19.08	34.50	30.63	-43.69	31.21	34.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-4.18	10.47	9.20	-12.27	7.84	8.05	30.86	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.86	-7.14	-5.83	7.99	-5.10	-5.54	-15.59	-10.81	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.65	-6.81	-6.58	9.28	-6.06	-5.91	-18.80	-12.79	5.83	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.61	-8.19	-7.52	9.18	-5.41	-5.21	-15.25	-10.64	4.87	5.74	-	-	-	-	-	-	-	-	-	-	-	-
H12	7.11	-11.30	-7.55	11.16	-7.52	-10.74	-16.61	-4.80	4.00	3.11	2.90	-	-	-	-	-	-	-	-	-	-	-
H13	4.39	-27.30	-14.77	15.48	-8.06	-8.17	-15.17	-5.66	4.01	3.57	4.99	4.82	-	-	-	-	-	-	-	-	-	-
H14	4.62	-28.24	-15.34	19.98	-9.94	-10.68	-12.83	-4.03	2.95	2.78	3.07	5.08	8.68	-	-	-	-	-	-	-	-	-
H15	2.93	-14.58	-31.32	26.82	-9.86	-7.70	-11.19	-3.68	2.42	2.71	3.10	2.98	6.19	6.51	-	-	-	-	-	-	-	-
H16	3.59	-14.45	-30.78	26.50	-11.95	-8.87	-16.38	-5.06	2.97	3.71	4.32	3.33	6.15	5.21	9.31	-	-	-	-	-	-	-
F17	-4.16	14.63	24.63	-70.78	24.54	13.89	17.09	5.12	-3.32	-4.06	-3.89	-4.19	-5.91	-6.86	-10.97	-10.91	-	-	-	-	-	-
F18	-5.13	19.30	25.65	-72.97	25.54	18.23	17.70	5.26	-3.62	-3.99	-3.92	-5.30	-7.11	-10.91	-11.60	-8.90	23.00	-	-	-	-	-
H19	2.92	-8.09	-9.86	26.75	-31.10	-13.82	-11.37	-3.09	2.07	2.46	2.14	2.97	3.15	3.95	3.94	4.35	-10.91	-11.56	-	-	-	-
H20	3.68	-9.56	-12.30	27.23	-31.56	-14.14	-17.25	-4.24	2.63	3.41	2.89	3.41	3.77	4.10	4.48	6.33	-11.22	-9.14	9.53	-	-	-
H21	4.60	-8.92	-8.40	16.00	-15.25	-26.85	-16.80	-4.08	2.87	3.16	2.52	5.00	3.53	4.20	3.27	3.83	-6.12	-7.30	6.35	6.63	-	-
H22	4.47	-10.82	-9.58	19.18	-14.82	-26.04	-12.68	-3.42	2.48	2.54	2.30	4.93	3.93	6.00	3.80	3.86	-6.61	-10.41	6.32	5.20	8.64	-

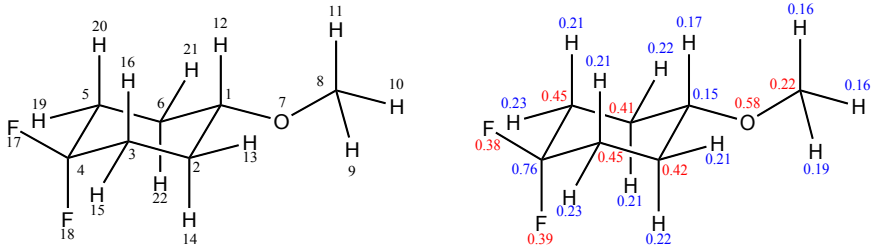


Table S11. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 4_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	F17	F18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.29	41.60	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	12.09	-42.95	-75.50	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-8.31	21.61	26.76	-75.74	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.35	22.82	20.67	-41.17	39.96	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-19.00	33.36	22.95	-34.84	23.37	33.17	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-4.27	10.33	7.47	-10.69	6.74	8.07	29.93	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.70	-8.18	-5.72	7.83	-4.64	-5.26	-14.94	-10.75	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.70	-6.74	-5.26	7.89	-5.03	-5.92	-18.21	-12.75	5.78	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.87	-6.86	-5.37	7.60	-4.84	-5.49	-14.90	-10.63	4.84	5.72	-	-	-	-	-	-	-	-	-	-	-	-
H12	6.40	-9.99	-8.26	11.74	-8.26	-9.56	-14.30	-4.30	2.65	2.75	3.52	-	-	-	-	-	-	-	-	-	-	-
H13	4.47	-27.10	-14.60	15.42	-7.98	-8.16	-14.68	-5.57	5.01	3.52	3.81	4.28	-	-	-	-	-	-	-	-	-	-
H14	4.66	-27.76	-14.90	19.53	-9.68	-10.53	-15.57	-4.71	3.86	3.28	2.93	3.58	8.50	-	-	-	-	-	-	-	-	-
H15	3.03	-14.72	-31.27	27.14	-9.91	-7.84	-9.50	-3.25	2.59	2.36	2.32	3.05	6.28	6.52	-	-	-	-	-	-	-	-
H16	3.51	-13.82	-29.15	25.48	-11.40	-8.54	-9.92	-3.38	2.54	2.39	2.59	4.14	5.97	4.95	9.11	-	-	-	-	-	-	-
F17	-4.24	14.54	24.28	-70.65	24.33	13.92	13.32	4.32	-3.18	-3.27	-3.15	-4.48	-5.91	-6.74	-11.11	-10.55	-	-	-	-	-	-
F18	-5.15	18.83	24.93	-72.06	24.99	18.02	16.59	5.08	-3.79	-3.85	-3.47	-4.71	-6.96	-10.48	-11.59	-8.46	22.69	-	-	-	-	-
H19	3.04	-8.19	-9.90	27.19	-31.42	-14.12	-9.69	-2.87	1.98	2.22	2.04	3.05	3.20	3.95	4.07	4.26	-11.10	-11.62	-	-	-	-
H20	3.50	-8.88	-11.34	25.45	-29.21	-13.21	-10.03	-3.05	2.07	2.27	2.30	4.11	3.53	3.77	4.25	5.69	-10.55	-8.45	9.12	-	-	-
H21	4.69	-8.87	-8.27	15.95	-15.07	-26.89	-16.22	-4.09	2.55	3.15	2.86	4.46	3.52	4.15	3.32	3.67	-6.11	-7.20	6.47	6.14	-	-
H22	4.66	-11.00	-9.66	19.53	-14.94	-26.52	-16.08	-3.96	2.68	3.02	2.55	3.58	3.99	6.02	3.94	3.78	-6.73	-10.46	6.53	4.94	8.81	-

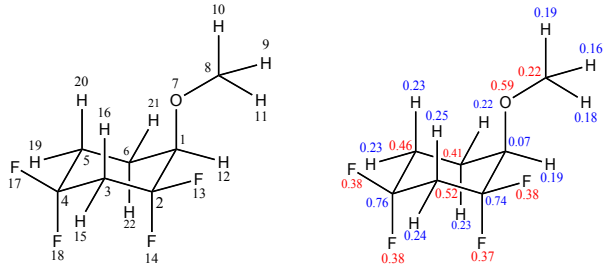


Table S12. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 5_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	F17	F18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	11.81	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-5.00	-85.66	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	6.30	75.24	-87.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-4.41	-38.58	31.38	-76.68	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-6.56	-40.98	24.41	-41.89	40.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-10.21	-60.90	34.69	-43.38	31.23	34.08	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-2.21	-16.72	9.40	-11.50	7.68	8.22	30.17	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	1.50	10.91	-6.00	7.71	-5.26	-5.97	-15.61	-10.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	1.41	11.53	-7.16	9.07	-6.07	-6.03	-18.58	-12.64	5.85	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	1.62	14.80	-8.08	9.26	-5.75	-5.98	-17.18	-12.03	5.57	6.47	-	-	-	-	-	-	-	-	-	-	-	-
H12	4.31	22.58	-9.80	12.58	-8.52	-12.28	-18.50	-5.68	4.60	3.52	4.32	-	-	-	-	-	-	-	-	-	-	-
F13	-3.86	-68.31	28.08	-25.95	13.76	14.00	26.67	9.08	-5.74	-6.20	-9.60	-9.30	-	-	-	-	-	-	-	-	-	-
F14	-3.87	-67.78	27.56	-31.70	16.10	17.76	20.61	6.26	-4.46	-4.48	-5.52	-9.61	21.51	-	-	-	-	-	-	-	-	-
H15	1.71	28.22	-39.11	28.87	-10.72	-8.61	-12.08	-3.60	2.36	2.80	3.21	3.72	-11.61	-11.83	-	-	-	-	-	-	-	-
H16	2.12	28.78	-39.45	29.42	-13.19	-9.96	-17.92	-4.87	2.95	3.86	4.18	4.19	-12.21	-9.36	11.25	-	-	-	-	-	-	-
F17	-2.19	-25.24	27.99	-69.83	24.23	13.94	16.90	4.77	-3.19	-3.95	-3.87	-4.68	10.09	11.01	-11.52	-12.18	-	-	-	-	-	-
F18	-2.58	-31.41	28.18	-70.58	24.62	17.76	16.78	4.78	-3.35	-3.75	-3.92	-5.68	11.27	16.71	-12.18	-9.54	21.82	-	-	-	-	-
H19	1.61	14.56	-11.62	27.56	-32.09	-14.48	-11.68	-3.14	2.23	2.55	2.37	3.45	-5.55	-6.67	4.40	4.95	-10.99	-11.50	-	-	-	-
H20	2.02	17.15	-14.22	27.54	-32.04	-14.58	-17.67	-4.22	2.78	3.49	3.06	3.93	-6.65	-6.77	4.89	7.02	-11.25	-8.91	9.94	-	-	-
H21	2.52	16.00	-9.80	16.34	-15.59	-27.92	-16.70	-4.33	3.34	3.28	3.01	5.75	-6.19	-7.16	3.65	4.30	-6.16	-7.17	6.71	6.81	-	-
H22	2.56	20.47	-11.96	20.76	-15.89	-28.41	-13.41	-3.67	2.76	2.72	2.82	5.94	-7.10	-10.91	4.55	4.62	-7.00	-10.75	6.92	5.64	9.45	-

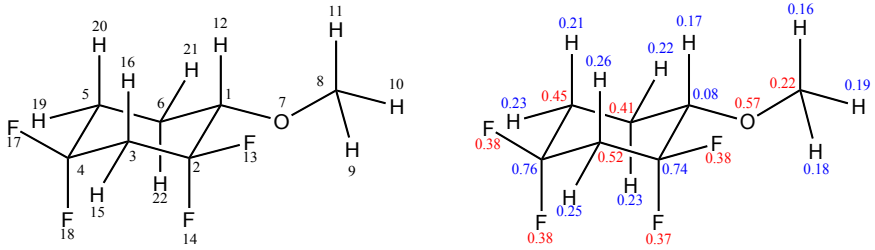


Table S13. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 5_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	F17	F18	H19	H20	H21	H22
C1		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	12.98	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-5.49	-83.91	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	6.96	73.99	-86.84	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-4.83	-37.70	30.93	-75.87	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-7.29	-40.36	24.25	-41.84	40.64	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-10.96	-56.85	25.88	-34.06	22.96	33.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-2.46	-17.53	8.42	-10.51	6.68	8.12	29.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	1.71	15.05	-7.07	8.48	-5.08	-5.86	-16.31	-11.96	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	1.55	11.29	-5.87	7.68	-4.95	-5.92	-17.50	-12.45	6.29	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	1.71	12.20	-6.25	7.69	-4.93	-5.66	-14.81	-10.79	5.49	5.70	-	-	-	-	-	-	-	-	-	-	-	-
H12	4.22	19.90	-10.61	13.14	-9.32	-10.88	-15.78	-4.78	3.24	3.07	4.05	-	-	-	-	-	-	-	-	-	-	-
F13	-4.32	-68.12	28.25	-26.18	13.80	14.09	24.60	9.69	-9.39	-6.06	-7.20	-8.58	-	-	-	-	-	-	-	-	-	-
F14	-4.19	-66.12	26.82	-30.63	15.37	16.96	25.23	7.78	-7.14	-5.36	-4.96	-6.43	21.30	-	-	-	-	-	-	-	-	-
H15	1.93	28.43	-39.34	29.25	-10.79	-8.74	-10.25	-3.50	3.07	2.50	2.57	3.74	-11.95	-11.91	-	-	-	-	-	-	-	-
H16	2.23	27.19	-37.42	28.15	-12.56	-9.54	-10.71	-3.67	3.02	2.57	2.88	5.06	-11.95	-8.80	10.98	-	-	-	-	-	-	-
F17	-2.42	-24.92	27.73	-69.66	23.99	13.93	12.86	4.20	-3.41	-3.15	-3.15	-4.98	10.22	10.72	-11.69	-11.68	-	-	-	-	-	-
F18	-2.84	-30.64	27.61	-69.76	24.12	17.58	15.54	4.79	-3.95	-3.59	-3.37	-5.07	11.20	15.92	-12.19	-9.04	21.54	-	-	-	-	-
H19	1.82	14.62	-11.74	27.99	-32.37	-14.75	-9.78	-2.93	2.24	2.25	2.14	3.54	-5.71	-6.54	4.55	4.84	-11.18	-11.55	-	-	-	-
H20	2.06	15.75	-13.18	25.64	-29.53	-13.51	-9.94	-3.06	2.30	2.27	2.37	4.70	-6.29	-6.11	4.64	6.29	-10.50	-8.21	9.46	-	-	-
H21	2.84	16.01	-9.86	16.51	-15.61	-28.23	-16.53	-4.23	2.92	3.26	3.00	5.17	-6.33	-6.98	3.76	4.17	-6.22	-7.18	6.91	6.37	-	-
H22	2.90	20.42	-12.02	21.01	-15.95	-28.72	-16.88	-4.20	3.16	3.17	2.77	4.30	-7.20	-10.46	4.68	4.48	-7.09	-10.79	7.13	5.31	9.72	-

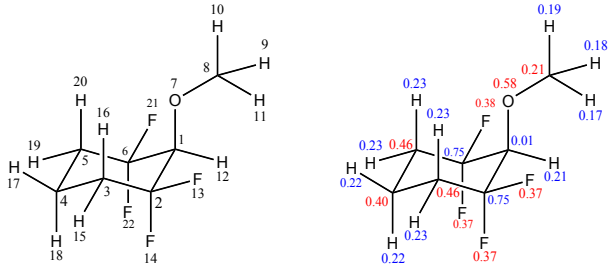


Table S14. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 6_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	H17	H18	H19	H20	F21	F22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	1.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-0.53	-75.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.40	-39.77	39.58	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.53	-38.81	27.57	39.59	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	1.44	73.78	-38.56	-39.48	-75.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-1.22	-60.93	29.92	21.67	29.69	-60.06	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.27	-15.11	7.54	5.80	7.89	-16.16	29.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.20	10.90	-5.56	-4.58	-6.56	14.08	-16.58	-11.72	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.17	11.21	-6.06	-4.68	-6.24	11.60	-18.33	-12.64	6.44	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.19	11.73	-5.55	-4.15	-5.32	10.93	-15.84	-11.13	5.68	6.13	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.56	24.03	-9.11	-7.03	-9.10	23.81	-19.14	-6.05	4.78	3.79	4.96	-	-	-	-	-	-	-	-	-	-	-
F13	-0.46	-67.51	23.74	13.20	13.44	-24.74	26.33	7.36	-5.02	-5.64	-6.26	-9.66	-	-	-	-	-	-	-	-	-	-
F14	-0.47	-68.38	24.23	17.08	16.25	-31.57	20.34	5.86	-4.52	-4.41	-4.72	-10.23	21.11	-	-	-	-	-	-	-	-	-
H15	0.20	27.01	-32.04	-13.92	-10.03	14.49	-11.30	-3.12	2.32	2.56	2.38	3.73	-10.81	-11.15	-	-	-	-	-	-	-	-
H16	0.24	26.90	-31.76	-13.89	-12.42	17.01	-16.66	-4.08	2.90	3.43	2.91	4.15	-10.87	-8.70	9.82	-	-	-	-	-	-	-
H17	0.16	15.67	-15.26	-26.29	-15.27	15.57	-9.67	-2.72	2.15	2.27	1.95	3.02	-5.89	-6.93	6.53	6.55	-	-	-	-	-	-
H18	0.19	19.59	-15.34	-26.38	-15.34	19.43	-9.87	-2.80	2.26	2.23	2.06	3.67	-6.63	-10.31	6.66	5.37	8.90	-	-	-	-	-
H19	0.20	14.58	-10.02	-13.92	-32.03	26.86	-11.21	-3.29	2.84	2.66	2.26	3.72	-5.40	-6.70	4.04	4.57	6.53	6.66	-	-	-	-
H20	0.24	17.01	-12.37	-13.84	-31.64	26.66	-16.39	-4.29	3.50	3.55	2.76	4.12	-6.40	-6.72	4.55	6.57	6.54	5.35	9.78	-	-	-
F21	-0.47	-25.37	13.73	13.47	24.27	-68.28	26.68	8.70	-8.87	-6.28	-5.60	-9.79	9.85	11.22	-5.52	-6.59	-6.01	-6.74	-11.00	-11.13	-	-
F22	-0.47	-31.36	16.04	16.85	24.11	-67.85	20.15	6.12	-5.39	-4.52	-4.49	-10.15	10.92	17.06	-6.62	-6.69	-6.86	-10.13	-11.14	-8.63	21.44	-

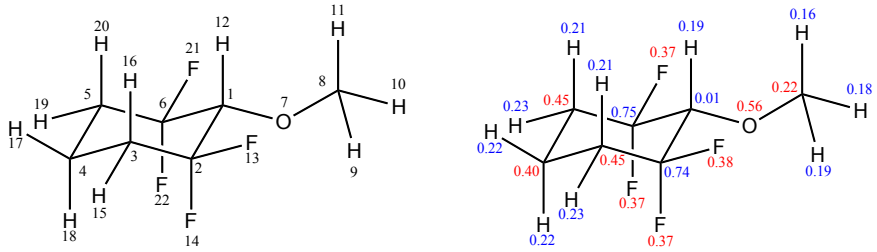


Table S15. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 6_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	H17	H18	H19	H20	F21	F22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	2.23	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-0.82	-73.69	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.62	-39.41	39.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.82	-37.88	27.10	39.30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	2.25	72.81	-38.24	-39.63	-73.98	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-1.85	-56.40	22.23	17.60	22.31	-57.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.42	-16.24	7.06	5.41	6.71	-14.98	28.18	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.31	14.07	-6.05	-4.37	-5.14	10.68	-15.80	-11.69	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.28	11.61	-5.29	-4.19	-5.15	11.23	-17.86	-12.86	6.47	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.29	10.63	-5.02	-3.94	-5.10	11.09	-14.66	-10.77	5.43	5.98	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.82	22.48	-10.49	-7.71	-10.47	22.76	-17.41	-5.70	4.33	3.61	4.57	-	-	-	-	-	-	-	-	-	-	-
F13	-0.75	-68.24	24.27	13.66	13.70	-25.47	24.71	8.78	-8.99	-6.22	-5.61	-9.64	-	-	-	-	-	-	-	-	-	-
F14	-0.72	-66.34	23.53	16.66	15.52	-30.34	24.76	6.95	-5.85	-5.43	-4.40	-7.23	21.24	-	-	-	-	-	-	-	-	-
H15	0.31	27.09	-32.18	-14.17	-10.07	14.71	-9.50	-3.14	2.76	2.43	2.21	4.00	-11.31	-11.17	-	-	-	-	-	-	-	-
H16	0.35	24.65	-29.32	-13.03	-11.50	15.87	-9.56	-3.25	2.83	2.40	2.41	5.25	-10.49	-7.93	9.32	-	-	-	-	-	-	-
H17	0.25	15.48	-15.12	-26.44	-15.07	15.58	-7.62	-2.47	2.02	1.95	1.83	3.34	-6.07	-6.77	6.63	6.12	-	-	-	-	-	-
H18	0.31	19.85	-15.55	-27.08	-15.49	19.95	-9.50	-2.86	2.30	2.28	2.03	3.60	-6.98	-10.26	6.89	5.13	9.11	-	-	-	-	-
H19	0.31	14.64	-10.12	-14.20	-32.11	27.37	-9.60	-2.96	2.25	2.36	2.26	4.01	-5.66	-6.58	4.17	4.35	6.64	6.90	-	-	-	-
H20	0.35	15.73	-11.53	-13.03	-29.19	24.84	-9.61	-3.09	2.40	2.35	2.46	5.25	-6.20	-6.11	4.34	5.79	6.12	5.12	9.33	-	-	-
F21	-0.73	-24.80	13.50	13.39	23.75	-67.73	24.76	7.26	-4.92	-5.62	-5.89	-9.53	10.05	10.70	-5.55	-6.10	-5.96	-6.83	-11.11	-10.33	-	-
F22	-0.72	-30.02	15.50	16.58	23.41	-66.81	25.13	6.44	-4.61	-5.21	-4.51	-7.24	10.89	15.74	-6.54	-6.09	-6.74	-10.18	-11.20	-7.92	20.79	-

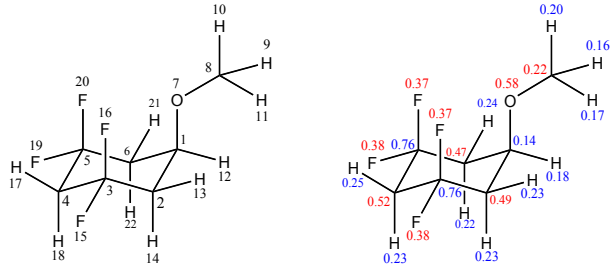


Table S16. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 7_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	F15	F16	H17	H18	F19	F20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-14.37	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	13.57	-81.78	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-7.84	33.14	-86.48	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	13.58	-42.18	76.62	-86.48	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-13.83	30.16	-40.24	31.55	-78.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-18.49	37.93	-47.57	27.53	-48.68	37.96	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-4.24	12.26	-15.29	8.29	-13.11	9.43	30.28	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.79	-8.17	9.47	-5.23	8.21	-6.20	-14.65	-10.71	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.71	-7.98	10.89	-6.27	10.11	-6.98	-18.60	-13.32	5.81	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.76	-9.98	13.17	-6.59	9.62	-6.44	-15.80	-11.61	5.06	6.29	-	-	-	-	-	-	-	-	-	-	-	-
H12	7.20	-13.30	12.84	-7.64	12.82	-12.68	-16.38	-4.92	3.91	3.24	3.09	-	-	-	-	-	-	-	-	-	-	-
H13	4.82	-34.82	27.82	-11.63	15.07	-10.45	-16.35	-6.51	4.50	4.09	5.95	5.38	-	-	-	-	-	-	-	-	-	-
H14	4.76	-33.69	27.11	-13.87	17.34	-12.64	-12.85	-4.31	3.07	2.98	3.40	5.49	1-	-	-	-	-	-	-	-	-	-
F15	-4.60	26.19	-70.03	27.86	-26.02	14.15	16.73	5.94	-3.86	-4.38	-5.24	-4.93	-11.27	-11.27	-	-	-	-	-	-	-	-
F16	-5.58	25.65	-69.09	27.11	-31.01	16.11	24.70	8.43	-4.81	-6.19	-7.86	-5.41	-11.33	-8.58	21.50	-	-	-	-	-	-	-
H17	2.85	-11.62	29.25	-39.14	29.30	-11.10	-11.03	-3.48	2.18	2.73	2.81	2.91	4.53	4.89	-11.72	-12.07	-	-	-	-	-	-
H18	3.09	-13.41	28.01	-37.01	27.98	-12.71	-10.34	-3.24	2.13	2.46	2.55	3.25	4.79	6.59	-11.81	-8.88	10.88	-	-	-	-	-
F19	-4.63	14.93	-26.14	28.00	-70.37	25.21	17.14	5.02	-3.26	-4.02	-3.69	-4.95	-5.70	-6.71	10.30	10.95	-11.74	-11.91	-	-	-	-
F20	-5.41	16.39	-30.31	26.72	-68.19	24.01	24.52	6.60	-3.92	-5.37	-4.81	-5.26	-6.43	-6.42	10.71	15.32	-11.98	-8.74	21.23	-	-	-
H21	5.08	-11.38	15.70	-12.06	28.92	-34.60	-18.40	-4.64	3.07	3.64	3.04	5.57	4.37	4.82	-5.88	-6.92	4.71	4.92	-11.62	-11.66	-	-
H22	4.65	-12.83	16.75	-13.40	26.59	-31.59	-12.89	-3.66	2.54	2.74	2.57	5.36	4.52	6.35	-6.43	-6.39	4.76	6.32	-11.25	-8.26	10.10	-

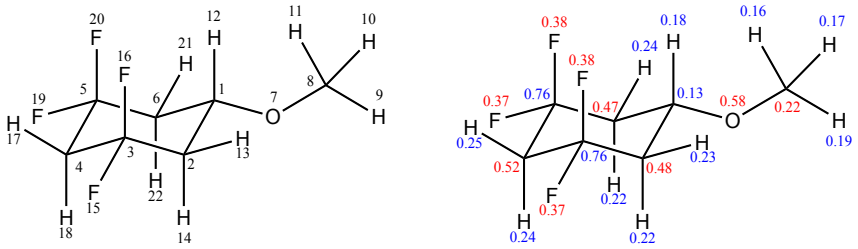


Table S17. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 7_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	F15	F16	H17	H18	F19	F20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-13.63	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	13.13	-80.88	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-7.54	32.64	-86.40	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	13.14	-41.71	76.89	-86.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-13.19	29.77	-40.25	31.45	-77.84	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-17.67	37.95	-38.81	23.29	-39.33	37.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-4.01	11.65	-12.62	7.20	-11.44	9.31	29.79	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.56	-7.78	9.05	-5.40	8.63	-6.90	-18.38	-13.01	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.77	-7.86	9.25	-5.28	8.51	-6.59	-15.40	-11.11	6.04	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.56	-9.30	9.76	-5.29	7.89	-6.05	-14.91	-10.83	5.90	5.05	-	-	-	-	-	-	-	-	-	-	-	-
H12	7.19	-13.59	16.68	-9.44	16.67	-13.11	-16.98	-5.22	3.35	4.40	3.28	-	-	-	-	-	-	-	-	-	-	-
H13	4.58	-34.12	27.76	-11.53	14.98	-10.32	-16.00	-5.99	3.91	4.12	5.49	5.64	-	-	-	-	-	-	-	-	-	-
H14	4.50	-32.89	26.62	-13.59	17.10	-12.53	-16.14	-4.83	3.45	3.07	3.92	4.45	9.72	-	-	-	-	-	-	-	-	-
F15	-4.37	25.52	-69.42	27.46	-25.70	13.93	14.97	5.16	-3.84	-3.74	-4.16	-5.62	-11.08	-10.83	-	-	-	-	-	-	-	-
F16	-5.54	25.83	-69.88	27.54	-31.80	16.41	17.01	5.94	-4.25	-4.68	-4.53	-8.60	-11.51	-8.58	21.51	-	-	-	-	-	-	-
H17	2.74	-11.46	29.22	-39.05	29.18	-11.04	-9.02	-2.92	2.23	2.20	2.16	3.70	4.49	4.80	-11.58	-12.24	-	-	-	-	-	-
H18	2.99	-13.34	28.25	-37.38	28.21	-12.84	-10.07	-3.10	2.37	2.20	2.30	3.56	4.78	6.51	-11.68	-9.09	10.97	-	-	-	-	-
F19	-4.36	14.43	-25.67	27.40	-69.21	24.53	15.20	4.56	-3.59	-3.37	-3.15	-5.61	-5.54	-6.45	9.95	11.02	-11.55	-11.66	-	-	-	-
F20	-5.53	17.01	-31.82	27.54	-69.79	24.84	17.21	5.37	-4.05	-4.25	-3.66	-8.59	-6.71	-6.61	11.04	16.60	-12.25	-9.09	21.45	-	-	-
H21	4.78	-11.10	15.49	-11.88	28.44	-33.94	-17.49	-4.52	3.50	3.32	2.81	5.87	4.27	4.73	-5.73	-6.94	4.63	4.93	-11.32	-11.80	-	-
H22	4.51	-13.01	17.12	-13.59	26.59	-31.66	-16.63	-4.12	3.19	2.77	2.77	4.45	4.57	6.49	-6.46	-6.61	4.80	6.51	-10.82	-8.57	10.05	-

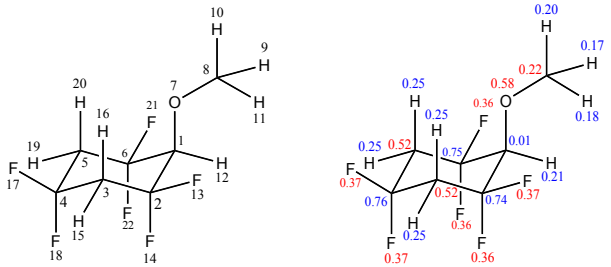


Table S18. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 8_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	F17	F18	H19	H20	F21	F22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	1.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-0.71	-85.54	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.89	75.00	-87.40	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.71	-43.89	35.74	-87.40	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	1.68	73.65	-44.17	75.55	-86.00	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-1.43	-60.29	34.35	-42.52	34.64	-61.12	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.31	-16.11	9.07	-11.26	8.70	-15.15	29.23	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.22	11.04	-6.19	8.13	-6.50	11.95	-16.11	-11.31	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.21	11.75	-7.29	9.24	-7.09	11.38	-18.65	-12.85	6.31	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.23	14.06	-7.54	8.87	-6.41	10.97	-16.73	-11.80	5.79	6.57	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.67	24.56	-10.73	13.82	-10.75	24.77	-19.77	-6.23	5.16	3.96	4.97	-	-	-	-	-	-	-	-	-	-	-
F13	-0.54	-67.15	27.47	-25.39	15.42	-24.92	26.34	8.50	-5.54	-6.24	-8.66	-9.92	-	-	-	-	-	-	-	-	-	-
F14	-0.52	-65.48	26.40	-30.22	17.54	-30.12	19.44	5.87	-4.36	-4.40	-5.18	-10.03	20.25	-	-	-	-	-	-	-	-	-
H15	0.25	28.97	-40.07	29.64	-12.57	15.95	-12.26	-3.57	2.49	2.93	3.08	4.17	-11.60	-11.67	-	-	-	-	-	-	-	-
H16	0.31	29.21	-39.96	29.78	-15.26	18.46	-18.13	-4.74	3.09	3.98	3.88	4.66	-12.19	-9.12	11.70	-	-	-	-	-	-	-
F17	-0.31	-24.89	27.57	-68.84	27.56	-25.03	16.45	4.63	-3.34	-3.99	-3.65	-5.08	9.76	10.37	-11.62	-12.23	-	-	-	-	-	-
F18	-0.35	-30.02	27.04	-68.15	27.04	-30.27	15.76	4.51	-3.38	-3.68	-3.65	-5.97	10.56	15.17	-12.05	-9.31	20.70	-	-	-	-	-
H19	0.25	15.84	-12.57	29.64	-40.07	29.11	-12.35	-3.40	2.64	2.84	2.54	4.18	-5.93	-6.96	4.90	5.42	-11.62	-12.04	-	-	-	-
H20	0.31	18.46	-15.32	29.85	-40.09	29.45	-18.44	-4.52	3.28	3.86	3.21	4.70	-7.07	-7.01	5.44	7.66	-12.24	-9.33	11.74	-	-	-
F21	-0.53	-24.32	15.11	-24.93	26.92	-66.43	25.99	7.29	-6.31	-5.65	-4.99	-9.80	9.52	10.32	-5.82	-6.87	9.56	10.40	-11.41	-11.92	-	-
F22	-0.53	-30.29	17.76	-30.60	26.51	-65.92	19.60	5.64	-4.60	-4.30	-4.36	-10.09	10.58	15.71	-7.06	-7.04	10.46	15.44	-11.66	-9.17	19.94	-

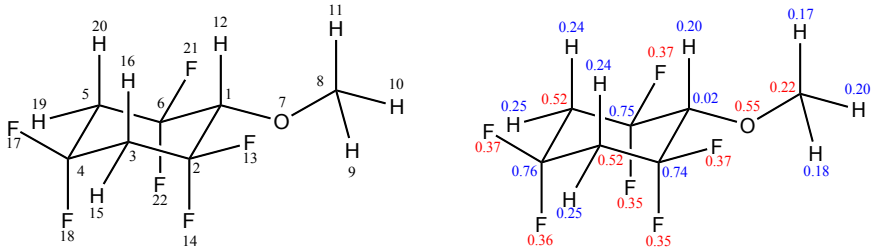


Table S19. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 8_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	F17	F18	H19	H20	F21	F22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	2.71	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-1.14	-84.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	1.44	74.33	-86.61	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-1.14	-43.18	35.21	-86.43	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	2.74	72.66	-43.59	74.85	-84.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-2.24	-56.05	25.31	-33.11	25.44	-57.60	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.51	-16.32	8.13	-10.33	7.73	-15.03	28.07	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.37	14.17	-6.99	8.38	-5.93	10.74	-15.79	-11.82	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.34	11.78	-6.16	8.08	-6.00	11.41	-18.01	-13.11	6.62	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.35	10.73	-5.82	7.60	-5.91	11.17	-14.68	-10.92	5.52	6.13	-	-	-	-	-	-	-	-	-	-	-	-
H12	1.00	22.52	-12.09	14.93	-12.08	22.82	-17.36	-5.74	4.35	3.67	4.63	-	-	-	-	-	-	-	-	-	-	-
F13	-0.89	-67.20	27.58	-25.64	15.46	-25.08	24.15	8.69	-8.92	-6.21	-5.59	-9.53	-	-	-	-	-	-	-	-	-	-
F14	-0.84	-63.94	25.79	-29.65	17.00	-29.12	23.63	6.71	-5.67	-5.29	-4.26	-6.97	20.08	-	-	-	-	-	-	-	-	-
H15	0.41	29.17	-40.25	29.97	-12.62	16.07	-10.26	-3.42	3.01	2.68	2.42	4.35	-11.92	-11.68	-	-	-	-	-	-	-	-
H16	0.47	27.27	-37.47	28.12	-14.33	17.38	-10.53	-3.63	3.17	2.71	2.70	5.82	-11.64	-8.46	11.25	-	-	-	-	-	-	-
F17	-0.50	-24.70	27.35	-68.71	27.29	-24.90	12.38	4.12	-3.38	-3.28	-3.10	-5.62	9.87	10.19	-11.78	-11.58	-	-	-	-	-	-
F18	-0.56	-29.53	26.51	-67.32	26.44	-29.72	14.42	4.45	-3.59	-3.60	-3.19	-5.51	10.56	14.78	-12.03	-8.70	20.44	-	-	-	-	-
H19	0.41	15.98	-12.67	30.01	-40.21	29.49	-10.36	-3.23	2.46	2.60	2.47	4.36	-6.09	-6.92	5.04	5.21	-11.79	-12.05	-	-	-	-
H20	0.47	17.22	-14.36	28.13	-37.40	27.54	-10.59	-3.45	2.67	2.65	2.76	5.82	-6.73	-6.46	5.21	6.85	-11.60	-8.71	11.27	-	-	-
F21	-0.88	-24.38	15.20	-25.15	27.01	-66.74	24.22	7.16	-4.87	-5.61	-5.83	-9.42	9.74	10.10	-5.96	-6.61	9.69	10.34	-11.70	-11.46	-	-
F22	-0.84	-28.78	16.96	-29.51	25.71	-64.48	23.99	6.21	-4.46	-5.08	-4.37	-6.98	10.29	14.48	-6.88	-6.44	10.17	14.68	-11.71	-8.46	19.66	-

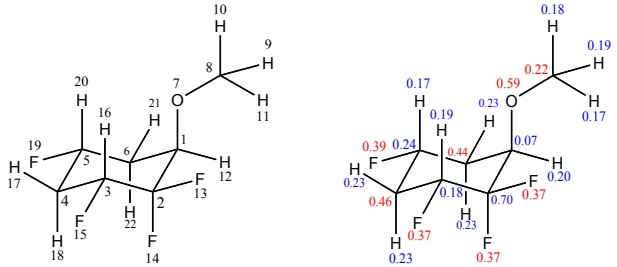


Table S20. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 9_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	F15	H16	H17	H18	F19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	11.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	1.79	28.34	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-3.82	-43.09	-18.57	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	2.36	19.43	5.92	-24.24	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-7.10	-41.42	-9.20	26.87	-23.28	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-10.30	-57.54	-12.31	25.83	-16.42	36.48	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-2.24	-15.95	-3.36	6.93	-4.07	8.85	30.30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	1.43	10.97	2.55	-5.45	3.21	-6.51	-18.68	-12.80	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	1.64	14.12	2.89	-5.60	3.05	-6.44	-17.27	-12.19	6.56	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	1.54	10.48	2.15	-4.67	2.79	-6.45	-15.75	-11.00	5.95	5.66	-	-	-	-	-	-	-	-	-	-	-	-
H12	4.39	21.57	3.49	-7.66	4.55	-13.29	-18.64	-5.76	3.57	4.34	4.70	-	-	-	-	-	-	-	-	-	-	-
F13	-3.79	-63.17	-9.54	15.22	-7.09	14.58	25.79	8.88	-6.04	-9.38	-5.68	-9.17	-	-	-	-	-	-	-	-	-	-
F14	-3.87	-63.67	-9.62	19.56	-8.60	18.93	20.38	6.22	-4.46	-5.46	-4.45	-9.51	20.74	-	-	-	-	-	-	-	-	-
F15	-2.43	-36.53	-16.38	23.74	-7.97	12.94	17.24	5.29	-4.13	-4.75	-3.49	-5.36	16.37	16.69	-	-	-	-	-	-	-	-
H16	1.65	20.61	10.48	-13.16	5.37	-8.18	-13.94	-3.79	3.00	3.25	2.29	3.24	-8.88	-7.04	-11.40	-	-	-	-	-	-	-
H17	1.42	15.51	6.52	-32.02	8.47	-9.68	-10.55	-2.98	2.43	2.42	2.01	3.01	-6.20	-7.23	-10.53	5.69	-	-	-	-	-	-
H18	1.65	19.11	6.45	-31.51	8.41	-11.95	-10.50	-2.98	2.32	2.44	2.08	3.57	-6.87	-10.65	-10.62	4.57	9.64	-	-	-	-	-
F19	-2.56	-21.81	-6.42	25.09	-22.37	24.06	18.35	5.07	-4.13	-3.84	-3.63	-5.60	8.65	10.79	10.03	-5.92	-11.12	-11.18	-	-	-	-
H20	1.51	12.06	3.77	-12.14	12.60	-11.69	-12.98	-3.13	2.59	2.28	2.08	2.95	-4.79	-5.05	-5.17	4.03	5.25	4.20	-11.05	-	-	-
H21	2.60	15.48	3.55	-10.07	8.47	-30.67	-17.16	-4.46	3.40	3.10	3.43	5.90	-6.17	-7.26	-5.34	3.39	4.02	4.53	-11.11	5.27	-	-
H22	2.57	19.21	4.17	-12.53	8.47	-30.37	-13.37	-3.69	2.73	2.82	2.78	5.98	-6.89	-10.80	-6.38	3.51	4.56	6.61	-11.24	4.23	9.65	-

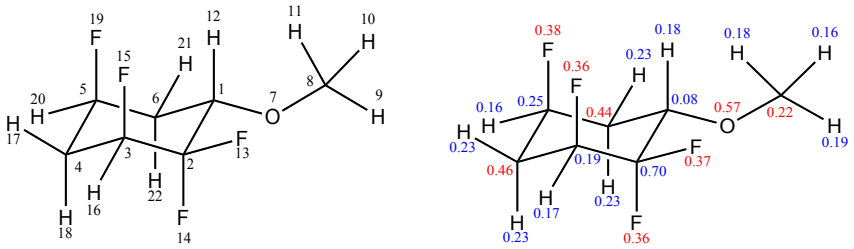


Table S21. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 9_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	F15	H16	H17	H18	F19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	9.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	1.57	28.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-3.41	-43.74	-18.99	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	2.06	19.33	5.84	-24.64	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-6.27	-41.85	-9.25	27.24	-23.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-8.80	-55.25	-9.31	20.96	-12.25	35.50	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-1.97	-15.90	-2.95	6.39	-3.59	8.85	29.16	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	1.25	10.82	2.11	-4.76	2.67	-6.47	-17.85	-12.61	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	1.34	10.42	2.10	-4.64	2.68	-6.37	-14.99	-10.81	5.80	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	1.42	13.90	2.54	-5.21	2.75	-6.36	-16.42	-11.95	6.39	5.50	-	-	-	-	-	-	-	-	-	-	-	-
H12	3.97	22.27	4.52	-9.54	5.80	-13.75	-18.52	-5.87	3.63	4.79	4.33	-	-	-	-	-	-	-	-	-	-	-
F13	-3.32	-63.03	-9.56	15.43	-6.99	14.61	24.55	8.77	-5.89	-5.62	-9.13	-9.34	-	-	-	-	-	-	-	-	-	-
F14	-3.41	-64.26	-9.91	20.23	-8.79	19.35	25.36	7.11	-5.29	-4.49	-6.10	-7.65	20.87	-	-	-	-	-	-	-	-	-
F15	-2.76	-37.47	-16.71	24.54	-9.95	15.62	16.93	5.83	-4.13	-4.43	-5.07	-9.75	16.87	13.30	-	-	-	-	-	-	-	-
H16	1.15	20.31	10.43	-13.27	4.25	-6.96	-7.73	-2.55	1.89	1.80	2.27	3.32	-8.72	-9.08	-11.50	-	-	-	-	-	-	-
H17	1.29	15.91	6.73	-33.45	8.70	-9.95	-8.45	-2.71	2.05	2.02	2.23	3.88	-6.35	-7.49	-11.29	5.67	-	-	-	-	-	-
H18	1.46	19.31	6.70	-33.09	8.69	-11.98	-9.78	-2.95	2.25	2.09	2.41	3.87	-7.00	-10.93	-8.77	5.89	10.22	-	-	-	-	-
F19	-2.89	-26.13	-8.07	26	-22.74	24.72	17.85	5.68	-4.2	-4.52	-4.37	-9.96	10.53	11.17	17.42	-6.05	-12.02	-9.26	-	-	-	-
H20	1.08	10.43	3.07	-12.54	12.70	-11.85	-7.28	-2.19	1.69	1.63	1.67	3.06	-4.05	-5.22	-5.38	2.48	5.35	5.53	-11.41	-	-	-
H21	2.31	15.69	3.59	-10.32	8.56	-31.06	-16.64	-4.46	3.38	3.39	3.06	6.20	-6.20	-7.42	-6.66	2.85	4.18	4.61	-11.8	5.28	-	-
H22	2.30	19.51	4.19	-12.49	8.50	-30.76	-16.79	-4.14	3.19	2.83	3.03	5.01	-6.97	-11.13	-6.69	3.39	4.61	6.44	-9.10	5.35	9.86	-

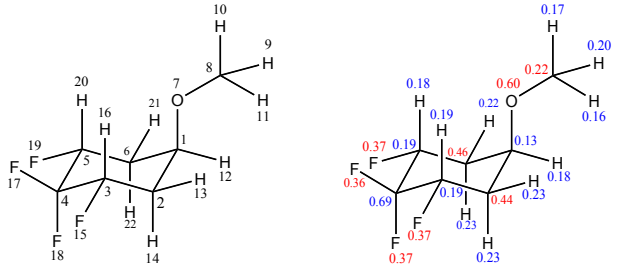


Table S22. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 10_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	F15	H16	F17	F18	F19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.89	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	3.30	-18.00	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	10.43	-40.31	27.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	3.30	-9.30	4.57	27.82	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-13.41	27.04	-9.73	-42.23	-18.81	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-18.68	37.19	-12.80	-39.04	-12.51	37.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-4.13	8.88	-3.23	-11.00	-3.74	11.36	31.10	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.65	-6.61	2.53	8.47	2.72	-7.53	-19.21	-13.23	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.85	-6.21	2.13	7.26	2.38	-7.75	-15.92	-11.17	6.09	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.61	-5.76	2.22	8.21	3.04	-8.96	-15.49	-10.94	5.97	5.06	-	-	-	-	-	-	-	-	-	-	-	-
H12	7.36	-12.39	3.25	10.59	3.25	-12.95	-17.49	-5.16	3.36	4.34	3.17	-	-	-	-	-	-	-	-	-	-	-
H13	4.74	-31.00	6.63	15.22	3.62	-10.20	-17.72	-4.38	3.43	3.13	2.71	5.55	-	-	-	-	-	-	-	-	-	-
H14	4.67	-30.52	6.56	18.73	4.20	-12.55	-13.57	-3.71	2.79	2.72	2.50	5.54	9.76	-	-	-	-	-	-	-	-	-
F15	-4.40	22.80	-16.51	-35.67	-6.13	13.54	17.61	4.89	-3.99	-3.35	-3.38	-4.92	-10.60	-10.72	-	-	-	-	-	-	-	-
H16	2.99	-12.78	10.67	20.16	4.19	-8.63	-14.37	-3.55	2.90	2.23	2.41	2.99	5.82	4.65	-11.49	-	-	-	-	-	-	-
F17	-3.80	14.18	-9.32	-59.98	-9.32	14.84	15.89	4.77	-3.85	-3.14	-3.61	-4.13	-6.06	-6.71	15.83	-8.65	-	-	-	-	-	-
F18	-4.68	18.56	-9.60	-61.41	-9.61	19.49	16.42	4.90	-3.77	-3.40	-3.65	-5.22	-7.18	-10.57	16.57	-7.00	19.88	-	-	-	-	-
F19	-4.40	12.93	-6.13	-35.62	-16.50	23.82	17.27	5.76	-4.36	-3.84	-4.86	-4.92	-5.38	-6.36	9.56	-5.72	15.85	16.53	-	-	-	-
H20	2.91	-8.04	4.08	19.57	10.33	-12.95	-13.62	-4.15	3.12	2.46	3.49	2.91	3.37	3.44	-5.55	4.42	-8.39	-6.79	-11.15	-	-	-
H21	4.53	-9.42	3.49	14.75	6.41	-31.36	-16.07	-5.98	3.84	4.17	5.38	5.35	3.94	4.44	-5.21	3.33	-5.86	-7.00	-10.34	5.41	-	-
H22	4.78	-12.34	4.33	19.30	6.71	-32.63	-13.62	-4.31	3.02	3.15	3.31	5.67	4.70	6.78	-6.56	3.63	-6.89	-10.95	-10.89	4.61	9.74	-

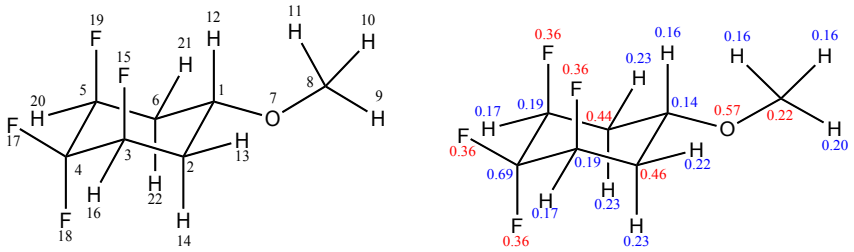


Table S23. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 10_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	F15	H16	F17	F18	F19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-12.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	3.16	-19.07	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	9.99	-42.26	28.46	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	3.13	-9.68	4.56	28.21	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-12.26	27.09	-9.42	-40.74	-18.22	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-17.25	36.34	-9.62	-31.58	-9.68	36.23	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-3.88	11.01	-3.11	-9.66	-2.80	8.84	29.77	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	2.47	-7.36	2.22	7.21	2.10	-6.54	-18.31	-12.84	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	2.68	-7.41	2.28	7.09	2.09	-6.28	-15.40	-11.01	5.97	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	2.47	-8.73	2.39	7.04	1.91	-5.71	-14.79	-10.65	5.79	4.97	-	-	-	-	-	-	-	-	-	-	-	-
H12	6.98	-12.93	4.12	12.80	4.09	-12.49	-16.99	-5.20	3.31	4.38	3.26	-	-	-	-	-	-	-	-	-	-	-
H13	4.32	-31.40	6.60	14.95	3.52	-9.51	-15.63	-5.77	3.76	3.92	5.28	5.42	-	-	-	-	-	-	-	-	-	-
H14	4.44	-31.79	6.64	18.62	4.22	-12.14	-16.38	-4.82	3.46	3.07	3.87	4.49	9.53	-	-	-	-	-	-	-	-	-
F15	-5.34	24.2	-17	-36.51	-7.68	15.49	16.93	5.87	-4.19	-4.62	-4.46	-8.56	-10.8	-8.54	-	-	-	-	-	-	-	-
H16	2.24	-13.03	10.64	20.01	3.31	-6.97	-7.74	-2.61	1.93	1.90	2.08	2.95	5.48	5.66	-11.47	-	-	-	-	-	-	-
F17	-3.57	14.58	-9.34	-59.82	-9.25	14.05	12.28	3.98	-3.04	-2.99	-2.92	-4.97	-5.83	-6.54	16.17	-8.27	-	-	-	-	-	-
F18	-4.51	19.71	-10.09	-62.89	-10.00	18.99	15.92	4.83	-3.72	-3.41	-3.56	-5.43	-7.15	-10.63	13.22	-9.18	19.95	-	-	-	-	-
F19	-5.35	16.08	-7.75	-36.55	-16.85	23.3	17.14	5.33	-4	-4.23	-3.61	-8.57	-6.41	-6.63	16.47	-5.76	16.19	13.23	-	-	-	-
H20	2.26	-7.27	3.36	20.10	10.61	-12.62	-7.91	-2.34	1.83	1.74	1.61	2.97	2.79	3.41	-5.78	2.70	-8.31	-9.21	-11.53	-	-	-
H21	4.52	-10.24	3.67	15.44	6.73	-31.31	-17.12	-4.38	3.39	3.23	2.70	5.65	3.99	4.65	-6.63	2.87	-6.02	-7.38	-11.11	5.66	-	-
H22	4.44	-12.58	4.26	18.61	6.58	-30.58	-16.84	-4.14	3.20	2.79	2.75	4.49	4.47	6.69	-6.62	3.39	-6.54	-10.62	-8.53	5.68	9.86	-

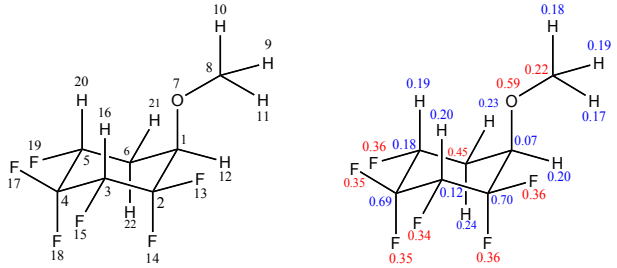


Table S24. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 11_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	F15	H16	F17	F18	F19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	11.11	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	1.17	18.91	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	5.63	63.78	18.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	1.78	14.71	2.99	27.60	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-7.11	-42.20	-6.26	-41.06	-18.10	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-10.17	-57.75	-8.25	-39.10	-12.71	37.23	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-2.21	-15.94	-2.24	-10.43	-3.13	9.03	30.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	1.43	11.13	1.73	8.33	2.51	-6.72	-18.98	-13.01	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	1.63	14.16	1.93	8.43	2.35	-6.60	-17.41	-12.28	6.69	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	1.53	10.55	1.45	7.09	2.18	-6.66	-15.97	-11.15	6.10	5.76	-	-	-	-	-	-	-	-	-	-	-	-
H12	4.46	22.28	2.40	11.78	3.59	-13.95	-19.24	-5.94	3.73	4.53	4.88	-	-	-	-	-	-	-	-	-	-	-
F13	-3.69	-62.55	-6.35	-22.46	-5.35	14.68	25.71	8.78	-6.08	-9.30	-5.63	-9.31	-	-	-	-	-	-	-	-	-	-
F14	-3.66	-61.58	-6.17	-27.40	-6.20	18.45	19.67	6.00	-4.35	-5.30	-4.32	-9.47	19.75	-	-	-	-	-	-	-	-	-
F15	-2.23	-33.97	-10.32	-33.22	-5.66	12.36	16.07	4.90	-3.88	-4.40	-3.27	-5.15	14.97	15.01	-	-	-	-	-	-	-	-
H16	1.76	22.38	7.65	21.78	4.45	-9.05	-15.15	-4.11	3.30	3.52	2.51	3.63	-9.66	-7.37	-11.58	-	-	-	-	-	-	-
F17	-2.05	-22.39	-6.18	-59.66	-9.15	14.30	15.91	4.52	-3.78	-3.67	-3.07	-4.58	9.11	9.93	14.50	-9.39	-	-	-	-	-	-
F18	-2.38	-27.58	-6.09	-59.36	-9.12	17.97	15.58	4.46	-3.54	-3.67	-3.16	-5.48	10.06	14.94	14.90	-7.26	18.94	-	-	-	-	-
F19	-2.36	-20.31	-4.00	-35.26	-16.13	22.83	17.36	4.78	-3.95	-3.63	-3.46	-5.39	8.00	9.54	8.78	-6.06	15.37	15.75	-	-	-	-
H20	1.67	13.48	2.80	20.48	10.71	-13.18	-14.84	-3.56	2.98	2.59	2.38	3.41	-5.34	-5.38	-5.39	4.93	-8.76	-6.82	-11.48	-	-	-
H21	2.63	15.93	2.44	15.55	6.69	-32.12	-17.58	-4.59	3.53	3.20	3.59	6.28	-6.27	-7.18	-5.14	3.78	-6.12	-7.02	-10.71	5.98	-	-
H22	2.68	20.54	2.99	20.05	6.86	-32.88	-14.23	-3.92	2.94	3.02	2.98	6.50	-7.24	-11.02	-6.43	4.09	-7.06	-10.73	-11.07	4.99	10.53	-

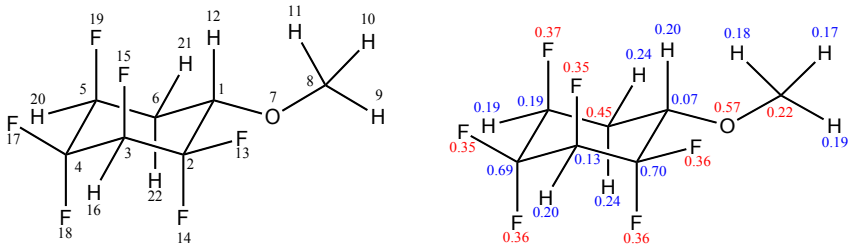


Table S25. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 11$_{eq}$.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	F15	H16	F17	F18	F19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	10.29	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	1.12	19.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	5.24	63.89	19.13	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	1.65	14.70	3.06	27.91	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-6.61	-42.34	-6.46	-41.29	-18.36	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-9.09	-54.74	-6.36	-30.81	-9.41	35.99	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-2.05	-16.06	-2.04	-9.48	-2.77	9.01	29.05	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	1.31	10.90	1.47	7.11	2.09	-6.67	-17.92	-12.79	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	1.41	10.72	1.48	6.97	2.09	-6.49	-15.03	-10.95	5.91	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	1.47	14.02	1.75	7.71	2.12	-6.48	-16.41	-12.08	6.50	5.59	-	-	-	-	-	-	-	-	-	-	-	-
H12	4.11	22.13	3.08	14.14	4.50	-13.95	-18.38	-5.83	3.66	4.87	4.21	-	-	-	-	-	-	-	-	-	-	-
F13	-3.40	-62.14	-6.54	-22.46	-5.32	14.66	23.85	8.76	-5.83	-5.81	-9.07	-9.29	-	-	-	-	-	-	-	-	-	-
F14	-3.39	-61.85	-6.50	-27.85	-6.33	18.67	24.35	6.98	-5.17	-4.44	-6.08	-7.32	19.77	-	-	-	-	-	-	-	-	-
F15	-2.66	-35.03	-10.89	-34.33	-7.16	14.81	15.67	5.44	-3.89	-4.21	-4.69	-8.96	15.89	11.97	-	-	-	-	-	-	-	-
H16	1.30	21.80	7.82	21.48	3.56	-7.74	-8.33	-2.78	2.06	1.99	2.46	3.57	-9.18	-9.47	-11.68	-	-	-	-	-	-	-
F17	-1.86	-21.87	-6.24	-58.91	-9.03	14.05	11.87	3.88	-2.97	-2.93	-3.19	-5.46	8.88	9.82	15.17	-8.70	-	-	-	-	-	-
F18	-2.26	-28.23	-6.50	-60.69	-9.51	18.39	14.78	4.50	-3.48	-3.20	-3.68	-5.73	10.27	15.56	11.95	-9.53	18.88	-	-	-	-	-
F19	-2.85	-24.61	-5.22	-36.33	-16.64	23.59	16.83	5.38	-4.02	-4.32	-4.11	-9.56	9.91	9.99	-6.20	15.40	15.95	12.66	-	-	-	-
H20	1.24	11.46	2.34	20.76	10.87	-13.26	-8.01	-2.43	1.89	1.82	1.86	3.40	-4.43	-5.42	-5.62	3.02	-8.40	-9.17	-11.85	-	-	-
H21	2.47	16.11	2.54	15.77	6.83	-32.59	-17.21	-4.59	3.54	3.46	3.15	6.34	-6.31	-7.31	-6.37	3.21	-6.07	-7.23	-11.30	6.00	-	-
H22	2.52	20.66	3.08	19.85	6.94	-33.18	-17.53	-4.37	3.40	2.99	3.23	5.28	-7.27	-11.20	-6.67	3.98	-6.85	-10.78	-9.05	6.23	10.76	-

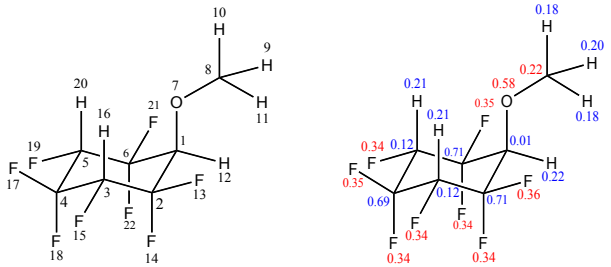


Table S26. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 12_{ax}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	F15	H16	F17	F18	F19	H20	F21	F22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	1.62	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.17	18.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.82	63.79	18.46	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.17	9.75	1.99	18.37	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	1.63	65.96	9.85	64.24	18.99	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-1.46	-57.37	-8.21	-38.53	-8.24	-58.16	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.32	-15.33	-2.16	-10.21	-2.07	-14.46	29.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.21	11.32	1.76	8.49	1.71	11.00	-19.05	-13.16	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.24	13.45	1.81	8.09	1.53	10.53	-17.00	-12.03	6.78	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.23	10.65	1.49	7.47	1.56	11.58	-16.47	-11.60	6.54	5.97	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.71	24.01	2.61	12.82	2.60	24.23	-20.40	-6.43	4.14	5.17	5.39	-	-	-	-	-	-	-	-	-	-	-
F13	-0.53	-61.70	-6.25	-22.07	-3.50	-22.77	25.45	8.20	-6.10	-8.38	-5.42	-9.86	-	-	-	-	-	-	-	-	-	-
F14	-0.51	-59.52	-5.93	-26.17	-3.93	-27.22	18.59	5.60	-4.25	-4.97	-4.21	-9.77	18.63	-	-	-	-	-	-	-	-	-
F15	-0.32	-33.54	-10.20	-32.79	-3.71	-19.08	15.70	4.65	-3.89	-4.05	-3.29	-5.49	14.39	14.22	-	-	-	-	-	-	-	-
H16	0.26	22.76	7.78	22.09	3.00	14.56	-15.39	-4.00	3.40	3.28	2.63	4.00	-9.68	-7.18	-11.58	-	-	-	-	-	-	-
F17	-0.30	-22.21	-6.13	-59.11	-6.10	-22.34	15.59	4.39	-3.83	-3.49	-3.21	-4.94	8.88	9.39	14.14	-9.47	-	-	-	-	-	-
F18	-0.33	-26.42	-5.86	-57.33	-5.83	-26.62	14.68	4.20	-3.46	-3.41	-3.19	-5.70	9.45	13.59	14.14	-7.08	18.03	-	-	-	-	-
F19	-0.32	-18.94	-3.73	-32.78	-10.14	-33.69	15.79	4.43	-3.77	-3.33	-3.50	-5.50	7.34	8.51	8.06	-5.72	14.13	14.12	-	-	-	-
H20	0.26	14.56	3.03	22.18	7.78	23.00	-15.65	-3.82	3.31	2.72	2.81	4.03	-5.69	-5.57	-5.75	5.40	-9.50	-7.11	-11.63	-	-	-
F21	-0.52	-22.21	-3.44	-21.65	-6.09	-61.03	25.12	7.08	-5.55	-4.88	-6.22	-9.74	8.85	9.48	7.20	-5.53	8.70	9.30	14.13	-9.48	-	-
F22	-0.51	-27.37	-3.99	-26.47	-5.93	-60.01	18.76	5.40	-4.17	-4.20	-4.46	-9.84	9.73	14.27	8.62	-5.58	9.47	13.80	14.21	-7.25	18.36	-

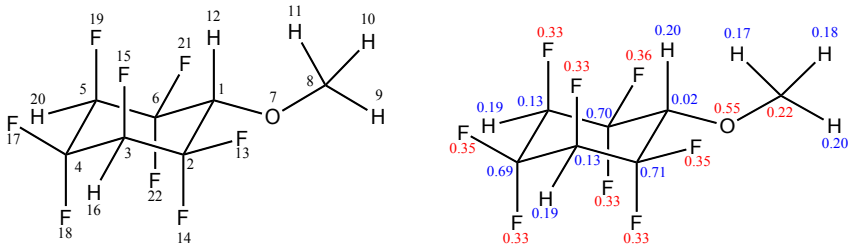


Table S27. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 12_{eq}.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	F15	H16	F17	F18	F19	H20	F21	F22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	0.61	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.07	19.66	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.30	64.23	19.12	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.07	10.07	2.09	19.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.60	66.02	10.08	63.94	19.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-0.52	-54.77	-6.26	-30.00	-6.20	-53.93	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.12	-14.45	-1.91	-9.32	-1.96	-15.21	27.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.08	10.97	1.49	7.36	1.51	11.24	-18.12	-13.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.09	10.26	1.47	7.52	1.68	12.98	-15.70	-11.68	6.59	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.08	11.31	1.53	7.14	1.45	10.32	-15.20	-11.25	6.36	5.65	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.26	24.64	3.41	15.53	3.38	24.40	-19.63	-6.53	4.19	5.11	5.32	-	-	-	-	-	-	-	-	-	-	-
F13	-0.20	-60.92	-6.34	-21.68	-3.52	-22.18	23.14	7.00	-5.45	-4.74	-6.07	-10.07	-	-	-	-	-	-	-	-	-	-
F14	-0.19	-60.21	-6.25	-26.54	-4.10	-27.23	23.08	6.02	-4.94	-4.29	-4.48	-7.73	18.36	-	-	-	-	-	-	-	-	-
F15	-0.15	-35.17	-10.86	-34.12	-4.91	-23.18	15.30	5.12	-3.93	-4.00	-4.33	-9.86	15.37	11.44	-	-	-	-	-	-	-	-
H16	0.08	22.68	8.07	22.10	2.51	12.39	-8.43	-2.65	2.14	2.01	2.13	4.06	-9.09	-9.39	-11.96	-	-	-	-	-	-	-
F17	-0.11	-21.75	-6.17	-58.04	-6.14	-21.64	11.42	3.78	-3.04	-3.10	-2.96	-5.93	8.48	9.27	14.92	-8.85	-	-	-	-	-	-
F18	-0.13	-27.34	-6.25	-58.54	-6.22	-27.21	13.87	4.24	-3.46	-3.38	-3.17	-6.06	9.52	14.22	11.43	-9.41	17.90	-	-	-	-	-
F19	-0.15	-23.29	-4.94	-34.09	-10.81	-34.96	15.25	5.29	-4.00	-4.67	-4.08	-9.83	9.07	8.96	14.58	-6.03	14.9	11.43	-	-	-	-
H20	0.08	12.43	2.52	22.07	8.02	22.49	-8.38	-2.74	2.18	2.38	2.00	4.04	-4.62	-5.55	-6.02	3.34	-8.83	-9.40	-11.94	-	-	-
F21	-0.20	-22.62	-3.59	-21.98	-6.38	-61.24	23.22	7.93	-5.88	-7.88	-5.18	-10.15	8.78	9.64	9.19	-4.69	8.59	9.65	15.55	-9.19	-	-
F22	-0.19	-27.44	-4.13	-26.59	-6.22	-59.83	22.92	6.31	-5.09	-5.17	-4.20	-7.72	9.51	14.28	8.97	-5.57	9.28	14.26	11.44	-9.37	18.62	-

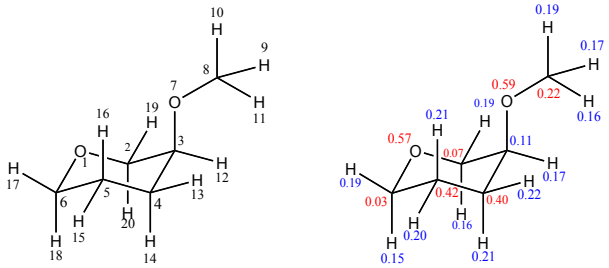


Table S28. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 13_{ax}.

	O1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20
O1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	9.16	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.23	-1.55	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	26.60	3.62	-9.22	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	33.18	3.34	-5.93	36.92	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	4.41	0.31	-0.40	1.75	3.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	38.05	5.37	-14.52	33.25	28.24	1.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	12.03	1.70	-3.24	8.02	7.39	0.54	30.57	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-10.38	-1.37	2.09	-5.44	-5.41	-0.43	-15.71	-11.21	-	-	-	-	-	-	-	-	-	-	-	-
H10	-8.25	-1.07	2.02	-5.78	-5.54	-0.39	-18.28	-12.73	5.93	-	-	-	-	-	-	-	-	-	-	-
H11	-7.43	-1.13	2.14	-5.26	-4.60	-0.34	-14.83	-10.53	4.92	5.57	-	-	-	-	-	-	-	-	-	-
H12	-9.47	-1.75	5.30	-10.25	-6.78	-0.47	-15.81	-4.59	2.86	2.96	3.65	-	-	-	-	-	-	-	-	-
H13	-10.66	-1.41	3.51	-26.36	-13.92	-0.68	-16.60	-4.06	2.63	3.10	2.69	4.71	-	-	-	-	-	-	-	-
H14	-11.35	-1.60	3.21	-23.97	-12.78	-0.77	-11.64	-3.21	2.24	2.34	2.22	4.48	7.97	-	-	-	-	-	-	-
H15	-11.60	-1.20	2.07	-12.57	-26.35	-1.04	-10.19	-2.86	2.09	2.22	1.83	2.64	5.73	5.40	-	-	-	-	-	-
H16	-15.05	-1.47	2.69	-13.25	-27.57	-1.09	-15.79	-4.07	2.96	3.16	2.40	3.11	6.20	4.57	8.23	-	-	-	-	-
H17	-17.81	-1.30	1.71	-7.26	-12.18	-1.88	-8.66	-2.70	2.19	2.05	1.69	2.14	3.13	3.23	5.07	5.43	-	-	-	-
H18	-13.86	-1.29	1.60	-7.18	-9.73	-1.48	-6.92	-2.12	1.67	1.56	1.40	2.06	2.82	3.72	4.12	3.48	5.27	-	-	-
H19	-17.90	-3.90	3.03	-7.31	-6.92	-0.63	-13.46	-5.25	4.72	3.21	3.69	4.17	3.16	3.27	2.64	3.29	2.94	2.64	-	-
H20	-15.02	-3.32	2.66	-7.92	-7.07	-0.68	-9.42	-3.06	2.40	2.07	2.19	3.75	3.11	4.14	2.75	2.94	2.84	3.38	5.78	-

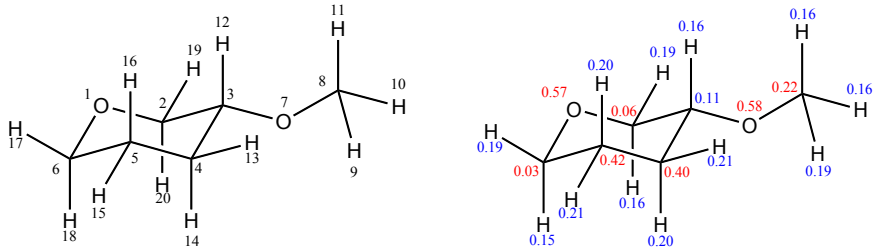


Table S29. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 13_{eq}.

	O1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20
O1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	8.23	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-8.40	-1.42	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	26.80	3.28	-9.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	32.97	2.98	-5.98	36.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	4.52	0.29	-0.42	1.80	3.08	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	30.12	4.83	-14.62	32.80	21.75	1.57	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	9.64	1.46	-3.27	7.98	6.25	0.48	29.81	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-6.77	-0.96	2.05	-5.81	-4.63	-0.35	-18.07	-12.58	-	-	-	-	-	-	-	-	-	-	-	-
H10	-7.42	-1.16	2.07	-5.16	-4.31	-0.35	-14.81	-10.60	5.68	-	-	-	-	-	-	-	-	-	-	-
H11	-6.93	-0.97	2.22	-5.55	-4.56	-0.34	-15.10	-10.72	5.74	4.85	-	-	-	-	-	-	-	-	-	-
H12	-11.30	-1.51	5.16	-9.94	-8.01	-0.54	-14.92	-4.53	2.85	2.83	3.75	-	-	-	-	-	-	-	-	-
H13	-10.52	-1.25	3.52	-26.12	-13.59	-0.69	-15.54	-3.97	3.02	2.46	2.86	4.58	-	-	-	-	-	-	-	-
H14	-11.64	-1.48	3.36	-24.61	-12.96	-0.81	-15.20	-3.70	2.82	2.46	2.43	3.51	8.06	-	-	-	-	-	-	-
H15	-11.83	-1.10	2.15	-12.89	-26.66	-1.08	-8.89	-2.62	2.01	1.81	1.90	2.92	5.77	5.62	-	-	-	-	-	-
H16	-14.06	-1.23	2.54	-12.38	-25.49	-1.04	-9.40	-2.86	2.11	1.96	2.19	4.02	5.66	4.35	7.85	-	-	-	-	-
H17	-17.79	-1.17	1.74	-7.29	-12.08	-1.93	-7.02	-2.24	1.68	1.66	1.64	2.45	3.08	3.30	5.15	5.08	-	-	-	-
H18	-14.27	-1.20	1.68	-7.45	-9.98	-1.57	-6.93	-2.09	1.57	1.55	1.44	2.07	2.87	3.93	4.33	3.36	5.44	-	-	-
H19	-17.60	-3.46	3.03	-7.22	-6.75	-0.64	-12.97	-4.79	3.06	4.35	3.24	3.99	3.06	3.30	2.65	3.01	2.89	2.68	-	-
H20	-14.73	-2.96	2.66	-7.82	-6.89	-0.68	-11.70	-3.45	2.42	2.78	2.15	2.79	3.02	4.18	2.76	2.69	2.80	3.44	5.57	-

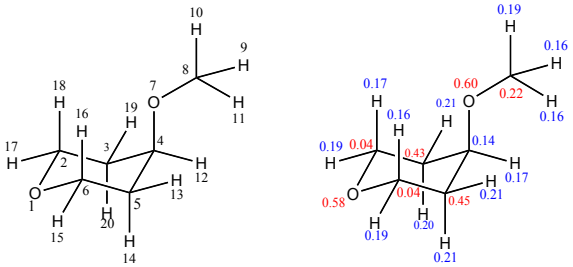


Table S30. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 14_{ax}.

	O1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20
O1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	5.15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	34.20	3.59	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-9.04	-0.69	-12.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	35.76	2.00	26.09	-13.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	5.29	0.21	1.97	-0.70	3.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	32.60	2.58	36.34	-18.96	36.49	2.58	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	9.12	0.65	8.57	-4.14	10.96	0.76	30.74	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-5.96	-0.42	-5.88	2.82	-7.42	-0.48	-15.44	-10.68	-	-	-	-	-	-	-	-	-	-	-	-
H10	-6.85	-0.50	-6.27	2.61	-7.12	-0.54	-18.62	-12.64	5.73	-	-	-	-	-	-	-	-	-	-	-
H11	-6.78	-0.45	-5.54	2.59	-8.55	-0.61	-15.19	-10.59	4.82	5.68	-	-	-	-	-	-	-	-	-	-
H12	-8.36	-0.61	-11.15	6.90	-11.64	-0.63	-16.19	-4.70	3.90	3.02	2.84	-	-	-	-	-	-	-	-	-
H13	-11.78	-0.68	-8.61	4.28	-28.41	-1.24	-15.04	-5.54	3.83	3.48	4.94	4.54	-	-	-	-	-	-	-	-
H14	-14.99	-0.82	-10.95	4.43	-28.88	-1.27	-12.36	-3.88	2.83	2.66	2.95	4.81	8.20	-	-	-	-	-	-	-
H15	-17.71	-0.72	-6.97	2.43	-12.89	-2.22	-9.22	-2.98	1.95	2.19	2.47	2.42	5.07	5.26	-	-	-	-	-	-
H16	-15.12	-0.79	-7.20	2.64	-11.30	-1.92	-11.91	-3.56	2.10	2.61	2.96	2.39	4.48	3.71	5.67	-	-	-	-	-
H17	-17.65	-2.15	-12.32	2.42	-7.26	-0.74	-9.39	-2.55	1.70	2.02	1.76	2.41	2.62	3.20	2.85	2.81	-	-	-	-
H18	-15.58	-1.93	-11.18	2.72	-7.73	-0.83	-12.59	-3.10	1.92	2.47	2.12	2.46	2.83	2.98	2.91	3.81	5.82	-	-	-
H19	-12.25	-1.26	-28.34	4.51	-9.38	-0.73	-16.78	-4.05	2.82	3.13	2.50	4.74	3.44	3.98	2.74	2.88	5.23	4.85	-	-
H20	-14.51	-1.21	-26.99	4.31	-11.07	-0.81	-12.29	-3.31	2.39	2.45	2.22	4.68	3.72	5.50	3.10	2.81	5.13	3.74	8.26	-

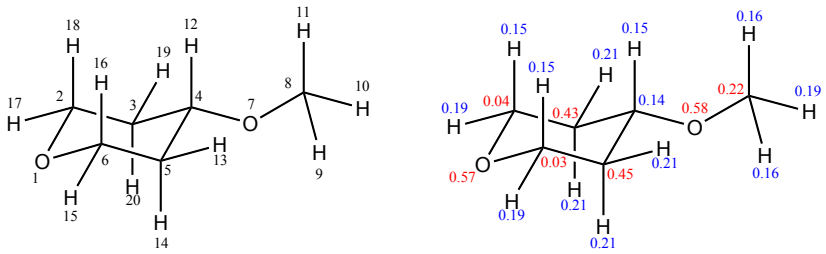


Table S31. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 14_{eq}.

	O1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20
O1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	4.74	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	33.93	3.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-8.98	-0.64	-12.89	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	35.34	1.85	26.17	-13.39	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	4.54	0.17	1.70	-0.61	3.32	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	26.57	1.83	35.32	-18.56	35.49	1.72	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	8.13	0.53	8.61	-4.18	11.04	0.56	30.04	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-5.96	-0.36	-5.61	2.65	-8.74	-0.43	-14.92	-10.73	-	-	-	-	-	-	-	-	-	-	-	-
H10	-5.95	-0.39	-6.25	2.62	-7.14	-0.39	-18.11	-12.69	5.72	-	-	-	-	-	-	-	-	-	-	-
H11	-5.70	-0.38	-5.81	2.78	-7.28	-0.40	-14.86	-10.60	4.80	5.66	-	-	-	-	-	-	-	-	-	-
H12	-8.84	-0.65	-10.27	6.28	-10.72	-0.62	-14.39	-4.32	2.65	2.74	3.50	-	-	-	-	-	-	-	-	-
H13	-11.70	-0.63	-8.63	4.29	-28.44	-1.08	-14.24	-5.42	4.83	3.41	3.72	4.27	-	-	-	-	-	-	-	-
H14	-14.66	-0.75	-10.90	4.42	-28.79	-1.09	-15.21	-4.65	3.83	3.20	2.86	3.50	8.12	-	-	-	-	-	-	-
H15	-17.96	-0.68	-7.15	2.49	-13.19	-1.96	-7.98	-2.72	2.16	1.96	1.92	2.57	5.21	5.34	-	-	-	-	-	-
H16	-14.13	-0.69	-6.78	2.49	-10.64	-1.56	-7.17	-2.43	1.81	1.70	1.83	3.00	4.27	3.48	5.46	-	-	-	-	-
H17	-17.98	-2.05	-12.66	2.50	-7.46	-0.66	-8.13	-2.41	1.67	1.84	1.70	2.57	2.69	3.26	3.00	2.72	-	-	-	-
H18	-14.13	-1.63	-10.19	2.49	-7.05	-0.66	-7.24	-2.21	1.51	1.63	1.65	2.99	2.60	2.70	2.71	3.26	5.47	-	-	-
H19	-12.07	-1.16	-28.19	4.49	-9.34	-0.62	-15.67	-3.98	2.48	3.03	2.77	4.43	3.42	3.94	2.78	2.69	5.35	4.38	-	-
H20	-14.72	-1.14	-27.61	4.44	-11.41	-0.72	-15.75	-3.88	2.62	2.93	2.48	3.51	3.81	5.63	3.26	2.71	5.36	3.48	8.42	-

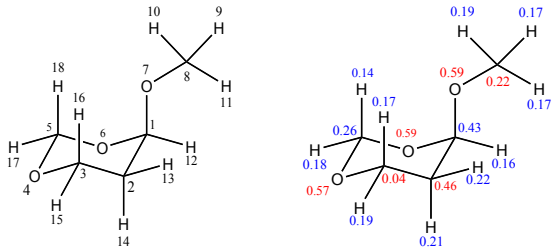


Table S32. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 15$_{ax}$.

	C1	C2	C3	O4	C5	O6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-42.48	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-2.42	4.22	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O4	-28.94	35.99	5.66	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	15.71	-14.21	-1.58	-35.47	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O6	-59.42	37.24	3.00	48.34	-36.40	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-60.18	38.15	2.84	32.64	-17.99	50.26	-	-	-	-	-	-	-	-	-	-	-	-
C8	-13.51	9.28	0.74	9.51	-5.53	15.62	31.34	-	-	-	-	-	-	-	-	-	-	-
H9	9.23	-6.51	-0.56	-7.70	4.87	-13.38	-16.63	-11.94	-	-	-	-	-	-	-	-	-	-
H10	8.19	-6.52	-0.55	-6.90	3.81	-9.72	-18.42	-12.92	6.15	-	-	-	-	-	-	-	-	-
H11	8.99	-6.29	-0.48	-6.13	3.42	-10.25	-15.75	-11.24	5.40	5.81	-	-	-	-	-	-	-	-
H12	20.69	-11.09	-0.65	-8.12	4.26	-15.78	-15.41	-4.63	3.09	2.83	3.76	-	-	-	-	-	-	-
H13	14.50	-30.54	-1.43	-12.43	5.08	-12.94	-17.12	-4.23	2.82	3.13	2.92	4.51	-	-	-	-	-	-
H14	14.16	-29.62	-1.40	-15.02	5.74	-15.44	-12.81	-3.56	2.59	2.53	2.54	4.67	8.76	-	-	-	-	-
H15	7.84	-13.29	-2.47	-17.87	5.10	-9.99	-9.52	-2.68	2.01	2.05	1.78	2.36	5.40	5.49	-	-	-	-
H16	8.65	-11.93	-2.19	-15.66	5.69	-10.49	-12.48	-3.21	2.36	2.47	1.97	2.36	5.02	3.94	6.07	-	-	-
H17	7.68	-7.14	-0.77	-16.67	14.08	-17.30	-9.12	-3.11	2.84	2.20	2.00	2.35	2.71	3.13	2.78	2.80	-	-
H18	7.31	-6.50	-0.74	-12.60	10.71	-13.01	-10.49	-3.27	2.94	2.33	1.87	2.00	2.53	2.48	2.42	3.27	4.43	-

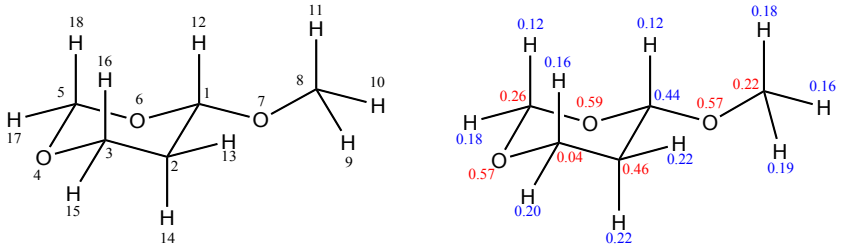


Table S33. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 15$_{eq}$.

	C1	C2	C3	O4	C5	O6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-43.73	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-2.42	4.12	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O4	-29.52	35.80	5.51	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	16.38	-14.45	-1.56	-35.71	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O6	-60.38	37.53	2.93	48.23	-37.04	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-59.42	36.31	2.11	26.54	-14.03	48.82	-	-	-	-	-	-	-	-	-	-	-	-
C8	-13.90	9.30	0.64	8.59	-4.81	15.85	29.80	-	-	-	-	-	-	-	-	-	-	-
H9	8.43	-6.54	-0.46	-6.06	3.23	-9.85	-17.55	-12.95	-	-	-	-	-	-	-	-	-	-
H10	9.88	-6.81	-0.50	-7.13	4.19	-14.21	-16.54	-12.49	6.43	-	-	-	-	-	-	-	-	-
H11	9.00	-6.16	-0.45	-5.88	3.33	-10.03	-14.62	-10.98	5.68	5.49	-	-	-	-	-	-	-	-
H12	16.22	-8.68	-0.61	-7.32	4.20	-11.92	-11.39	-3.59	2.20	2.50	2.85	-	-	-	-	-	-	-
H13	14.60	-30.17	-1.37	-12.18	5.07	-12.76	-15.20	-4.06	2.99	2.85	2.79	3.60	-	-	-	-	-	-
H14	15.14	-30.87	-1.41	-15.41	6.06	-16.30	-16.33	-4.22	3.10	3.19	2.65	2.99	8.97	-	-	-	-	-
H15	8.24	-13.63	-2.46	-18.25	5.28	-10.27	-8.13	-2.54	1.87	1.98	1.75	2.12	5.45	5.79	-	-	-	-
H16	8.20	-11.04	-1.96	-14.43	5.28	-9.63	-7.27	-2.33	1.66	1.79	1.70	2.47	4.57	3.77	5.75	-	-	-
H17	8.03	-7.31	-0.76	-16.96	14.56	-17.65	-7.90	-2.89	2.00	2.63	1.98	2.09	2.72	3.33	2.91	2.63	-	-
H18	6.93	-5.96	-0.66	-11.42	9.82	-11.86	-6.02	-2.16	1.45	1.83	1.60	2.17	2.27	2.36	2.25	2.71	4.12	-

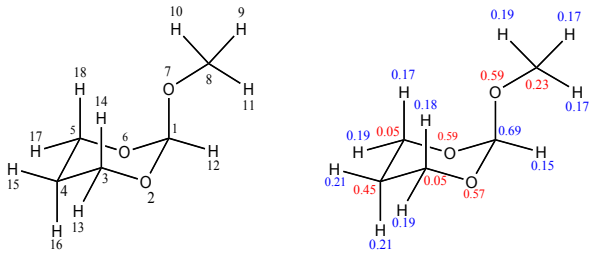


Table S34. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 16$_{ax}$.

	C1	O2	C3	C4	C5	O6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	-94.26	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-4.50	6.05	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-36.92	35.00	4.50	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-4.64	3.21	0.29	4.66	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O6	-96.62	47.69	3.22	36.33	6.50	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-97.59	49.66	3.25	25.96	3.31	50.21	-	-	-	-	-	-	-	-	-	-	-	-
C8	-22.29	12.12	0.84	7.63	1.04	15.93	31.78	-	-	-	-	-	-	-	-	-	-	-
H9	14.78	-8.24	-0.61	-6.01	-0.90	-13.22	-16.47	-12.02	-	-	-	-	-	-	-	-	-	-
H10	13.37	-8.36	-0.62	-5.48	-0.70	-9.73	-18.50	-13.17	6.12	-	-	-	-	-	-	-	-	-
H11	14.84	-8.19	-0.54	-4.89	-0.64	-10.49	-15.87	-11.52	5.41	5.90	-	-	-	-	-	-	-	-
H12	32.04	-14.30	-0.71	-6.07	-0.74	-14.89	-14.59	-4.42	2.86	2.70	3.58	-	-	-	-	-	-	-
H13	13.49	-17.75	-2.67	-13.03	-0.87	-9.92	-10.03	-2.81	2.02	2.12	1.87	2.40	-	-	-	-	-	-
H14	15.26	-16.09	-2.47	-12.18	-1.00	-10.69	-13.89	-3.51	2.47	2.67	2.14	2.45	6.30	-	-	-	-	-
H15	12.86	-11.83	-1.49	-28.85	-1.54	-12.28	-10.06	-3.11	2.47	2.32	1.98	2.24	5.18	5.03	-	-	-	-
H16	14.77	-14.32	-1.47	-28.20	-1.52	-14.89	-9.82	-3.03	2.38	2.17	2.03	2.64	5.31	3.96	8.17	-	-	-
H17	13.47	-9.58	-0.85	-13.06	-2.76	-18.46	-9.90	-3.46	3.11	2.40	2.23	2.41	2.81	2.94	5.20	5.32	-	-
H18	14.51	-9.84	-0.93	-11.61	-2.42	-15.87	-12.98	-4.21	3.79	2.94	2.40	2.33	2.80	3.75	4.79	3.78	6.01	-

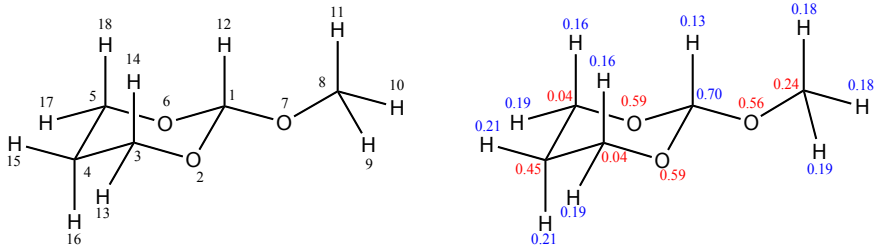


Table S35. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 16$_{eq}$.

	C1	O2	C3	C4	C5	O6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	-97.50	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-4.10	5.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-37.35	36.45	4.05	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-4.10	2.90	0.23	4.05	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O6	-97.50	49.72	2.90	36.45	5.67	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-94.99	48.05	2.16	20.49	2.16	48.05	-	-	-	-	-	-	-	-	-	-	-	-
C8	-23.27	16.55	0.79	7.90	0.79	16.55	30.55	-	-	-	-	-	-	-	-	-	-	-
H9	13.34	-9.72	-0.50	-5.02	-0.50	-9.72	-17.05	-13.37	-	-	-	-	-	-	-	-	-	-
H10	15.87	-14.22	-0.65	-6.29	-0.57	-11.02	-16.13	-13.01	6.28	-	-	-	-	-	-	-	-	-
H11	15.87	-11.02	-0.57	-6.29	-0.65	-14.22	-16.13	-13.01	6.28	6.12	-	-	-	-	-	-	-	-
H12	26.93	-12.13	-0.67	-5.99	-0.67	-12.13	-11.82	-3.04	1.96	2.11	2.11	-	-	-	-	-	-	-
H13	13.85	-18.72	-2.44	-13.28	-0.77	-10.10	-8.36	-3.25	2.12	2.84	2.35	2.29	-	-	-	-	-	-
H14	14.03	-14.99	-1.97	-10.96	-0.79	-9.65	-7.60	-2.62	1.73	2.10	1.89	2.80	5.75	-	-	-	-	-
H15	13.06	-12.31	-1.34	-28.98	-1.34	-12.31	-7.70	-2.98	1.97	2.37	2.37	2.27	5.28	4.52	-	-	-	-
H16	14.95	-15.00	-1.33	-28.58	-1.33	-15.00	-8.97	-3.76	2.37	3.10	3.10	2.26	5.43	3.59	8.26	-	-	-
H17	13.85	-10.10	-0.77	-13.28	-2.44	-18.72	-8.37	-3.25	2.12	2.35	2.84	2.29	2.90	2.69	5.28	5.43	-	-
H18	14.03	-9.65	-0.79	-10.96	-1.97	-14.99	-7.60	-2.62	1.73	1.89	2.10	2.80	2.69	3.19	4.52	3.59	5.75	-

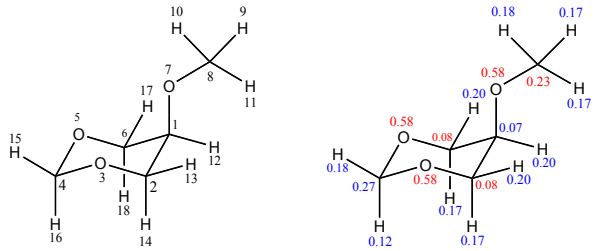


Table S36. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 17_{ax}.

	C1	C2	O3	C4	O5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-1.21	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O3	-5.62	10.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	2.28	-2.96	-36.69	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O5	-5.62	5.31	47.65	-36.69	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-1.21	0.80	5.31	-2.96	10.44	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-9.79	6.02	34.97	-13.86	34.97	6.02	-	-	-	-	-	-	-	-	-	-	-	-
C8	-2.30	1.97	14.35	-5.68	14.35	1.97	31.33	-	-	-	-	-	-	-	-	-	-	-
H9	1.53	-1.64	-13.23	4.63	-10.31	-1.30	-16.02	-12.26	-	-	-	-	-	-	-	-	-	-
H10	1.33	-1.18	-8.51	3.45	-8.51	-1.18	-17.43	-12.92	5.94	-	-	-	-	-	-	-	-	-
H11	1.53	-1.30	-10.31	4.63	-13.23	-1.64	-16.02	-12.26	5.68	5.94	-	-	-	-	-	-	-	-
H12	4.27	-2.35	-11.17	4.72	-11.17	-2.35	-18.87	-4.57	3.07	2.97	3.07	-	-	-	-	-	-	-
H13	2.26	-4.81	-19.27	5.59	-10.46	-1.53	-15.12	-5.09	4.50	3.22	3.11	5.10	-	-	-	-	-	-
H14	1.89	-3.98	-15.79	5.74	-9.95	-1.53	-9.74	-3.21	2.57	2.06	2.22	4.73	6.47	-	-	-	-	-
H15	1.13	-1.42	-17.10	14.70	-17.10	-1.42	-7.62	-3.33	2.78	2.11	2.78	2.46	3.02	2.82	-	-	-	-
H16	0.95	-1.23	-11.54	9.95	-11.54	-1.23	-5.51	-2.11	1.67	1.34	1.67	2.14	2.34	2.91	4.09	-	-	-
H17	2.26	-1.53	-10.46	5.59	-19.27	-4.81	-15.12	-5.09	3.11	3.22	4.50	5.10	3.25	2.97	3.02	2.34	-	-
H18	1.89	-1.53	-9.95	5.74	-15.79	-3.97	-9.74	-3.21	2.22	2.06	2.57	4.73	2.97	3.44	2.82	2.91	6.47	-

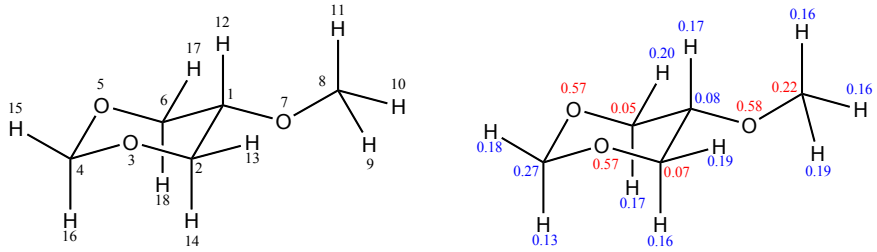


Table S37. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 17_{eq}.

	C1	C2	O3	C4	O5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-1.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O3	-6.00	9.15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	2.45	-2.62	-36.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O5	-6.00	4.64	46.18	-36.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-0.85	0.47	3.46	-1.95	6.79	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-10.45	5.39	29.86	-12.75	30.24	4.15	-	-	-	-	-	-	-	-	-	-	-	-
C8	-2.34	1.63	9.48	-3.83	8.62	1.01	29.60	-	-	-	-	-	-	-	-	-	-	-
H9	1.49	-1.09	-6.76	2.85	-6.45	-0.74	-18.17	-12.70	-	-	-	-	-	-	-	-	-	-
H10	1.61	-1.09	-6.87	2.76	-6.35	-0.71	-15.27	-10.87	5.88	-	-	-	-	-	-	-	-	-
H11	1.51	-1.31	-7.36	2.83	-5.99	-0.66	-14.86	-10.65	5.78	4.96	-	-	-	-	-	-	-	-
H12	3.91	-1.78	-11.78	4.65	-11.76	-1.33	-15.65	-4.75	3.03	3.97	3.01	-	-	-	-	-	-	-
H13	2.22	-3.99	-17.83	5.21	-9.58	-0.94	-12.97	-4.77	3.12	3.28	4.36	4.31	-	-	-	-	-	-
H14	1.95	-3.41	-15.00	5.58	-9.68	-1.01	-12.07	-3.57	2.54	2.25	2.92	3.02	5.86	-	-	-	-	-
H15	1.21	-1.26	-16.84	14.63	-16.81	-0.93	-6.81	-2.15	1.63	1.59	1.60	2.51	2.82	2.73	-	-	-	-
H16	1.01	-1.11	-11.55	10.08	-11.54	-0.82	-5.82	-1.73	1.32	1.20	1.29	1.81	2.23	2.88	4.13	-	-	-
H17	2.31	-1.30	-9.91	5.37	-18.28	-3.06	-14.13	-3.63	2.79	2.67	2.28	4.49	2.90	2.86	2.90	2.30	-	-
H18	1.96	-1.37	-9.74	5.61	-15.05	-2.55	-12.50	-3.04	2.35	2.03	2.04	3.04	2.77	3.51	2.74	2.89	6.08	-

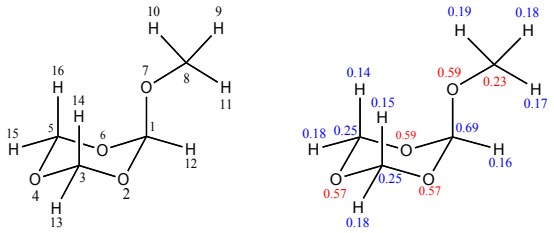


Table S38. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 18_{ax}.

	C1	O2	C3	O4	C5	O6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	-93.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	24.95	-33.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O4	-47.60	46.14	-34.20	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	24.83	-17.71	9.37	-34.19	-	-	-	-	-	-	-	-	-	-	-	-
O6	-95.52	47.92	-18.41	47.96	-35.16	-	-	-	-	-	-	-	-	-	-	-
O7	-96.57	49.30	-17.80	32.86	-17.48	49.87	-	-	-	-	-	-	-	-	-	-
C8	-22.31	12.20	-4.70	9.73	-5.48	15.90	31.78	-	-	-	-	-	-	-	-	-
H9	14.88	-8.33	3.41	-7.65	4.69	-13.27	-16.57	-12.27	-	-	-	-	-	-	-	-
H10	13.49	-8.48	3.44	-7.02	3.76	-9.85	-18.67	-13.49	6.30	-	-	-	-	-	-	-
H11	14.84	-8.26	3.02	-6.27	3.39	-10.42	-15.92	-11.72	5.53	6.05	-	-	-	-	-	-
H12	32.76	-14.65	4.08	-8.12	4.08	-15.28	-14.94	-4.61	3.01	2.83	3.73	-	-	-	-	-
H13	12.82	-16.95	14.14	-16.96	4.76	-9.72	-9.46	-2.70	1.95	2.04	1.79	2.36	-	-	-	-
H14	12.87	-13.57	11.45	-13.65	4.87	-9.32	-11.55	-2.97	2.12	2.27	1.81	2.12	4.98	-	-	-
H15	12.78	-9.36	4.76	-16.98	14.13	-17.62	-9.31	-3.23	2.87	2.28	2.08	2.37	2.73	2.52	-	-
H16	12.21	-8.55	4.65	-13.00	10.86	-13.41	-10.77	-3.43	3.00	2.43	1.97	2.02	2.39	2.96	4.74	-

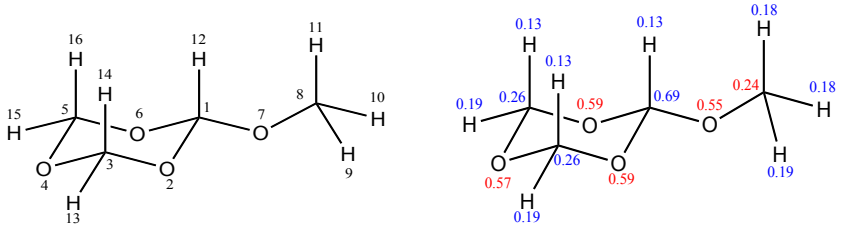


Table S39. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 18_{eq}.

	C1	O2	C3	O4	C5	O6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	-96.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	25.52	-35.69	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O4	-47.86	47.82	-34.53	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	25.52	-18.64	9.58	-34.53	-	-	-	-	-	-	-	-	-	-	-	-
O6	-96.09	49.87	-18.64	47.82	-35.69	-	-	-	-	-	-	-	-	-	-	-
O7	-93.92	47.55	-13.43	26.27	-13.43	47.55	-	-	-	-	-	-	-	-	-	-
C8	-23.12	16.54	-4.95	10.26	-4.95	16.54	30.38	-	-	-	-	-	-	-	-	-
H9	13.39	-9.81	3.16	-6.54	3.16	-9.81	-17.13	-13.56	-	-	-	-	-	-	-	-
H10	15.97	-14.40	4.17	-8.30	3.68	-11.18	-16.26	-13.25	6.45	-	-	-	-	-	-	-
H11	15.97	-11.18	3.68	-8.30	4.17	-14.40	-16.26	-13.25	6.45	6.31	-	-	-	-	-	-
H12	28.18	-12.76	4.40	-8.05	4.40	-12.76	-12.41	-3.21	2.10	2.26	2.26	-	-	-	-	-
H13	13.15	-17.89	14.56	-17.25	4.90	-9.90	-7.94	-3.14	2.06	2.77	2.32	2.30	-	-	-	-
H14	11.61	-12.45	10.15	-12.04	4.35	-8.24	-6.25	-2.18	1.45	1.76	1.61	2.44	4.48	-	-	-
H15	13.15	-9.90	4.90	-17.25	14.56	-17.89	-7.94	-3.14	2.06	2.32	2.77	2.30	2.83	2.26	-	-
H16	11.61	-8.24	4.35	-12.04	10.15	-12.45	-6.25	-2.18	1.45	1.61	1.76	2.44	2.26	2.42	4.48	-

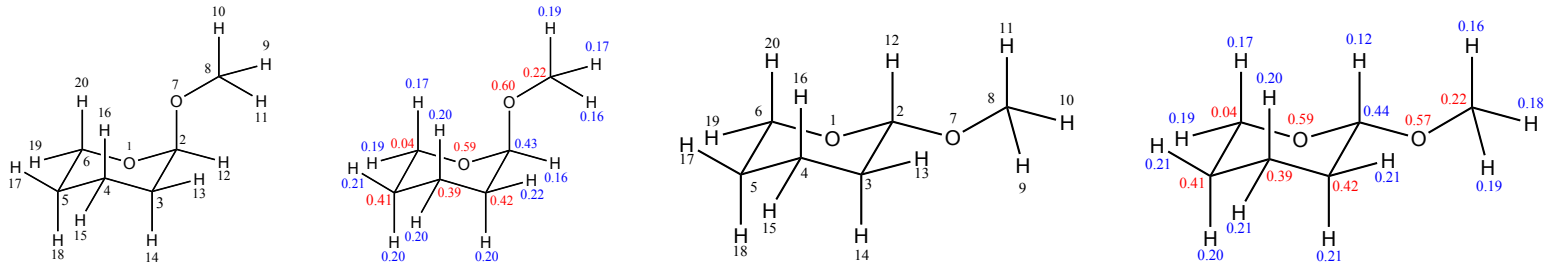


Table S40. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 1. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	O1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20
O1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	1.42	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-0.38	1.31	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.07	0.62	0.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.33	0.66	-0.08	0.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.76	-0.27	0.28	0.31	0.52	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	0.98	-0.35	1.49	6.46	4.47	1.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.21	0.40	-0.03	0.85	0.71	0.25	1.45	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-3.60	0.83	0.01	-0.84	-1.24	-0.37	0.89	0.90	-	-	-	-	-	-	-	-	-	-	-	-
H10	4.56	-1.74	0.29	-0.41	0.14	-0.04	-1.72	-0.38	-0.26	-	-	-	-	-	-	-	-	-	-	-
H11	-0.25	-0.03	-0.12	-0.21	-0.17	-0.10	-1.08	-0.29	-0.23	0.29	-	-	-	-	-	-	-	-	-	-
H12	-3.94	4.55	-2.32	-0.27	-0.52	-0.11	-4.05	-1.05	0.90	0.35	0.92	-	-	-	-	-	-	-	-	-
H13	-0.09	-0.22	-0.20	-0.20	-0.08	-0.11	-1.33	-0.09	-0.20	0.22	0.10	0.99	-	-	-	-	-	-	-	-
H14	0.84	-0.97	1.13	0.37	0.35	-0.09	3.41	0.61	-0.46	-0.63	-0.09	1.60	-0.24	-	-	-	-	-	-	-
H15	0.31	-0.44	0.33	0.46	0.33	-0.10	-1.54	-0.18	0.15	0.09	0.03	0.27	-0.06	-0.30	-	-	-	-	-	-
H16	-0.83	0.40	-0.87	-1.76	-0.82	-0.21	-6.25	-1.03	0.81	0.80	0.29	-0.13	0.46	0.15	0.34	-	-	-	-	-
H17	0.04	-0.22	0.01	-0.07	0.04	-0.19	-2.06	-0.39	0.59	0.10	0.09	0.17	0.04	-0.11	-0.10	0.36	-	-	-	-
H18	0.47	-0.41	0.22	0.26	0.74	-0.15	-0.43	0.02	0.24	-0.34	0.00	0.50	-0.03	-0.26	-0.26	0.18	-0.18	-	-	-
H19	0.31	-0.36	0.12	0.08	0.22	-0.29	-1.35	-0.30	1.01	-0.45	0.05	0.29	-0.01	-0.17	-0.11	0.17	-0.07	-0.20	-	-
H20	-1.04	0.26	-0.45	-0.58	-0.73	-0.44	-5.29	-1.37	1.95	0.59	0.30	-0.22	0.23	0.08	0.15	0.59	0.34	0.16	0.32	-

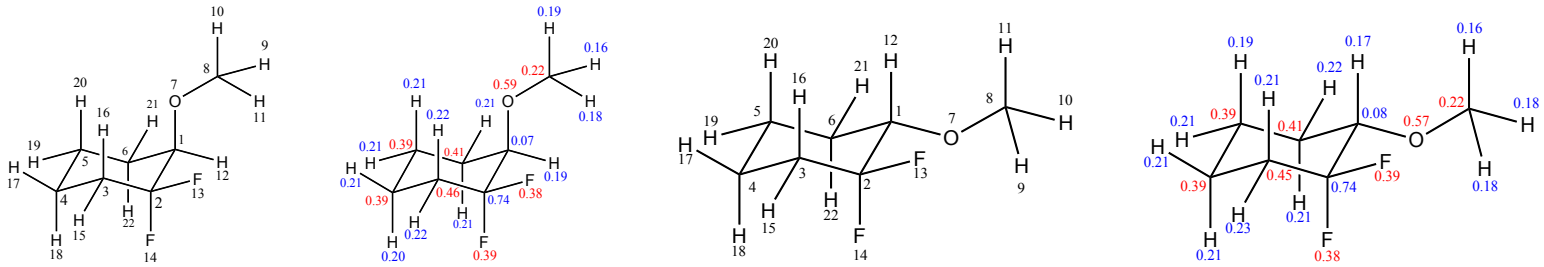


Table S41. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 2. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	H17	H18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-0.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.36	-1.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.31	-0.40	0.19	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.30	-0.77	0.36	0.12	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.61	-0.63	0.18	-0.09	0.32	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	0.69	-3.54	7.47	4.06	6.58	0.77	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	0.20	0.51	0.96	0.45	0.83	0.13	1.00	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-0.19	-3.95	0.90	0.47	-0.08	-0.08	0.98	1.15	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.11	0.31	-1.13	-0.62	-0.90	-0.11	-0.91	-0.24	-0.47	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	-0.06	2.81	-1.67	-0.78	-0.70	-0.31	-2.25	-1.32	0.06	0.79	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.01	1.96	0.97	0.43	0.85	-1.00	-2.01	-0.71	1.18	0.34	0.08	-	-	-	-	-	-	-	-	-	-	-
F13	0.40	-0.45	0.01	-0.16	0.01	-0.04	1.62	-0.50	3.70	-0.15	-2.63	-0.57	-	-	-	-	-	-	-	-	-	-
F14	0.27	-1.81	0.75	0.43	0.63	0.80	-4.91	-1.37	2.55	0.82	-0.66	-2.97	0.31	-	-	-	-	-	-	-	-	-
H15	-0.18	-0.22	0.17	0.29	0.08	0.13	-1.60	-0.13	-0.64	0.29	0.63	-0.15	0.33	0.07	-	-	-	-	-	-	-	-
H16	-0.06	1.87	-2.14	-0.68	-0.62	-0.48	-6.72	-1.18	-0.03	1.21	1.24	-0.91	-0.46	-0.66	0.34	-	-	-	-	-	-	-
H17	-0.12	0.17	-0.15	0.15	-0.10	0.00	-2.02	-0.28	-0.17	0.39	0.39	-0.21	0.07	-0.15	-0.13	0.34	-	-	-	-	-	-
H18	-0.18	-0.23	0.18	0.68	0.19	0.25	-0.34	0.07	-0.40	0.04	0.25	0.11	0.19	-0.05	-0.22	0.16	-0.20	-	-	-	-	-
H19	-0.16	-0.09	0.11	0.31	0.30	0.26	-1.51	-0.18	-0.03	0.25	0.20	-0.16	0.14	-0.09	-0.14	0.13	-0.13	-0.24	-	-	-	-
H20	0.00	1.35	-0.88	-0.84	-2.07	-1.02	-6.63	-1.03	0.40	1.05	0.62	-0.73	-0.39	-0.65	0.22	0.69	0.41	0.23	0.42	-	-	-
H21	-0.25	0.09	-0.01	0.09	-0.05	0.13	-0.29	-0.14	0.38	0.05	0.01	0.37	0.08	-0.22	-0.08	0.17	-0.03	-0.12	-0.16	0.44	-	-
H22	-0.28	-0.02	0.06	0.20	0.09	0.37	3.55	0.49	-0.38	-0.43	0.02	1.37	0.11	-0.38	-0.13	0.15	-0.07	-0.23	-0.22	0.29	-0.23	-

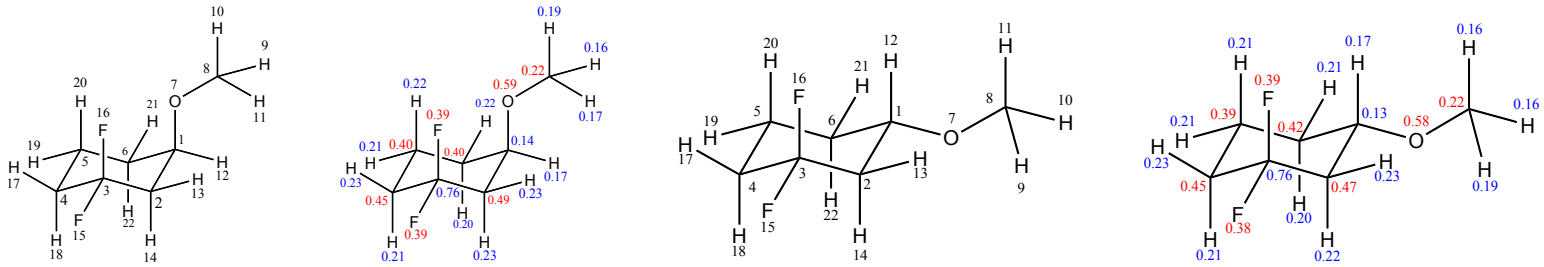


Table S42. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 3. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	F15	F16	H17	H18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-0.85	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.10	-3.95	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.11	1.37	-0.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.21	1.31	-0.34	0.44	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.31	0.10	1.70	-1.05	-1.19	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-0.58	0.52	-8.95	4.14	6.70	0.32	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.11	2.95	-3.86	0.97	0.49	-2.02	0.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.19	-1.35	0.97	0.07	0.25	1.33	3.32	2.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.04	-1.78	2.82	-0.77	-0.31	2.14	-3.59	-2.23	-0.11	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	-0.01	-3.57	4.90	-1.26	-0.45	1.21	-0.96	-0.75	-0.75	1.24	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.24	-0.84	-2.76	1.02	1.42	0.38	-0.49	0.00	0.76	0.11	-0.93	-	-	-	-	-	-	-	-	-	-	-
H13	-0.09	-0.84	-0.58	0.24	0.10	0.66	0.95	-1.91	1.00	1.16	2.63	-0.20	-	-	-	-	-	-	-	-	-	-
H14	0.14	-2.03	0.50	-0.12	-0.19	0.36	3.72	-0.16	-0.09	0.14	0.69	1.23	-0.05	-	-	-	-	-	-	-	-	-
F15	-0.14	1.73	-0.96	0.41	0.35	-0.33	1.81	1.40	-0.32	-1.18	-1.99	0.37	0.08	-0.53	-	-	-	-	-	-	-	-
F16	0.15	0.84	0.74	-0.44	-0.39	-1.21	8.11	3.19	-0.86	-2.52	-3.92	2.75	0.41	0.00	0.06	-	-	-	-	-	-	-
H17	0.04	-0.52	0.06	0.01	-0.14	0.40	-1.96	-0.52	-0.02	0.49	0.62	-0.46	-0.09	0.05	-0.12	0.12	-	-	-	-	-	-
H18	0.00	-0.33	-0.35	0.50	0.07	0.59	-0.25	-0.10	-0.22	0.08	0.34	-0.10	-0.18	-0.07	-0.13	0.26	-0.15	-	-	-	-	-
H19	0.00	-0.26	-0.27	0.24	0.16	0.83	-1.62	0.07	-0.31	-0.10	-0.01	-0.40	-0.14	-0.03	0.00	0.30	-0.10	-0.19	-	-	-	-
H20	0.31	-1.23	1.22	-0.94	-2.00	-0.31	-6.96	-0.96	0.18	0.86	0.58	-1.15	0.18	0.31	-0.50	-0.25	0.38	0.23	0.38	-	-	-
H21	0.32	-0.94	0.56	-0.39	-0.64	0.07	-2.15	1.32	-0.73	-1.78	-1.00	0.24	0.07	0.24	-0.31	-0.05	0.15	0.11	0.12	0.65	-	-
H22	-0.03	-0.28	-0.30	0.16	0.10	1.63	2.95	1.12	-0.82	-1.16	-0.45	0.88	-0.20	-0.08	-0.02	0.29	-0.07	-0.15	-0.21	0.22	0.17	-

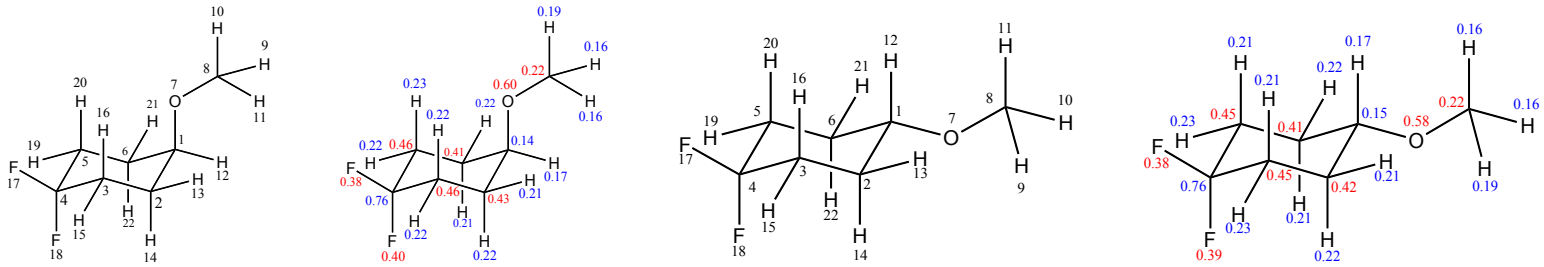


Table S43. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 4. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	F17	F18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	0.21	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.05	0.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.20	-0.44	-1.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.09	0.32	0.60	-0.84	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.28	0.07	0.21	0.04	0.21	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-0.08	1.14	7.68	-8.85	7.84	0.92	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	0.09	0.14	1.73	-1.58	1.10	-0.02	0.93	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.16	1.04	-0.11	0.16	-0.46	-0.28	-0.65	-0.06	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.05	-0.07	-1.32	1.39	-1.03	0.01	-0.59	-0.04	0.05	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	-0.26	-1.33	-2.15	1.58	-0.57	0.28	-0.35	-0.01	0.03	0.02	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.71	-1.31	0.71	-0.58	0.74	-1.18	-2.31	-0.50	1.35	0.36	-0.62	-	-	-	-	-	-	-	-	-	-	-
H13	-0.08	-0.20	-0.17	0.06	-0.08	-0.01	-0.49	-0.09	-1.00	0.05	1.18	0.54	-	-	-	-	-	-	-	-	-	-
H14	-0.04	-0.48	-0.44	0.45	-0.26	-0.15	2.74	0.68	-0.91	-0.50	0.14	1.50	0.18	-	-	-	-	-	-	-	-	-
H15	-0.10	0.14	-0.05	-0.32	0.05	0.14	-1.69	-0.43	-0.17	0.35	0.78	-0.07	-0.09	-0.01	-	-	-	-	-	-	-	-
H16	0.08	-0.63	-1.63	1.02	-0.55	-0.33	-6.46	-1.68	0.43	1.32	1.73	-0.81	0.18	0.26	0.20	-	-	-	-	-	-	-
F17	0.08	0.09	0.35	-0.13	0.21	-0.03	3.77	0.80	-0.14	-0.79	-0.74	0.29	0.00	-0.12	0.14	-0.36	-	-	-	-	-	-
F18	0.02	0.47	0.72	-0.91	0.55	0.21	1.11	0.18	0.17	-0.14	-0.45	-0.59	-0.15	-0.43	-0.01	-0.44	0.31	-	-	-	-	-
H19	-0.12	0.10	0.04	-0.44	0.32	0.30	-1.68	-0.22	0.09	0.24	0.10	-0.08	-0.05	0.00	-0.13	0.09	0.19	0.06	-	-	-	-
H20	0.18	-0.68	-0.96	1.78	-2.35	-0.93	-7.22	-1.19	0.56	1.14	0.59	-0.70	0.24	0.33	0.23	0.64	-0.67	-0.69	0.41	-	-	-
H21	-0.09	-0.05	-0.13	0.05	-0.18	0.04	-0.58	0.01	0.32	0.01	-0.34	0.54	0.01	0.05	-0.05	0.16	-0.01	-0.10	-0.12	0.49	-	-
H22	-0.19	0.18	0.08	-0.35	0.12	0.48	3.40	0.54	-0.20	-0.48	-0.25	1.35	-0.06	-0.02	-0.14	0.08	0.12	0.05	-0.21	0.26	-0.17	-

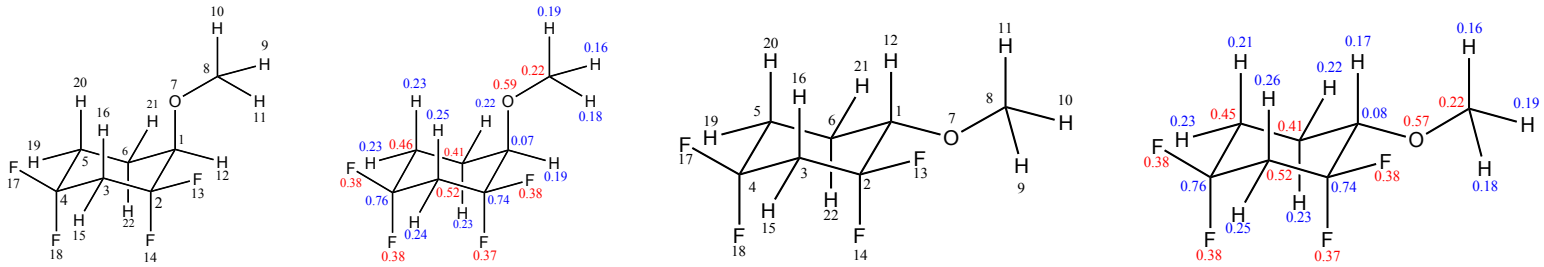


Table S44. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 5. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	F17	F18	H19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-1.17	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.49	-1.75	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.66	1.25	-0.81	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.42	-0.88	0.45	-0.81	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.73	-0.62	0.16	-0.05	0.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	0.75	-4.05	8.81	-9.32	8.27	1.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	0.25	0.81	0.98	-0.99	1.00	0.10	1.15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-0.21	-4.14	1.07	-0.77	-0.18	-0.11	0.70	1.13	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.14	0.24	-1.29	1.39	-1.12	-0.11	-1.08	-0.19	-0.44	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	-0.09	2.60	-1.83	1.57	-0.82	-0.32	-2.37	-1.24	0.08	0.77	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.09	2.68	0.81	-0.56	0.80	-1.40	-2.72	-0.90	1.36	0.45	0.27	-	-	-	-	-	-	-	-	-	-	-
F13	0.46	-0.19	-0.17	0.23	-0.04	-0.09	2.07	-0.61	3.65	-0.14	-2.40	-0.72	-	-	-	-	-	-	-	-	-	-
F14	0.32	-1.66	0.74	-1.07	0.73	0.80	-4.62	-1.52	2.68	0.88	-0.56	-3.18	0.21	-	-	-	-	-	-	-	-	-
H15	-0.22	-0.21	0.23	-0.38	0.07	0.13	-1.83	-0.10	-0.71	0.30	0.64	-0.02	0.34	0.08	-	-	-	-	-	-	-	-
H16	-0.11	1.59	-2.03	1.27	-0.63	-0.42	-7.21	-1.20	-0.07	1.29	1.30	-0.87	-0.26	-0.56	0.27	-	-	-	-	-	-	-
F17	0.23	-0.32	0.26	-0.17	0.24	0.01	4.04	0.57	0.22	-0.80	-0.72	0.30	-0.13	0.29	0.17	-0.50	-	-	-	-	-	-
F18	0.26	-0.77	0.57	-0.82	0.50	0.18	1.24	-0.01	0.60	-0.16	-0.55	-0.61	0.07	0.79	0.01	-0.50	0.28	-	-	-	-	-
H19	-0.21	-0.06	0.12	-0.43	0.28	0.27	-1.90	-0.21	-0.01	0.30	0.23	-0.09	0.16	-0.13	-0.15	0.11	0.19	0.05	-	-	-	-
H20	-0.04	1.40	-1.04	1.90	-2.51	-1.07	-7.73	-1.16	0.48	1.22	0.69	-0.77	-0.36	-0.66	0.25	0.73	-0.75	-0.70	0.48	-	-	-
H21	-0.32	-0.01	0.06	-0.17	0.02	0.31	-0.17	-0.10	0.42	0.02	0.01	0.58	0.14	-0.18	-0.11	0.13	0.06	0.01	-0.20	0.44	-	-
H22	-0.34	0.05	0.06	-0.25	0.06	0.31	3.47	0.53	-0.40	-0.45	0.05	1.64	0.10	-0.45	-0.13	0.14	0.09	0.04	-0.21	0.33	-0.27	-

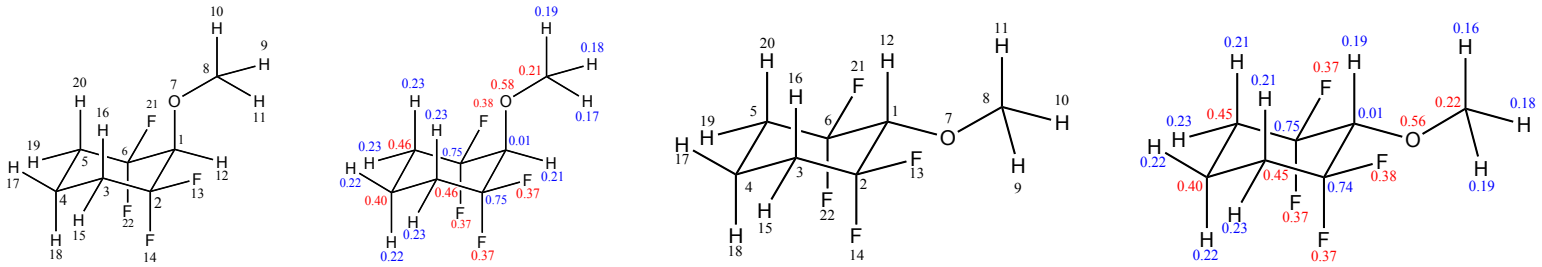


Table S45. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 6. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	H17	H18	H19	H20	F21	F22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-0.78	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.29	-1.75	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.22	-0.36	0.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.29	-0.93	0.47	0.29	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-0.81	0.97	-0.32	0.15	-1.06	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	0.63	-4.53	7.69	4.07	7.38	-2.21	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	0.15	1.13	0.48	0.39	1.18	-1.18	0.96	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-0.11	-3.17	0.49	-0.21	-1.42	3.40	-0.78	-0.03	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.11	-0.40	-0.77	-0.49	-1.09	0.37	-0.47	0.22	-0.03	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	-0.10	1.10	-0.53	-0.21	-0.22	-0.16	-1.18	-0.36	0.25	0.15	-	-	-	-	-	-	-	-	-	-	-	-
H12	-0.26	1.55	1.38	0.68	1.37	1.05	-1.73	-0.35	0.45	0.18	0.39	-	-	-	-	-	-	-	-	-	-	-
F13	0.29	0.73	-0.53	-0.46	-0.26	0.73	1.62	-1.42	3.97	0.58	-0.65	-0.02	-	-	-	-	-	-	-	-	-	-
F14	0.25	-2.04	0.70	0.42	0.73	-1.23	-4.42	-1.09	1.33	1.02	-0.32	-3.00	-0.13	-	-	-	-	-	-	-	-	-
H15	-0.11	-0.08	0.14	0.25	0.04	-0.22	-1.80	0.02	-0.44	0.13	0.17	-0.27	0.50	0.02	-	-	-	-	-	-	-	-
H16	-0.11	2.25	-2.44	-0.86	-0.92	1.14	-7.10	-0.83	0.07	1.03	0.50	-1.10	-0.38	-0.77	0.50	-	-	-	-	-	-	-
H17	-0.09	0.19	-0.14	0.15	-0.20	-0.01	-2.05	-0.25	0.13	0.32	0.12	-0.32	0.18	-0.16	-0.10	0.43	-	-	-	-	-	-
H18	-0.12	-0.26	0.21	0.70	0.15	-0.52	-0.37	0.06	-0.04	-0.05	0.03	0.07	0.35	-0.05	-0.23	0.24	-0.21	-	-	-	-	-
H19	-0.11	-0.06	0.10	0.28	0.08	-0.51	-1.61	-0.33	0.59	0.30	0.00	-0.29	0.26	-0.12	-0.13	0.22	-0.11	-0.24	-	-	-	-
H20	-0.11	1.28	-0.84	-0.81	-2.45	1.82	-6.78	-1.20	1.10	1.20	0.30	-1.13	-0.20	-0.61	0.21	0.78	0.42	0.23	0.45	-	-	-
F21	0.26	-0.57	0.23	0.08	0.52	-0.55	1.92	1.44	-3.95	-0.66	0.29	-0.26	-0.20	0.52	0.03	-0.49	-0.05	0.09	0.11	-0.80	-	-
F22	0.25	-1.34	0.54	0.27	0.70	-1.04	-4.98	-0.32	-0.78	0.69	0.02	-2.91	0.03	1.32	-0.08	-0.60	-0.12	0.05	0.06	-0.71	0.65	-

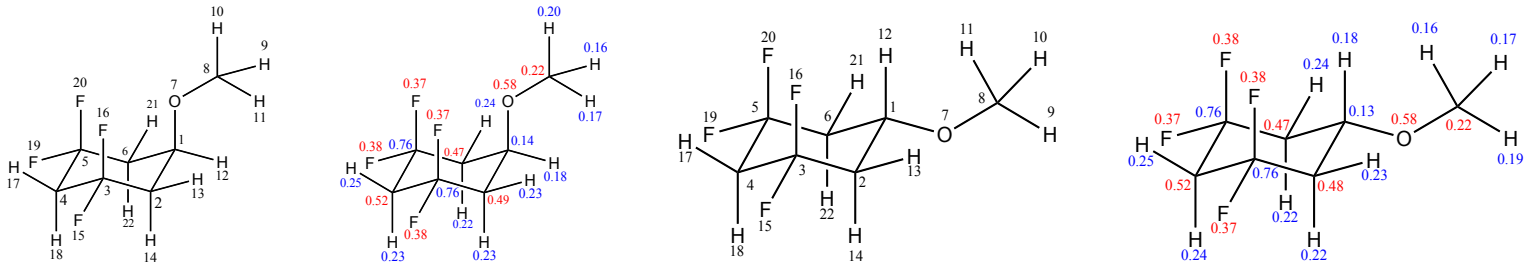


Table S46. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 7. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	F15	F16	H17	H18	F19	F20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-0.74	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.44	-0.90	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.30	0.50	-0.08	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.44	-0.47	-0.27	-0.21	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-0.64	0.39	0.01	0.10	-0.30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-0.82	-0.02	-8.76	4.24	-9.35	0.11	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.23	0.61	-2.67	1.09	-1.67	0.12	0.49	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.23	-0.39	0.42	0.17	-0.42	0.70	3.73	2.30	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.06	-0.12	1.64	-0.99	1.60	-0.39	-3.20	-2.21	-0.23	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.20	-0.68	3.41	-1.30	1.73	-0.39	-0.89	-0.78	-0.84	1.24	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.01	0.29	-3.84	1.80	-3.85	0.43	0.60	0.30	0.56	-1.16	-0.19	-	-	-	-	-	-	-	-	-	-	-
H13	0.24	-0.70	0.06	-0.10	0.09	-0.13	-0.35	-0.52	0.59	-0.03	0.46	-0.26	-	-	-	-	-	-	-	-	-	-
H14	0.26	-0.80	0.49	-0.28	0.24	-0.11	3.29	0.52	-0.38	-0.09	-0.52	1.04	0.28	-	-	-	-	-	-	-	-	-
F15	-0.23	0.67	-0.61	0.40	-0.32	0.22	1.76	0.78	-0.02	-0.64	-1.08	0.69	-0.19	-0.44	-	-	-	-	-	-	-	-
F16	-0.04	-0.18	0.79	-0.43	0.79	-0.30	7.65	2.49	-0.56	-1.51	-3.33	3.19	0.18	0.0	-0.01	-	-	-	-	-	-	-
H17	0.11	-0.16	0.03	-0.09	0.12	-0.06	-2.01	-0.56	-0.05	0.53	0.65	-0.79	0.04	0.09	-0.14	0.17	-	-	-	-	-	-
H18	0.10	-0.07	-0.24	0.37	-0.23	0.13	-0.27	-0.14	-0.24	0.26	0.25	-0.31	0.01	0.08	-0.13	0.21	-0.09	-	-	-	-	-
F19	-0.27	0.50	-0.47	0.60	-1.16	0.68	1.94	0.46	0.33	-0.65	-0.54	0.66	-0.16	-0.26	0.35	-0.07	-0.19	-0.25	-	-	-	-
F20	0.12	-0.62	1.51	-0.82	1.60	-0.83	7.31	1.23	0.13	-1.12	-1.15	3.33	0.28	0.19	-0.33	-1.28	0.27	0.35	-0.22	-	-	-
H21	0.30	-0.28	0.21	-0.18	0.48	-0.66	-0.91	-0.12	-0.43	0.32	0.23	-0.30	0.10	0.09	-0.15	0.02	0.08	-0.01	-0.30	0.14	-	-
H22	0.14	0.18	-0.37	0.19	0.00	0.07	3.74	0.46	-0.65	-0.03	-0.20	0.91	-0.05	-0.14	0.03	0.22	-0.04	-0.19	-0.43	0.31	0.05	-

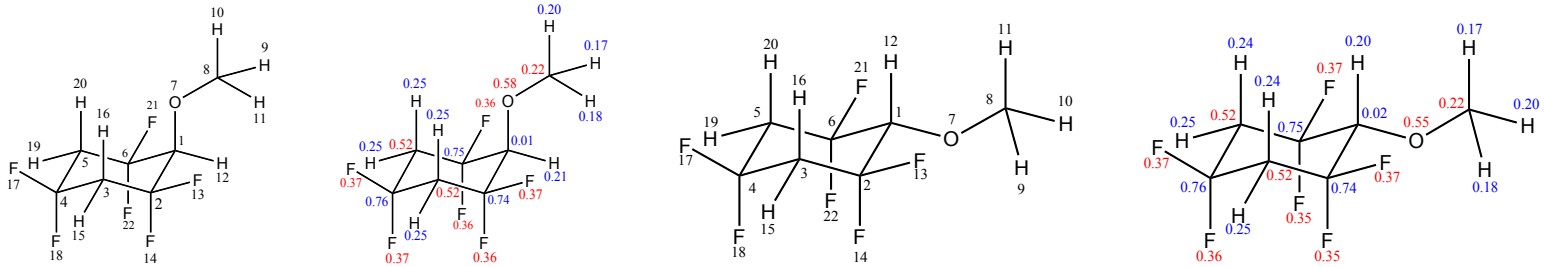


Table S47. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 8. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	H15	H16	F17	F18	H19	H20	F21	F22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-1.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.43	-1.40	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.55	0.67	-0.79	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.43	-0.71	0.53	-0.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-1.06	0.99	-0.58	0.70	-1.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	0.81	-4.24	9.04	-9.41	9.20	-3.52	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	0.20	0.21	0.94	-0.93	0.97	-0.12	1.16	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-0.15	-3.13	0.80	-0.25	-0.57	1.21	-0.32	0.51	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.13	-0.03	-1.13	1.16	-1.09	-0.03	-0.64	0.26	-0.31	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	-0.12	3.33	-1.72	1.27	-0.50	-0.20	-2.05	-0.88	0.27	0.44	-	-	-	-	-	-	-	-	-	-	-	-
H12	-0.33	2.04	1.36	-1.11	1.33	1.95	-2.41	-0.49	0.81	0.29	0.34	-	-	-	-	-	-	-	-	-	-	-
F13	0.35	0.05	-0.11	0.25	-0.04	0.16	2.19	-0.19	3.38	-0.03	-3.07	-0.39	-	-	-	-	-	-	-	-	-	-
F14	0.32	-1.54	0.61	-0.57	0.54	-1.00	-4.19	-0.84	1.31	0.89	-0.92	-3.06	0.17	-	-	-	-	-	-	-	-	-
H15	-0.16	-0.20	0.18	-0.33	0.05	-0.12	-2.00	-0.15	-0.52	0.25	0.66	-0.18	0.32	0.01	-	-	-	-	-	-	-	-
H16	-0.16	1.94	-2.49	1.66	-0.93	1.08	-7.60	-1.11	-0.08	1.27	1.18	-1.16	-0.55	-0.66	0.45	-	-	-	-	-	-	-
F17	0.19	-0.19	0.22	-0.13	0.27	-0.13	4.07	0.51	0.04	-0.71	-0.55	0.54	-0.11	0.18	0.16	-0.65	-	-	-	-	-	-
F18	0.21	-0.49	0.53	-0.83	0.60	-0.55	1.34	0.06	0.21	-0.08	-0.46	-0.46	0.00	0.39	-0.02	-0.61	0.26	-	-	-	-	-
H19	-0.16	-0.14	0.10	-0.37	0.14	-0.38	-1.99	-0.17	0.18	0.24	0.07	-0.18	0.16	-0.04	-0.14	0.21	0.17	0.01	-	-	-	-
H20	-0.16	1.24	-0.96	1.72	-2.69	1.91	-7.85	-1.07	0.61	1.21	0.45	-1.12	-0.34	-0.55	0.23	0.81	-0.64	-0.62	0.47	-	-	-
F21	0.35	0.06	-0.09	0.22	-0.09	0.31	1.77	0.13	-1.44	-0.04	0.84	-0.38	-0.22	0.22	0.14	-0.26	-0.13	0.06	0.29	-0.46	-	-
F22	0.31	-1.51	0.80	-1.09	0.80	-1.44	-4.39	-0.57	-0.14	0.78	0.01	-3.11	0.29	1.23	-0.18	-0.60	0.29	0.76	0.05	-0.71	0.28	-

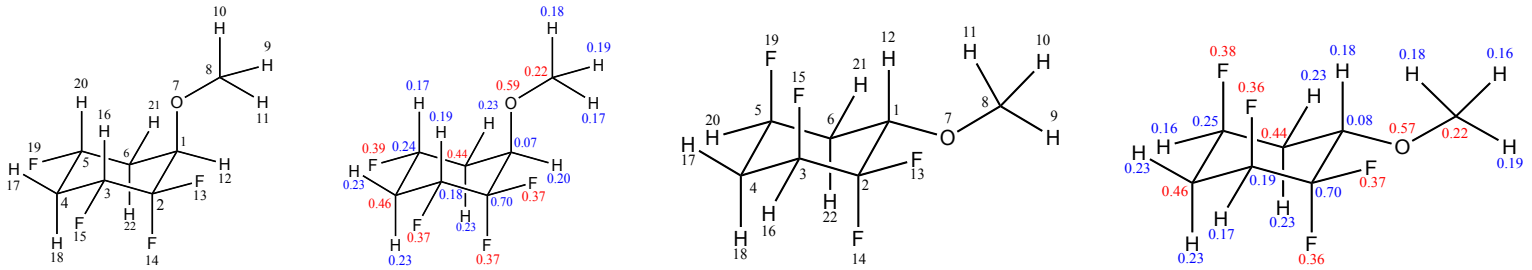


Table S48. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 9. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	F15	H16	H17	H18	F19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	1.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.22	-0.10	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.41	0.65	0.42	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.30	0.10	0.08	0.40	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-0.83	0.43	0.05	-0.37	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-1.50	-2.29	-3.00	4.87	-4.17	0.98	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.27	-0.05	-0.41	0.54	-0.48	0	1.14	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.18	0.15	0.44	-0.69	0.54	-0.04	-0.83	-0.19	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.3	3.7	0.79	-0.96	0.37	-0.07	-2.28	-1.38	0.76	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.12	-3.42	-0.39	0.54	0.04	-0.09	0.67	0.95	-0.44	0.16	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.42	-0.7	-1.03	1.88	-1.25	0.46	-0.12	0.11	-0.06	-0.45	0.37	-	-	-	-	-	-	-	-	-	-	-
F13	-0.47	-0.14	0.02	-0.21	-0.1	-0.03	1.24	0.11	-0.15	-3.76	3.45	0.17	-	-	-	-	-	-	-	-	-	-
F14	-0.46	0.59	0.29	-0.67	0.19	-0.42	-4.98	-0.89	0.83	-0.97	1.65	-1.86	-0.13	-	-	-	-	-	-	-	-	-
F15	0.33	0.94	0.33	-0.80	1.98	-2.68	0.31	-0.54	0.00	-0.32	1.58	4.39	-0.50	3.39	-	-	-	-	-	-	-	-
H16	0.5	0.3	0.05	0.11	1.12	-1.22	-6.21	-1.24	1.11	1.45	0.02	-0.08	-0.16	2.04	0.1	-	-	-	-	-	-	-
H17	0.13	-0.40	-0.21	1.43	-0.23	0.27	-2.10	-0.27	0.38	0.40	-0.22	-0.87	0.15	0.26	0.76	0.02	-	-	-	-	-	-
H18	0.19	-0.20	-0.25	1.58	-0.28	0.03	-0.72	-0.03	0.07	0.35	-0.33	-0.30	0.13	0.28	-1.85	-1.32	-0.58	-	-	-	-	-
F19	0.33	4.32	1.65	-0.91	0.37	-0.66	0.50	-0.61	0.07	0.68	0.74	4.36	-1.88	-0.38	-7.39	0.13	0.9	-1.92	-	-	-	-
H20	0.43	1.63	0.70	0.40	-0.10	0.16	-5.70	-0.94	0.90	0.65	0.41	-0.11	-0.74	0.17	0.21	1.55	-0.1	-1.33	0.36	-	-	-
H21	0.29	-0.21	-0.04	0.25	-0.09	0.39	-0.52	0.00	0.02	-0.29	0.37	-0.30	0.03	0.16	1.32	0.54	-0.16	-0.08	0.69	-0.01	-	-
H22	0.27	-0.30	-0.02	-0.04	-0.03	0.39	3.42	0.45	-0.46	-0.01	-0.25	0.97	0.08	0.33	0.31	0.12	-0.05	0.17	-2.14	-1.12	-0.21	-

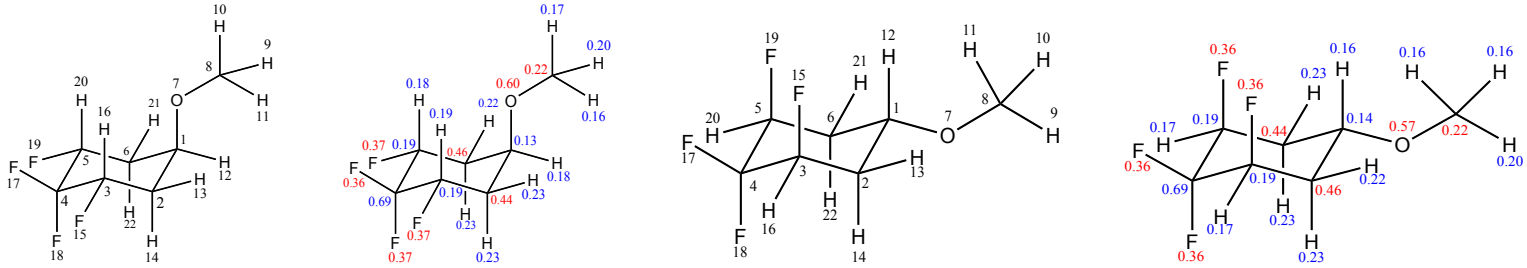


Table S49. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 10. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	F15	H16	F17	F18	F19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-0.22	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.14	1.07	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.44	1.95	-0.61	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.17	0.38	0.01	-0.39	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-1.15	-0.05	-0.31	-1.49	-0.59	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-1.43	0.85	-3.18	-7.46	-2.83	1.22	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.25	-2.13	-0.12	-1.34	-0.94	2.52	1.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.18	0.75	0.31	1.26	0.62	-0.99	-0.9	-0.39	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.17	1.2	-0.15	0.17	0.29	-1.47	-0.52	-0.16	0.12	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.14	2.97	-0.17	1.17	1.13	-3.25	-0.70	-0.29	0.18	0.09	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.38	0.54	-0.87	-2.21	-0.84	-0.46	-0.5	0.04	0.05	-0.04	-0.09	-	-	-	-	-	-	-	-	-	-	-
H13	0.42	0.4	0.03	0.27	0.1	-0.69	-2.09	1.39	-0.33	-0.79	-2.57	0.13	-	-	-	-	-	-	-	-	-	-
H14	0.23	1.27	-0.08	0.11	-0.02	-0.41	2.81	1.11	-0.67	-0.35	-1.37	1.05	0.23	-	-	-	-	-	-	-	-	-
F15	0.94	-1.4	0.49	0.84	1.55	-1.95	0.68	-0.98	0.20	1.27	1.08	3.64	0.20	-2.18	-	-	-	-	-	-	-	-
H16	0.75	0.25	0.03	0.15	0.88	-1.66	-6.63	-0.94	0.97	0.33	0.33	0.04	0.34	-1.01	-0.02	-	-	-	-	-	-	-
F17	-0.23	-0.40	0.02	-0.16	-0.07	0.79	3.61	0.79	-0.81	-0.15	-0.69	0.84	-0.23	-0.17	-0.34	-0.38	-	-	-	-	-	-
F18	-0.17	-1.15	0.49	1.48	0.39	0.50	0.50	0.07	-0.05	0.01	-0.09	0.21	-0.03	0.06	3.35	2.18	-0.07	-	-	-	-	-
F19	0.95	-3.15	1.62	0.93	0.35	0.52	0.13	0.43	-0.36	0.39	-1.25	3.65	1.03	0.27	-6.91	0.04	-0.34	3.3	-	-	-	-
H20	0.65	-0.77	0.72	-0.53	-0.28	-0.33	-5.71	-1.81	1.29	0.72	1.88	-0.06	0.58	0.03	0.23	1.72	-0.08	2.42	0.38	-	-	-
H21	0.01	0.82	-0.18	-0.69	-0.32	-0.05	1.05	-1.60	0.45	0.94	2.68	-0.30	-0.05	-0.21	1.42	0.46	0.16	0.38	0.77	-0.25	-	-
H22	0.34	0.24	0.07	0.69	0.13	-2.05	3.22	-0.17	-0.18	0.36	0.56	1.18	0.23	0.09	0.06	0.24	-0.35	-0.33	-2.36	-1.07	-0.12	-

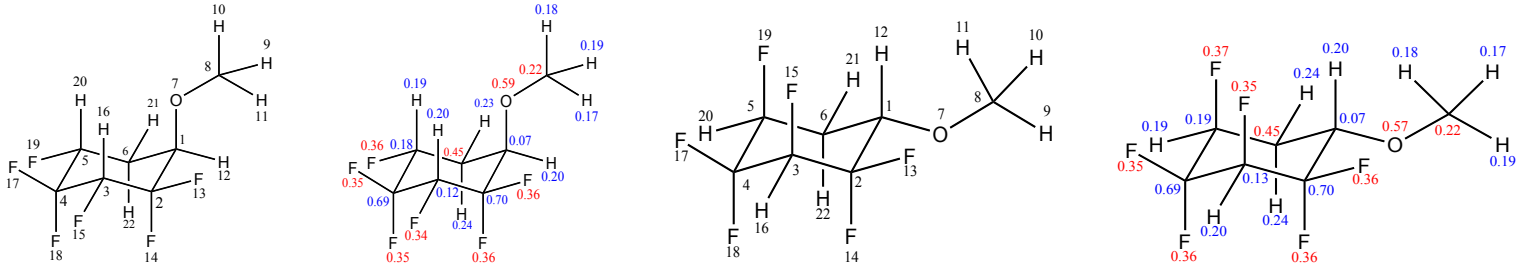


Table S50. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 11. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	F15	H16	F17	F18	F19	H20	H21	H22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	0.82	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.05	-0.54	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.39	-0.11	-0.68	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.13	0.01	-0.07	-0.31	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-0.50	0.14	0.20	0.23	0.26	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-1.08	-3.01	-1.89	-8.29	-3.3	1.24	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.16	0.12	-0.20	-0.95	-0.36	0.02	1.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.12	0.23	0.26	1.22	0.42	-0.05	-1.06	-0.22	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.22	3.44	0.45	1.46	0.26	-0.11	-2.38	-1.33	0.78	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.06	-3.47	-0.30	-0.62	0.06	-0.18	0.44	0.93	-0.40	0.17	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.35	0.15	-0.68	-2.36	-0.91	0.00	-0.86	-0.11	0.07	-0.34	0.67	-	-	-	-	-	-	-	-	-	-	-
F13	-0.29	-0.41	0.19	0.00	-0.03	0.02	1.86	0.02	-0.25	-3.49	3.44	-0.02	-	-	-	-	-	-	-	-	-	-
F14	-0.27	0.27	0.33	0.45	0.13	-0.22	-4.68	-0.98	0.82	-0.86	1.76	-2.15	-0.02	-	-	-	-	-	-	-	-	-
F15	0.43	1.06	0.57	1.11	1.50	-2.45	0.40	-0.54	0.01	-0.19	1.42	3.81	-0.92	3.04	-	-	-	-	-	-	-	-
H16	0.46	0.58	-0.17	0.30	0.89	-1.31	-6.82	-1.33	1.24	1.53	0.05	0.06	-0.48	2.1	0.1	-	-	-	-	-	-	-
F17	-0.19	-0.52	0.06	-0.75	-0.12	0.25	4.04	0.64	-0.81	-0.74	0.12	0.88	0.23	0.11	-0.67	-0.69	-	-	-	-	-	-
F18	-0.12	0.65	0.41	1.33	0.39	-0.42	0.8	-0.04	-0.06	-0.47	0.52	0.25	-0.21	-0.62	2.95	2.27	0.06	-	-	-	-	-
F19	0.49	4.30	1.22	1.07	0.51	-0.76	0.53	-0.60	0.07	0.69	0.65	4.17	-1.91	-0.45	14.98	-21.46	-0.58	3.09	-	-	-	-
H20	0.43	2.02	0.46	-0.28	-0.16	0.08	-6.83	-1.13	1.09	0.77	0.52	0.01	-0.91	0.04	0.23	1.91	-0.36	2.35	0.37	-	-	-
H21	0.16	-0.18	-0.10	-0.22	-0.14	0.47	-0.37	0.00	-0.01	-0.26	0.44	-0.06	0.04	0.13	1.23	0.57	-0.05	0.21	0.59	-0.02	-	-
H22	0.16	-0.12	-0.09	0.2	-0.08	0.30	3.30	0.45	-0.46	0.03	-0.25	1.22	0.03	0.18	0.24	0.11	-0.21	0.05	-2.02	-1.24	-0.23	-

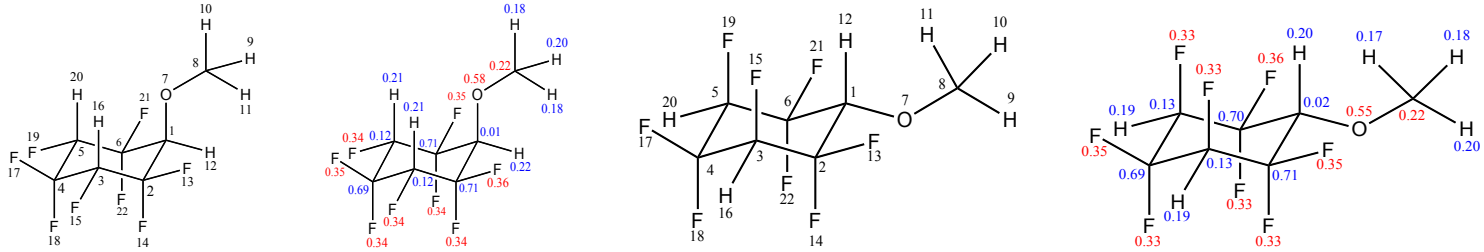


Table S51. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 12. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	F13	F14	F15	H16	F17	F18	F19	H20	F21	F22
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	1.01	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.1	-0.69	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.52	-0.44	-0.66	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.10	-0.32	-0.10	-0.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	1.03	-0.06	-0.23	0.3	-0.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-0.94	-2.60	-1.95	-8.53	-2.04	-4.23	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	-0.2	-0.88	-0.25	-0.89	-0.11	0.75	1.48	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.13	0.35	0.27	1.13	0.2	-0.24	-0.93	-0.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H10	0.15	3.19	0.34	0.57	-0.15	-2.45	-1.30	-0.35	0.19	-	-	-	-	-	-	-	-	-	-	-	-	-
H11	0.15	-0.66	-0.04	0.33	0.11	1.26	-1.27	-0.35	0.18	0.32	-	-	-	-	-	-	-	-	-	-	-	-
H12	0.45	-0.63	-0.8	-2.71	-0.78	-0.17	-0.77	0.10	-0.05	0.06	0.07	-	-	-	-	-	-	-	-	-	-	-
F13	-0.33	-0.78	0.09	-0.39	0.02	-0.59	2.31	1.20	-0.65	-3.64	0.65	0.21	-	-	-	-	-	-	-	-	-	-
F14	-0.32	0.69	0.32	0.37	0.17	0.01	-4.49	-0.42	0.69	-0.68	0.27	-2.04	0.27	-	-	-	-	-	-	-	-	-
F15	-0.17	1.63	0.66	1.33	1.20	4.10	0.40	-0.47	0.04	-0.05	1.04	4.37	-0.98	2.78	-	-	-	-	-	-	-	-
H16	0.18	0.08	-0.29	-0.01	0.49	2.17	-6.96	-1.35	1.26	1.27	0.50	-0.06	-0.59	2.21	0.38	-	-	-	-	-	-	-
F17	-0.19	-0.46	0.04	-1.07	0.04	-0.70	4.17	0.61	-0.79	-0.39	-0.25	0.99	0.40	0.12	-0.78	-0.62	-	-	-	-	-	-
F18	-0.20	0.92	0.39	1.21	0.39	0.59	0.81	-0.04	0.00	-0.03	-0.02	0.36	-0.07	-0.63	2.71	2.33	0.13	-	-	-	-	-
F19	-0.17	4.35	1.21	1.31	0.67	1.27	0.54	-0.86	0.23	1.34	0.58	4.33	-1.73	-0.45	-6.52	0.31	-0.77	2.69	-	-	-	-
H20	0.18	2.13	0.51	0.11	-0.24	0.51	-7.27	-1.08	1.13	0.34	0.81	-0.01	-1.07	-0.02	0.27	2.06	-0.67	2.29	0.31	-	-	-
F21	-0.32	0.41	0.15	0.33	0.29	0.21	1.90	-0.85	0.33	3.00	-1.04	0.41	0.07	-0.16	-1.99	-0.84	0.11	-0.35	-1.42	-0.29	-	-
F22	-0.32	0.07	0.14	0.12	0.29	-0.18	-4.16	-0.91	0.92	0.97	-0.26	-2.12	0.22	-0.01	-0.35	-0.01	0.19	-0.46	2.77	2.12	-0.26	-

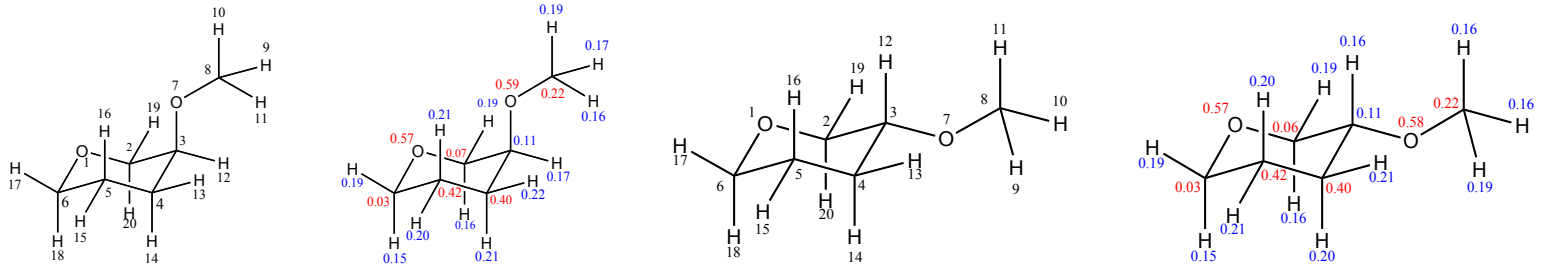


Table S52. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 13. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	O1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20
O1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	0.93	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.17	-0.13	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.20	0.34	0.22	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.21	0.36	0.05	0.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-0.11	0.02	0.02	-0.05	-0.06	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	7.93	0.54	0.10	0.45	6.49	0.26	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	2.39	0.24	0.03	0.04	1.14	0.06	0.76	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	-3.61	-0.41	0.04	0.37	-0.78	-0.08	2.36	1.37	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.83	0.09	-0.05	-0.62	-1.23	-0.04	-3.47	-2.13	0.25	-	-	-	-	-	-	-	-	-	-	-
H11	-0.50	-0.16	-0.08	0.29	-0.04	0.00	0.27	0.19	-0.82	0.72	-	-	-	-	-	-	-	-	-	-
H12	1.83	-0.24	0.14	-0.31	1.23	0.07	-0.89	-0.06	0.01	0.13	-0.10	-	-	-	-	-	-	-	-	-
H13	-0.14	-0.16	-0.01	-0.24	-0.33	0.01	-1.06	-0.09	-0.39	0.64	-0.17	0.13	-	-	-	-	-	-	-	-
H14	0.29	-0.12	-0.15	0.64	0.18	0.04	3.56	0.49	-0.58	-0.12	-0.21	0.97	-0.09	-	-	-	-	-	-	-
H15	0.23	-0.10	-0.08	0.32	0.31	0.04	-1.30	-0.24	0.08	0.41	-0.07	-0.28	-0.04	-0.22	-	-	-	-	-	-
H16	-0.99	-0.24	0.15	-0.87	-2.08	-0.05	-6.39	-1.21	0.85	1.20	0.21	-0.91	0.54	0.22	0.38	-	-	-	-	-
H17	-0.02	-0.13	-0.03	0.03	-0.10	0.05	-1.64	-0.46	0.51	0.39	0.05	-0.31	0.05	-0.07	-0.08	0.35	-	-	-	-
H18	0.41	-0.09	-0.08	0.27	0.25	0.09	0.01	-0.03	0.10	0.01	-0.04	-0.01	-0.05	-0.21	-0.21	0.12	-0.17	-	-	-
H19	-0.30	-0.44	0.00	-0.09	-0.17	0.01	-0.49	-0.46	1.66	-1.14	0.45	0.18	0.10	-0.03	-0.01	0.28	0.05	-0.04	-	-
H20	-0.29	-0.36	0.00	-0.10	-0.18	0.00	2.28	0.39	-0.02	-0.71	0.04	0.96	0.09	-0.04	-0.01	0.25	0.04	-0.06	0.21	-

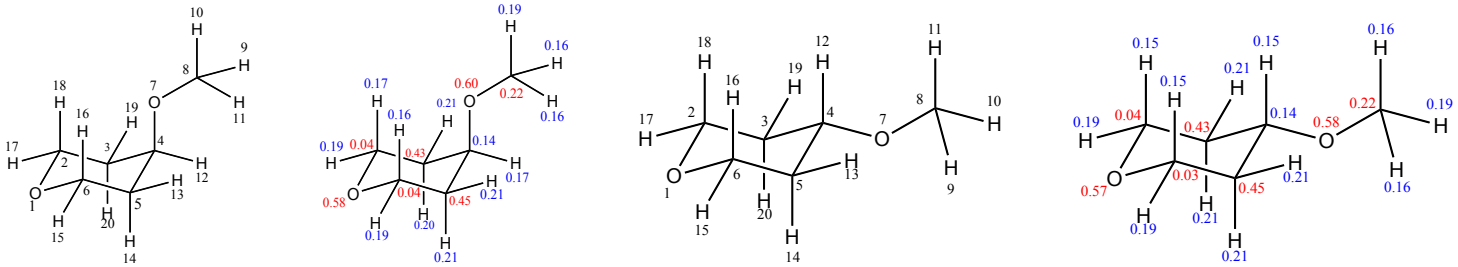


Table S53. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 14. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	O1	C2	C3	C4	C5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20
O1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	0.41	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.27	0.26	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.06	-0.05	0.06	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	0.42	0.15	-0.08	0.06	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	0.75	0.04	0.27	-0.09	0.53	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	6.03	0.75	1.02	-0.40	1.00	0.86	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8	0.99	0.12	-0.04	0.04	-0.08	0.20	0.70	-	-	-	-	-	-	-	-	-	-	-	-	-
H9	0.00	-0.06	-0.27	0.17	1.32	-0.05	-0.52	0.05	-	-	-	-	-	-	-	-	-	-	-	-
H10	-0.90	-0.11	-0.02	-0.01	0.02	-0.15	-0.51	0.05	0.01	-	-	-	-	-	-	-	-	-	-	-
H11	-1.08	-0.07	0.27	-0.19	-1.27	-0.21	-0.33	0.01	0.02	0.02	-	-	-	-	-	-	-	-	-	-
H12	0.48	0.04	-0.88	0.62	-0.92	-0.01	-1.80	-0.38	1.25	0.28	-0.66	-	-	-	-	-	-	-	-	-
H13	-0.08	-0.05	0.02	-0.01	0.03	-0.16	-0.80	-0.12	-1.00	0.07	1.22	0.27	-	-	-	-	-	-	-	-
H14	-0.33	-0.07	-0.05	0.01	-0.09	-0.18	2.85	0.77	-1.00	-0.54	0.09	1.31	0.08	-	-	-	-	-	-	-
H15	0.25	-0.04	0.18	-0.06	0.30	-0.26	-1.24	-0.26	-0.21	0.23	0.55	-0.15	-0.14	-0.08	-	-	-	-	-	-
H16	-0.99	-0.10	-0.42	0.15	-0.66	-0.36	-4.74	-1.13	0.29	0.91	1.13	-0.61	0.21	0.23	0.21	-	-	-	-	-
H17	0.33	-0.10	0.34	-0.08	0.20	-0.08	-1.26	-0.14	0.03	0.18	0.06	-0.16	-0.07	-0.06	-0.15	0.09	-	-	-	-
H18	-1.45	-0.30	-0.99	0.23	-0.68	-0.17	-5.35	-0.89	0.41	0.84	0.47	-0.53	0.23	0.28	0.20	0.55	0.35	-	-	-
H19	-0.18	-0.10	-0.15	0.02	-0.04	-0.11	-1.11	-0.07	0.34	0.10	-0.27	0.31	0.02	0.04	-0.04	0.19	-0.12	0.47	-	-
H20	0.21	-0.07	0.62	-0.13	0.34	-0.09	3.46	0.57	-0.23	-0.48	-0.26	1.17	-0.09	-0.13	-0.16	0.10	-0.23	0.26	-0.16	-

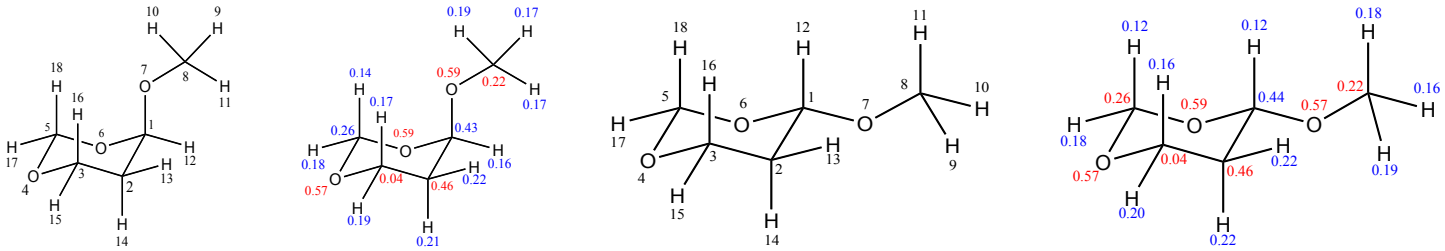


Table S54. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 15. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	C3	O4	C5	O6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	1.25	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	0.00	0.10	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O4	0.58	0.19	0.15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.67	0.24	-0.02	0.24	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O6	0.96	-0.29	0.07	0.11	0.64	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-0.76	1.84	0.73	6.10	-3.96	1.44	-	-	-	-	-	-	-	-	-	-	-	-
C8	0.39	-0.02	0.10	0.92	-0.72	-0.23	1.54	-	-	-	-	-	-	-	-	-	-	-
H9	0.80	0.03	-0.10	-1.64	1.64	-3.53	0.92	1.01	-	-	-	-	-	-	-	-	-	-
H10	-1.69	0.29	-0.05	0.23	-0.38	4.49	-1.88	-0.43	-0.28	-	-	-	-	-	-	-	-	-
H11	-0.01	-0.13	-0.03	-0.25	0.09	-0.22	-1.13	-0.26	-0.28	0.32	-	-	-	-	-	-	-	-
H12	4.47	-2.41	-0.04	-0.80	0.06	-3.86	-4.02	-1.04	0.89	0.33	0.91	-	-	-	-	-	-	-
H13	-0.10	-0.37	-0.06	-0.25	0.01	-0.18	-1.92	-0.17	-0.17	0.28	0.13	0.91	-	-	-	-	-	-
H14	-0.98	1.25	0.01	0.39	-0.32	0.86	3.52	0.66	-0.51	-0.66	-0.11	1.68	-0.21	-	-	-	-	-
H15	-0.40	0.34	-0.01	0.38	-0.18	0.28	-1.39	-0.14	0.14	0.07	0.03	0.24	-0.05	-0.30	-	-	-	-
H16	0.45	-0.89	-0.23	-1.23	0.41	-0.86	-5.21	-0.88	0.70	0.68	0.27	-0.11	0.45	0.17	0.32	-	-	-
H17	-0.35	0.17	-0.01	0.29	-0.48	0.35	-1.22	-0.22	0.84	-0.43	0.02	0.26	-0.01	-0.20	-0.13	0.17	-	-
H18	0.38	-0.54	-0.08	-1.18	0.89	-1.15	-4.47	-1.11	1.49	0.50	0.27	-0.17	0.26	0.12	0.17	0.56	0.31	-

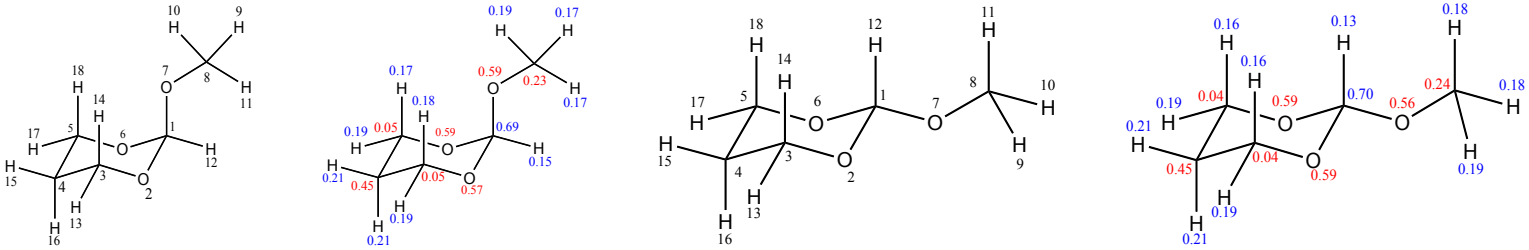


Table S55. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 16. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	O2	C3	C4	C5	O6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	3.24	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-0.40	0.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	0.43	-1.45	0.45	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.54	0.31	0.06	0.61	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O6	0.88	-2.03	0.32	-0.12	0.83	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	-2.60	1.61	1.09	5.47	1.15	2.16	-	-	-	-	-	-	-	-	-	-	-	-
C8	0.98	-4.43	0.05	-0.27	0.25	-0.62	1.23	-	-	-	-	-	-	-	-	-	-	-
H9	1.44	1.48	-0.11	-0.99	-0.40	-3.50	0.58	1.35	-	-	-	-	-	-	-	-	-	-
H10	-2.50	5.86	0.03	0.81	-0.13	1.29	-2.37	-0.16	-0.16	-	-	-	-	-	-	-	-	-
H11	-1.03	2.83	0.03	1.40	0.01	3.73	0.26	1.49	-0.87	-0.22	-	-	-	-	-	-	-	-
H12	5.11	-2.17	-0.04	-0.08	-0.07	-2.76	-2.77	-1.38	0.90	0.59	1.47	-	-	-	-	-	-	-
H13	-0.36	0.97	-0.23	0.25	-0.10	0.18	-1.67	0.44	-0.10	-0.72	-0.48	0.11	-	-	-	-	-	-
H14	1.23	-1.10	-0.50	-1.22	-0.21	-1.04	-6.29	-0.89	0.74	0.57	0.25	-0.35	0.55	-	-	-	-	-
H15	-0.20	0.48	-0.15	0.13	-0.20	0.03	-2.36	-0.13	0.50	-0.05	-0.39	-0.03	-0.10	0.51	-	-	-	-
H16	-0.18	0.68	-0.14	0.38	-0.19	0.11	-0.85	0.73	0.01	-0.93	-1.07	0.38	-0.12	0.37	-0.09	-	-	-
H17	-0.38	0.52	-0.08	0.22	-0.32	0.26	-1.53	-0.21	0.99	0.05	-0.61	0.12	-0.09	0.25	-0.08	-0.11	-	-
H18	0.48	-0.19	-0.14	-0.65	-0.45	-0.88	-5.38	-1.59	2.06	1.05	0.30	-0.47	0.11	0.56	0.27	0.19	0.26	-

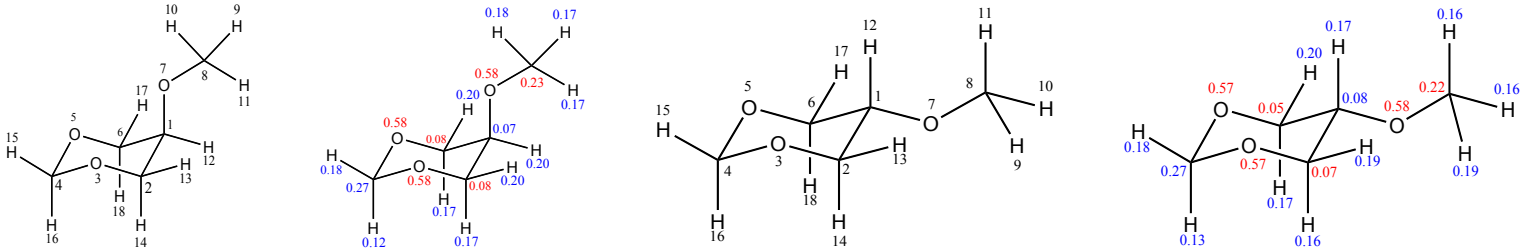


Table S56. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 17. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	C2	O3	C4	O5	C6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2	-0.07	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O3	0.38	1.29	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4	-0.17	-0.34	-0.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O5	0.38	0.67	1.47	-0.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6	-0.36	0.33	1.85	-1.01	3.65	-	-	-	-	-	-	-	-	-	-	-	-	-
O7	0.66	0.63	5.11	-1.11	4.73	1.87	-	-	-	-	-	-	-	-	-	-	-	-
C8	0.04	0.34	4.87	-1.85	5.73	0.96	1.73	-	-	-	-	-	-	-	-	-	-	-
H9	0.04	-0.55	-6.47	1.78	-3.86	-0.56	2.15	0.44	-	-	-	-	-	-	-	-	-	-
H10	-0.28	-0.09	-1.64	0.69	-2.16	-0.47	-2.16	-2.05	0.06	-	-	-	-	-	-	-	-	-
H11	0.02	0.01	-2.95	1.80	-7.24	-0.98	-1.16	-1.61	-0.10	0.98	-	-	-	-	-	-	-	-
H12	0.36	-0.57	0.61	0.07	0.59	-1.02	-3.22	0.18	0.04	-1.00	0.06	-	-	-	-	-	-	-
H13	0.04	-0.82	-1.44	0.38	-0.88	-0.59	-2.15	-0.32	1.38	-0.06	-1.25	0.79	-	-	-	-	-	-
H14	-0.06	-0.57	-0.79	0.16	-0.27	-0.52	2.33	0.36	0.03	-0.19	-0.70	1.71	0.61	-	-	-	-	-
H15	-0.08	-0.16	-0.26	0.07	-0.29	-0.49	-0.81	-1.18	1.15	0.52	1.18	-0.05	0.20	0.09	-	-	-	-
H16	-0.06	-0.12	0.01	-0.13	0.00	-0.41	0.31	-0.38	0.35	0.14	0.38	0.33	0.11	0.03	-0.04	-	-	-
H17	-0.05	-0.23	-0.55	0.22	-0.99	-1.75	-0.99	-1.46	0.32	0.55	2.22	0.61	0.35	0.11	0.12	0.04	-	-
H18	-0.07	-0.16	-0.21	0.13	-0.74	-1.42	2.76	-0.17	-0.13	0.03	0.53	1.69	0.20	-0.07	0.08	0.02	0.39	-

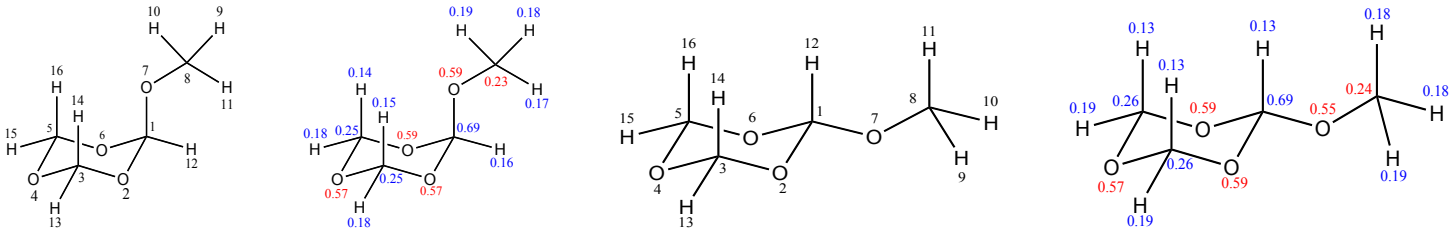


Table S57. Atom-atom electrostatic interactions (kcal mol^{-1}) obtained at M06-2X/aug-cc-pVTZ level using NPA charges for 18. Negative values are axial stabilizing and positive values are equatorial stabilizing.

	C1	O2	C3	O4	C5	O6	O7	C8	H9	H10	H11	H12	H13	H14	H15	H16
C1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	3.00	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3	-0.57	1.84	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O4	0.26	-1.68	0.33	-	-	-	-	-	-	-	-	-	-	-	-	-
C5	-0.69	0.93	-0.21	0.34	-	-	-	-	-	-	-	-	-	-	-	-
O6	0.57	-1.95	0.23	0.14	0.53	-	-	-	-	-	-	-	-	-	-	-
O7	-2.65	1.75	-4.37	6.59	-4.05	2.32	-	-	-	-	-	-	-	-	-	-
C8	0.81	-4.34	0.25	-0.53	-0.53	-0.64	1.40	-	-	-	-	-	-	-	-	-
H9	1.49	1.48	0.25	-1.11	1.53	-3.46	0.56	1.29	-	-	-	-	-	-	-	-
H10	-2.48	5.92	-0.73	1.28	0.08	1.33	-2.41	-0.24	-0.15	-	-	-	-	-	-	-
H11	-1.13	2.92	-0.66	2.03	-0.78	3.98	0.34	1.53	-0.92	-0.26	-	-	-	-	-	-
H12	4.58	-1.89	-0.32	-0.07	-0.32	-2.52	-2.53	-1.40	0.91	0.57	1.47	-	-	-	-	-
H13	-0.33	0.94	-0.42	0.29	-0.14	0.18	-1.52	0.44	-0.11	-0.73	-0.53	0.06	-	-	-	-
H14	1.26	-1.12	1.30	-1.61	0.52	-1.08	-5.30	-0.79	0.67	0.51	0.20	-0.32	0.50	-	-	-
H15	-0.37	0.54	-0.14	0.27	-0.43	0.27	-1.37	-0.09	0.81	-0.04	-0.69	0.07	-0.10	0.26	-	-
H16	0.60	-0.31	0.30	-0.96	0.71	-0.96	-4.52	-1.25	1.55	0.82	0.21	-0.42	0.13	0.54	0.26	-

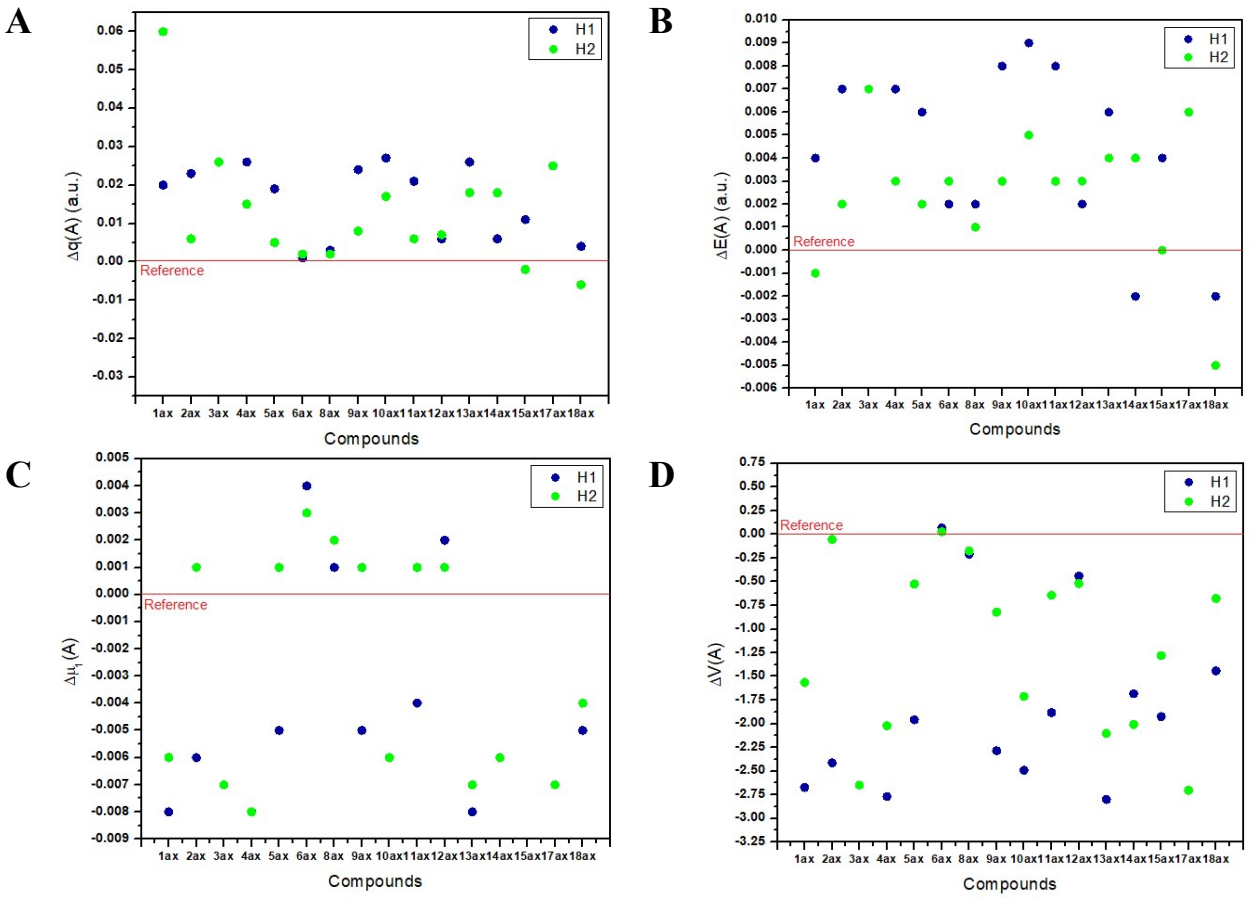
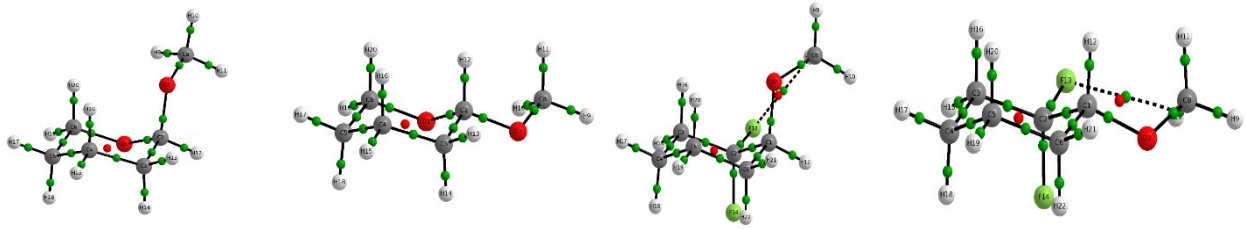
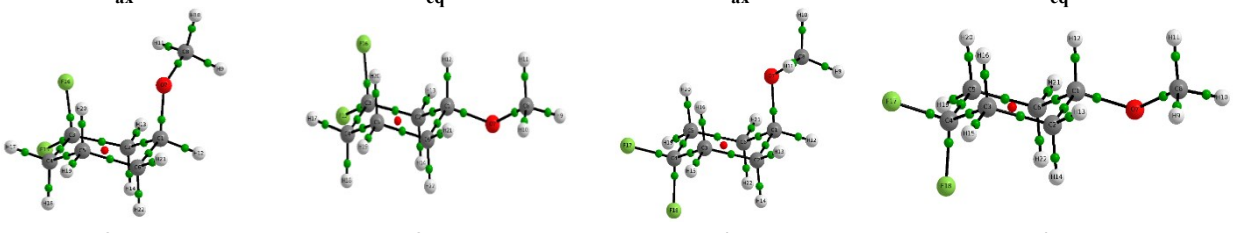


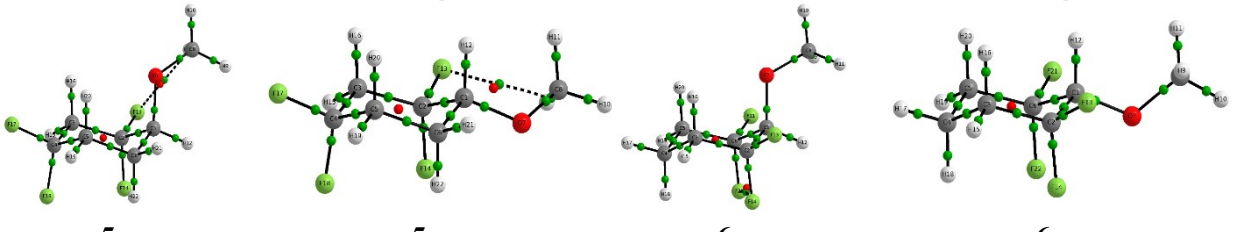
Figure S1. Popelier criterea parameters from QTAIM calculations run at the M06-2X/aug-cc-pVTZ wavefunction density for the molecules with axial hydrogens in positions 3 and/or 5 for compounds 1-18. The Popelier criteria is met for hydrogens with A) positive Δ atomic charge [Δq(A)]; B) positive Δ atomic energy [ΔE(A)]; C) positive Δ first intra-atomic dipole moment [Δμ1(A)] and D) negative Δ atomic volume [ΔV(A)].



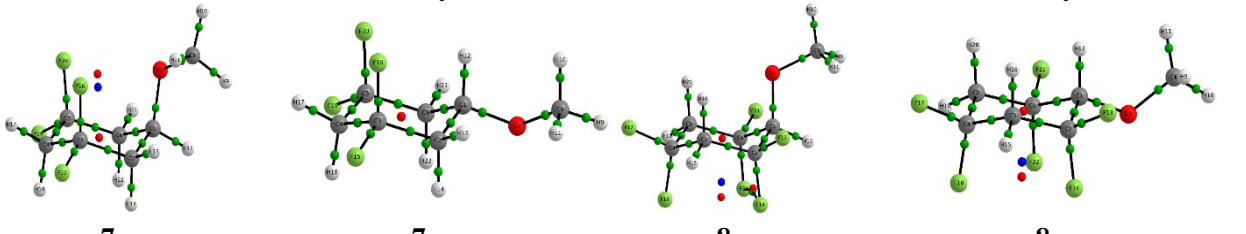
1_{ax} **1_{eq}** **2_{ax}** **2_{eq}**



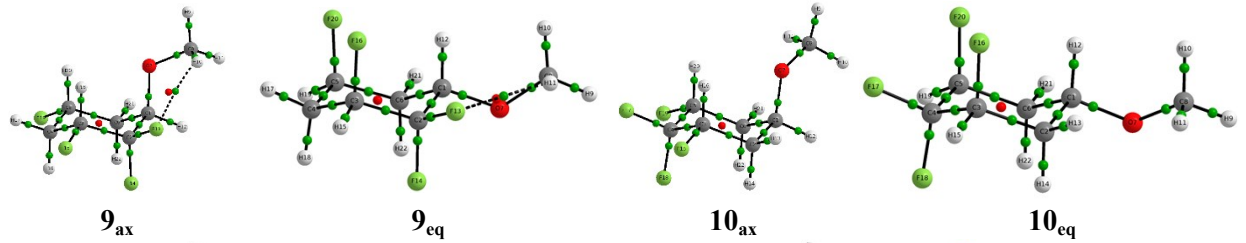
3_{ax} **3_{eq}** **4_{ax}** **4_{eq}**



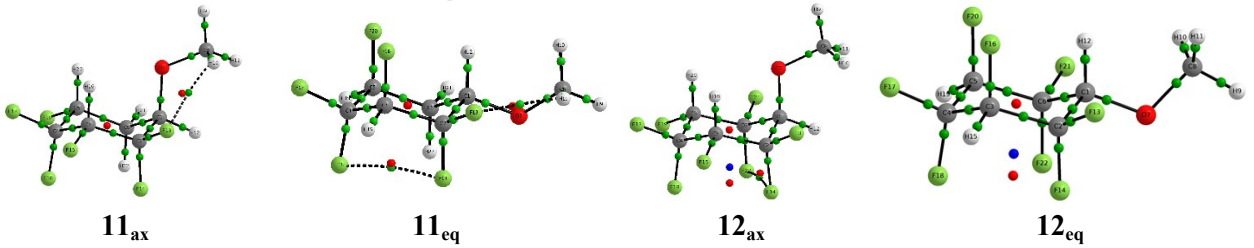
5_{ax} **5_{eq}** **6_{ax}** **6_{eq}**



7_{ax} **7_{eq}** **8_{ax}** **8_{eq}**



9_{ax} **9_{eq}** **10_{ax}** **10_{eq}**



11_{ax} **11_{eq}** **12_{ax}** **12_{eq}**

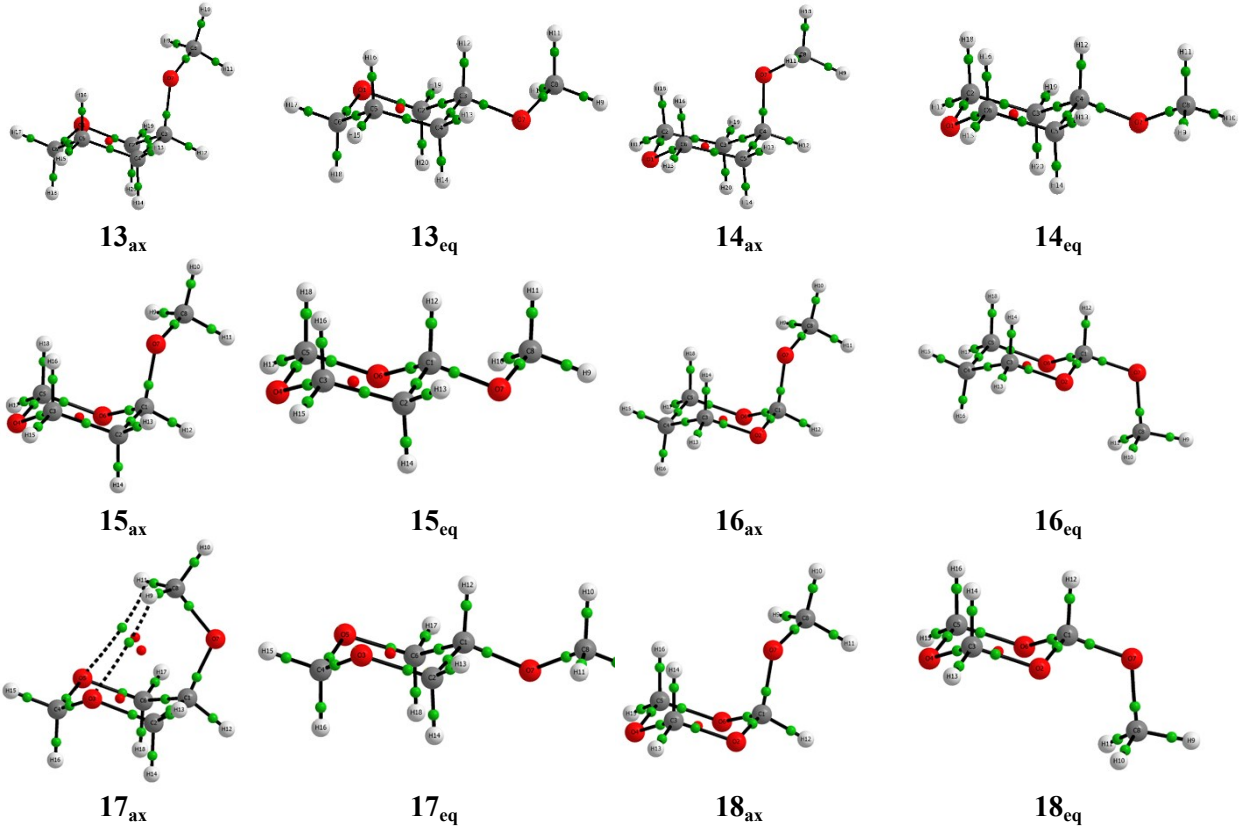
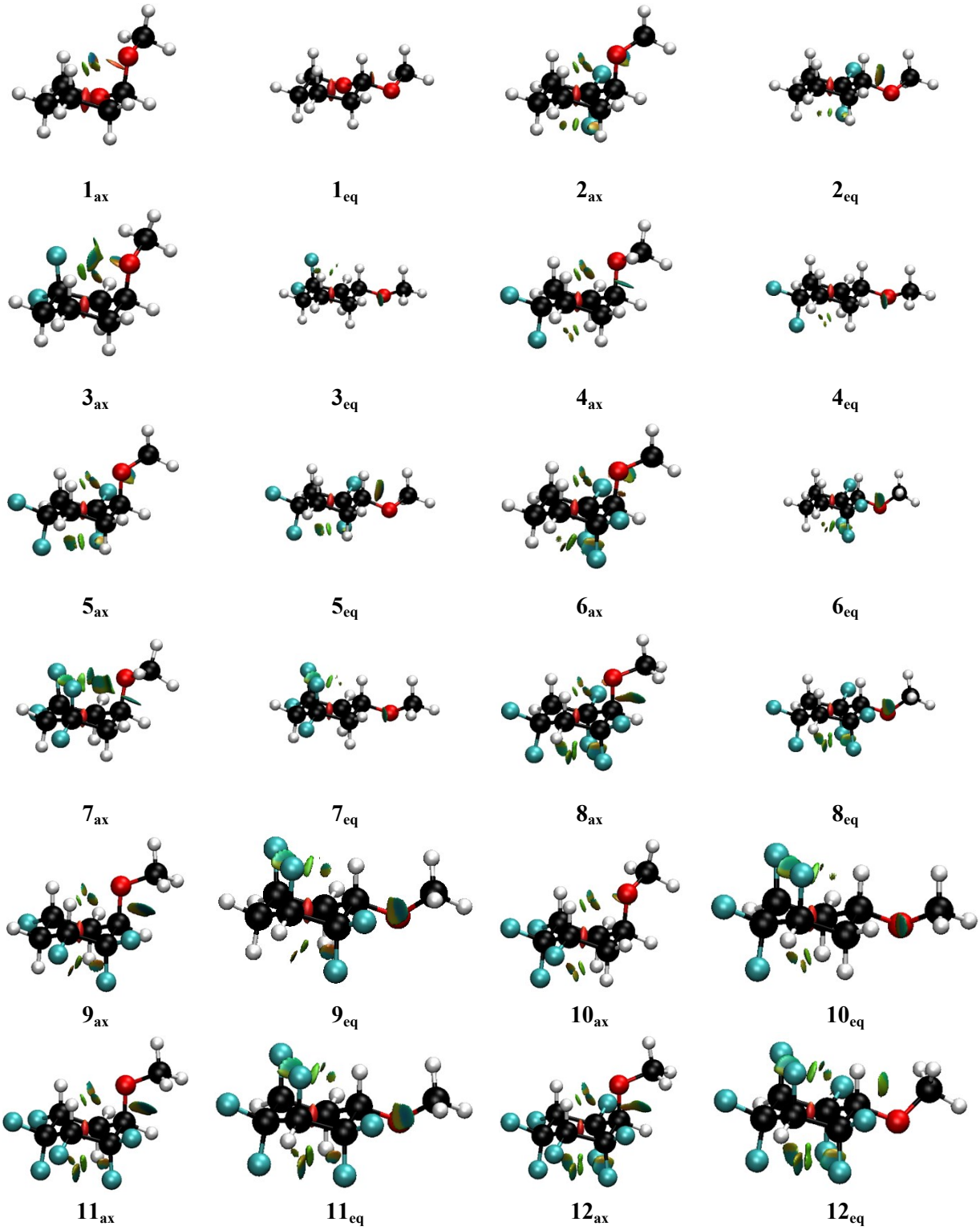


Figure S2. QTAIM molecular graphs for molecules 1-18. Bond critical points (green spheres), ring critical points (red spheres) and cage critical points (blue spheres).


1ax
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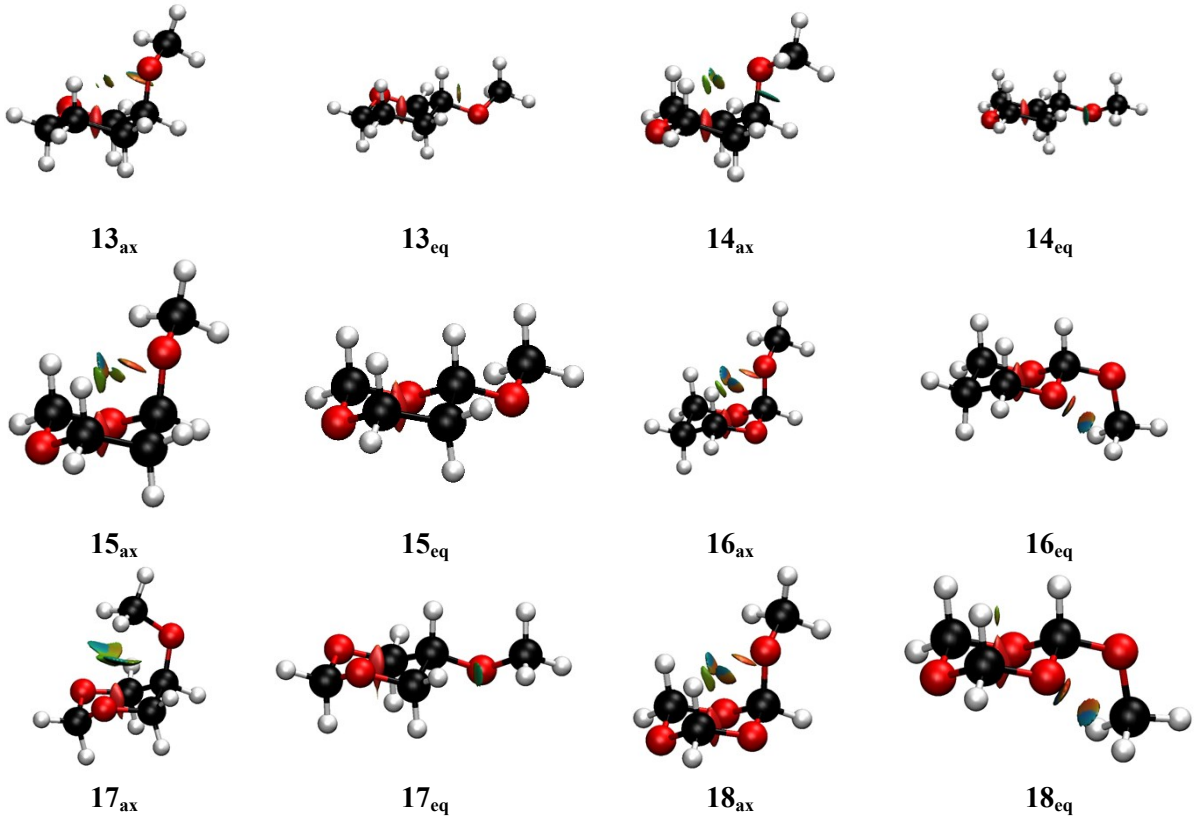
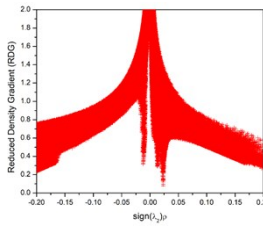
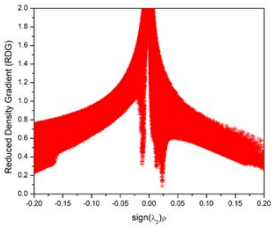


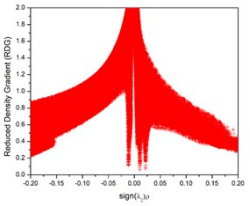
Figure S3. Isosurfaces from NCI for molecules 1-18, using reduced density gradient (RDG) = 0.5 and blue-green-red color scale ranging from -0.02 < sign(λ2)ρ(r) < +0.02 au.



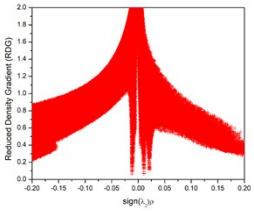
1$_{ax}$



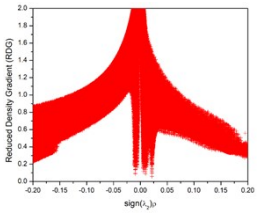
1$_{eq}$



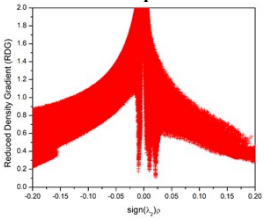
2$_{ax}$



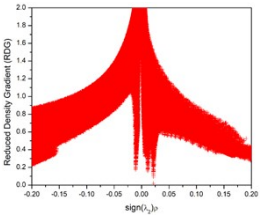
2$_{eq}$



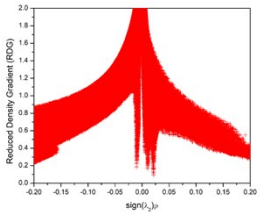
3$_{ax}$



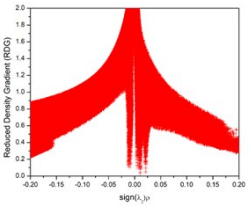
3$_{eq}$



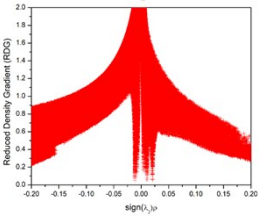
4$_{ax}$



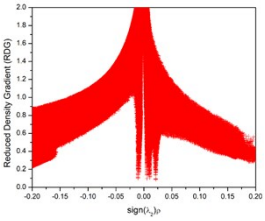
4$_{eq}$



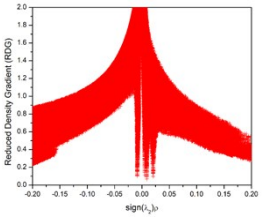
5$_{ax}$



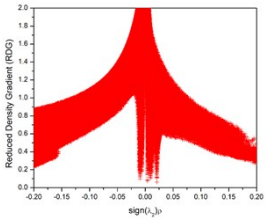
5$_{eq}$



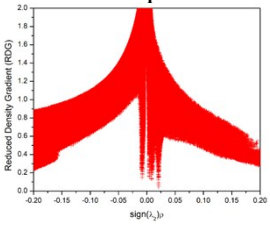
6$_{ax}$



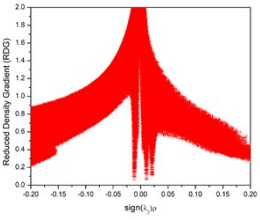
6$_{eq}$



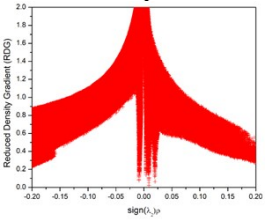
7$_{ax}$



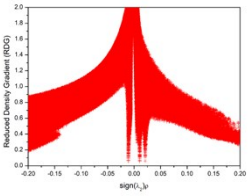
7$_{eq}$



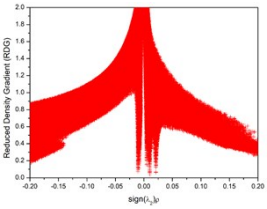
8$_{ax}$



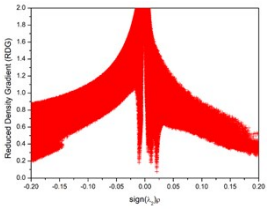
8$_{eq}$



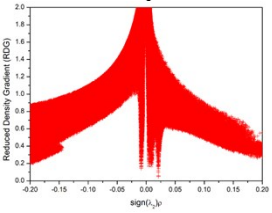
9$_{ax}$



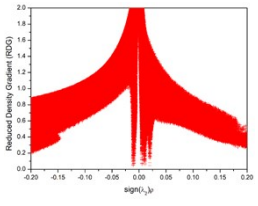
9$_{eq}$



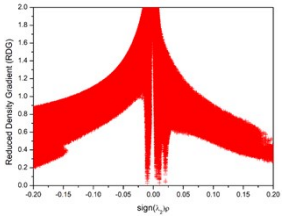
10$_{ax}$



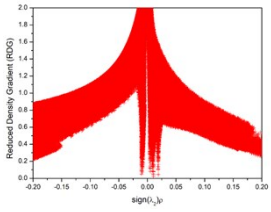
10$_{eq}$



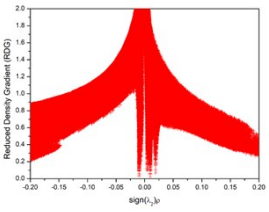
11$_{ax}$



11$_{eq}$



12$_{ax}$



12$_{eq}$

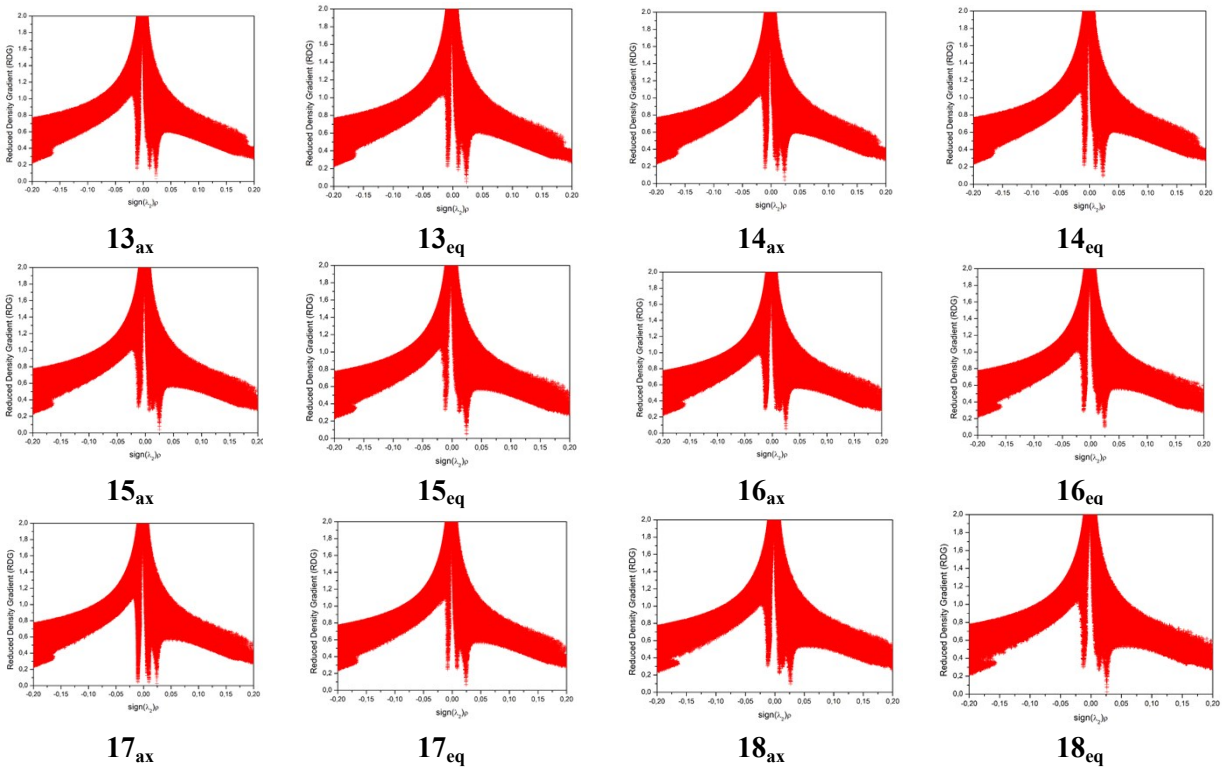
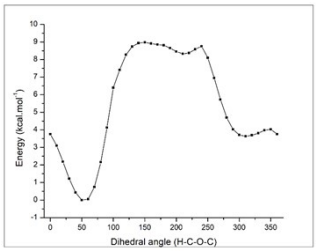


Figure S4. Reduced Density Gradient (RDG) versus sign(λ2)ρ obtained from M06-2X/aug-cc-VTZ electron densities for compounds 1-18.

Table S58. Calculated total relative energy Δ*E* values in kcal mol^{-1} and ax/eq population percentages obtained at DLPNO-CCSD(T)/def2-TZVP and M06-2X/aug-cc-pVTZ levels for compounds 1-18. Relative Gibbs free energies (kcal mol^{-1}) and population percentages are also shown in different solvents using the continuum polarizable model at the M06-2X/aug-cc-pVTZ level. Dipole moments (μ) calculated in each medium at M06-2X/aug-cc-pVTZ level are also given in Debyes. Negative values represent axial preference, and the positive ones equatorial preference.

		Gas-Phase			CH_3Cl		CH_2Cl_2		Acetone	
	DLPNO-CCSD(T)	M06-2X								
Compound	Δ*E*	Δ*E* (%P ax/eq)[a]	Δ*G* (%P ax/eq)[a]	μ (ax/eq)	Δ*G* (%P ax/eq)[a]	μ (ax/eq)	Δ*G* (%P ax/eq)[a]	μ (ax/eq)	Δ*G* (%P ax/eq)[a]	μ (ax/eq)
1	-1.23	-1.39 (91.3/8.7)	-1.10 (86.4/13.6)	0.17/0.72	-0.67 (75.5/24.5)	0.20/0.90	-0.55 (71.7/28.3)	0.21/0.95	-0.47 (68.7/31.3)	0.21/0.98
2	-1.54	-1.36 (90.8/9.2)	-1.22 (88.6/11.4)	0.62/1.03	-0.48 (69.3/30.7)	0.70/1.26	-0.32 (63.1/36.9)	0.72/1.31	-0.20 (58.5/41.5)	0.73/1.35
3	1.71	0.80 (20.6/79.4)	1.42 (8.4/91.6)	0.97/1.22	1.46 (7.8/92.2)	1.17/1.43	1.42 (8.3/91.7)	1.22/1.47	1.38 (8.9/91.1)	1.26/1.50
4	-1.09	-1.08 (86.0/14.0)	-0.74 (77.7/22.3)	1.24/1.12	-0.37 (65.0/35.0)	1.44/1.32	-0.28 (61.4/38.6)	1.48/1.37	-0.21 (58.7/41.3)	1.50/1.40
5	-2.42	-2.28 (97.9/2.1)	-2.06 (97.0/3.0)	1.26/1.24	-1.28 (89.7/10.3)	1.45/1.50	-1.07 (85.8/14.2)	1.49/1.56	-0.90 (81.9/18.1)	1.51/1.61
6	-2.80	-2.96 (99.3/0.7)	-2.56 (98.7/1.3)	0.90/1.53	-1.16 (87.6/12.4)	1.04/1.87	-0.75 (77.9/22.1)	1.06/1.95	-0.42 (66.9/33.1)	1.08/2.02
7	2.59	2.53 (1.4/98.6)	3.05 (0.6/99.4)	1.49/1.00	2.22 (2.3/97.7)	1.80/1.14	2.00 (3.3/96.7)	1.88/1.17	1.83 (4.4/95.6)	1.94/1.19
8	-3.61	-3.81 (99.8/0.2)	-3.40 (99.7/0.3)	1.28/1.59	-1.98 (96.6/3.4)	1.47/1.95	-1.51 (92.7/7.3)	1.50/2.04	-1.12 (86.8/13.2)	1.53/2.11
9	-0.94	-0.79 (79.2/20.8)	-0.59 (73.0/27.0)	1.18/1.81	-0.16 (56.8/43.2)	1.35/2.20	-0.04 (51.6/48.4)	1.39/2.29	0.05 (47.7/52.3)	1.41/2.35
10	-0.59	-0.60 (73.3/26.7)	-0.26 (60.8/39.2)	2.09/2.79	-0.83 (80.2/19.8)	2.42/3.18	-0.92 (82.5/17.5)	2.49/3.26	-1.01 (84.6/15.4)	2.53/3.32
11	-0.43	-0.41 (66.7/33.3)	0.25 (39.7/60.3)	2.06/0.75	-1.53 (93.0/7.0)	2.38/0.84	0.08 (46.7/53.3)	2.45/0.85	-0.36 (64.9/35.1)	2.50/0.86
12	-0.46	-0.47 (69.0/31.0)	-0.10 (54.1/45.9)	2.02/1.35	-1.64 (94.0/6.0)	2.34/1.55	-1.73 (94.9/5.1)	2.41/1.60	-1.81 (95.5/4.5)	2.46/1.64
13	0.42	0.35 (35.6/64.4)	0.87 (18.6/81.4)	0.58/0.19	0.90 (17.9/82.1)	0.75/0.22	0.83 (19.8/80.2)	0.80/0.22	0.74 (22.3/77.7)	0.83/0.22
14	0.23	0.25 (39.7/60.3)	0.36 (35.1/64.9)	0.80/0.74	0.67 (24.4/75.6)	0.97/0.91	0.72 (22.8/77.2)	1.01/0.96	0.76 (21.7/78.3)	1.03/0.99
15	-1.11	-1.26 (89.3/10.7)	-1.02 (84.7/15.3)	0.61/0.84	-0.60 (73.3/26.7)	0.72/1.05	-0.47 (69.0/31.0)	0.74/1.11	-0.38 (65.4/34.6)	0.76/1.15
16	-0.72	-0.90 (82.0/81.0)	-0.44 (67.8/32.2)	1.84/2.67	-0.25 (60.5/39.5)	2.22/3.19	-0.18 (57.4/42.6)	2.31/3.30	-0.11 (54.5-45.5)	2.38/3.38
17	1.88	1.59 (6.4/93.6)	1.81 (4.5/95.5)	0.65/0.65	1.89 (3.9/96.1)	0.81/0.77	1.91 (3.8/96.2)	0.85/0.79	1.91 (3.8/96.2)	0.88/0.81
18	0.20	-0.03 (51.3/48.7)	0.36 (35.1/64.9)	0.84/0.52	0.38 (34.4/65.6)	0.99/0.64	0.41 (33.3/66.7)	1.02/0.67	0.45 (32.0/68.0)	1.05/0.69

[a] Populations were measured using a Boltzmann Constant of 0.001987 kcal mol^{-1} and Temperature of 298.15 K.



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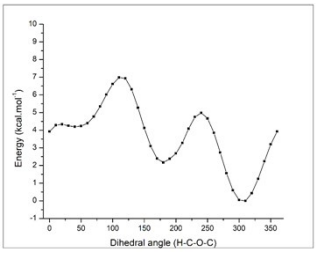

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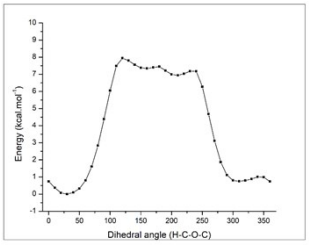

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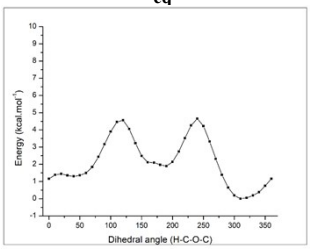

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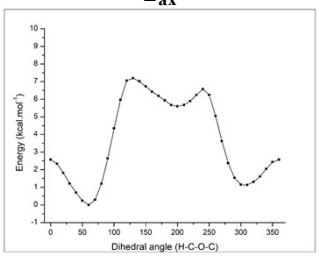

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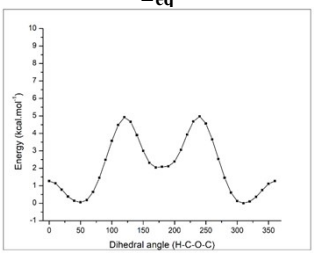

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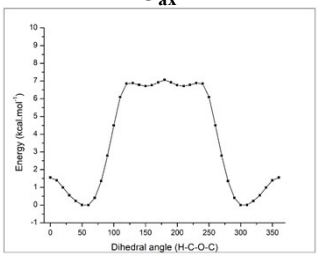

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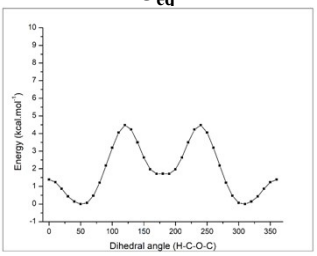

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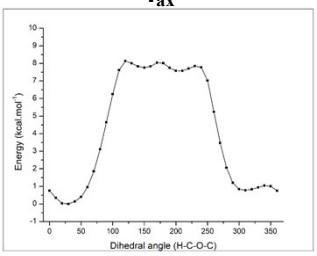

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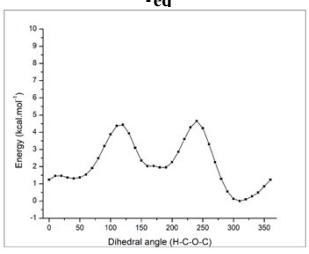

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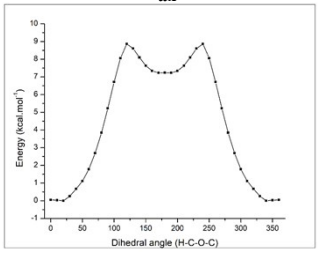

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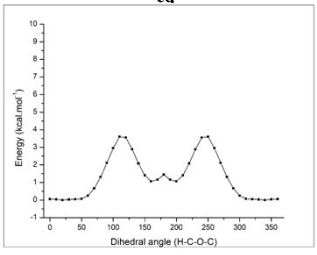

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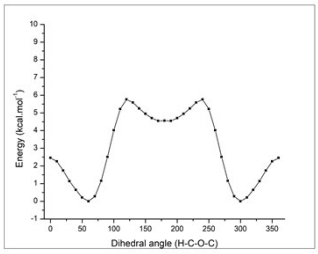

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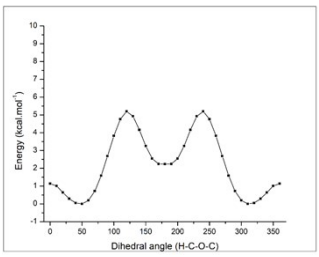

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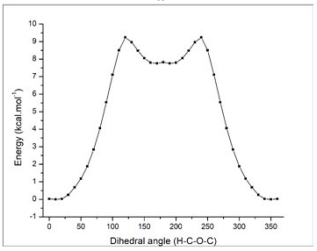

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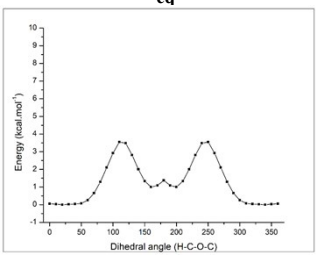

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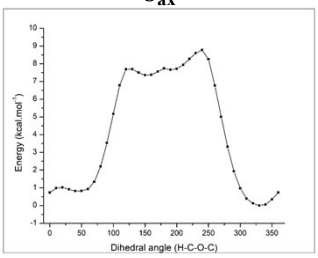

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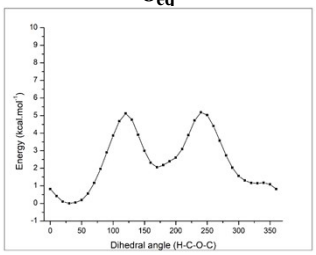

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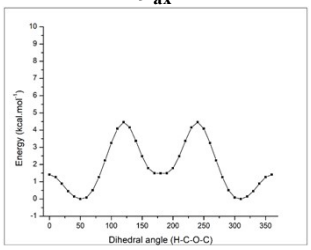

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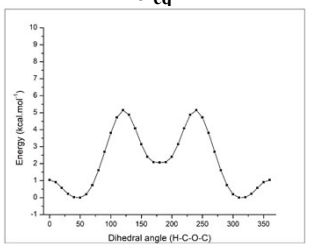

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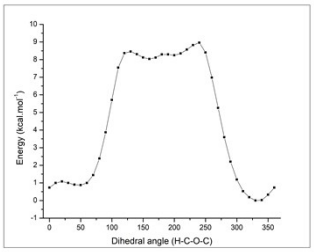

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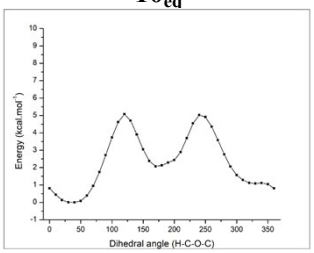

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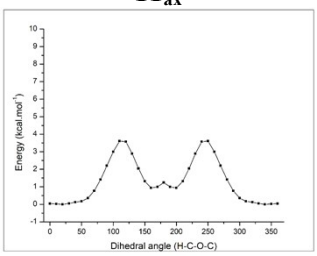

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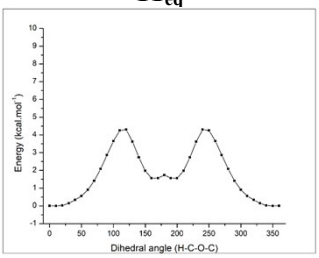

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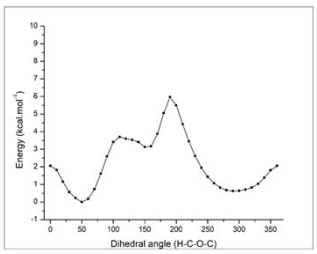

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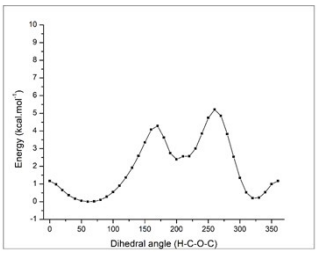

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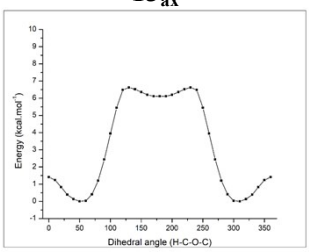

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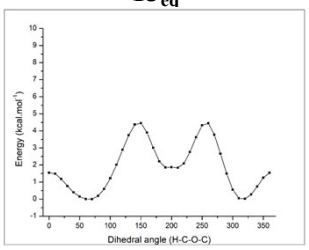

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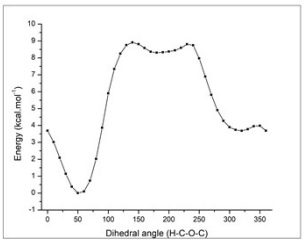

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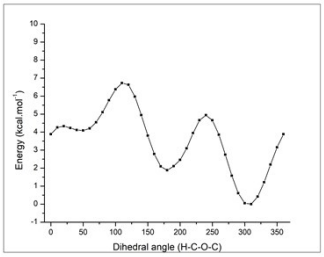

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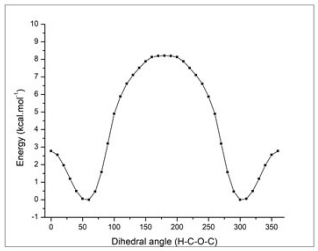

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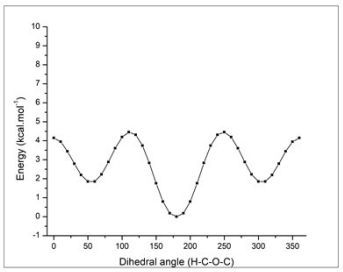

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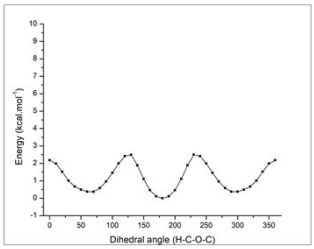

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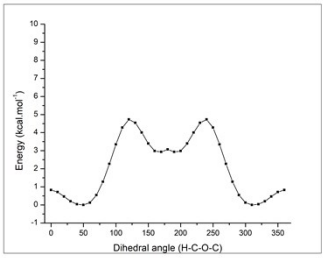

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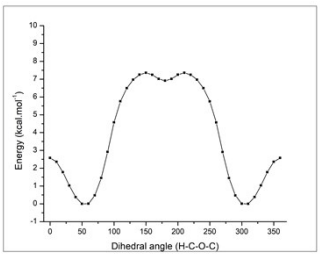

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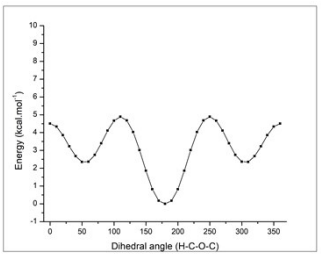

18_{eq}

Figure S5. Potential energy curves (kcal mol^{-1}) for the rotation of the H-C-O-C dihedral angle from 0 to 360º in steps of 10º for molecules 1-18 calculated at the M06-2X/cc-pVTZ level.

Table S59. Atomic charges obtained from QTAIM calculations from M06-2X/aug-cc-pVTZ wavefunctions for molecules 1-18.

Atomic Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
1_{ax}	-1.235	1.146	0.053	0.057	0.041	0.575	-1.256	0.588	0.027	0.022	0.010	0.014	0.004	-0.015	-0.015	-0.008	-0.008	-0.013	0.011	0.003	-	-	-	-	-
1_{eq}	-1.221	1.156	0.052	0.052	0.038	0.584	-1.264	0.588	0.022	0.039	0.005	-0.009	0.002	0.006	-0.008	-0.029	-0.008	-0.007	0.016	-0.012	-	-	-	-	-
2_{ax}	0.603	1.243	0.044	0.050	0.049	0.061	-1.248	0.588	0.023	0.007	0.040	0.017	-0.735	-0.733	0.021	0.021	-0.009	-0.013	-0.013	-0.006	-0.002	-0.010	-	-	-
2_{eq}	0.626	1.250	0.045	0.047	0.043	0.059	-1.245	0.594	0.020	0.036	0.006	0.000	-0.734	-0.733	0.027	0.001	-0.007	-0.006	-0.005	-0.030	0.002	0.004	-	-	-
3_{ax}	0.593	0.048	1.239	0.048	0.050	0.059	-1.238	0.597	0.002	0.025	0.023	-0.011	0.018	0.010	-0.729	-0.731	0.025	-0.002	-0.012	0.013	0.005	-0.033	-	-	-
3_{eq}	0.583	0.062	1.232	0.045	0.047	0.056	-1.237	0.602	0.026	0.007	0.009	-0.005	0.034	0.015	-0.729	-0.729	0.027	0.004	-0.005	-0.008	-0.017	-0.019	-	-	-
4_{ax}	0.573	0.053	0.045	1.234	0.050	0.061	-1.243	0.602	0.009	0.026	0.006	-0.011	-0.016	0.001	0.023	0.014	-0.731	-0.731	0.020	0.024	0.003	-0.011	-	-	-
4_{eq}	0.583	0.056	0.047	1.240	0.044	0.060	-1.239	0.604	0.008	0.026	0.006	-0.026	-0.016	0.003	0.029	0.002	-0.731	-0.732	0.028	0.001	0.004	0.005	-	-	-
5_{ax}	0.603	1.263	0.047	1.254	0.046	0.058	-1.247	0.580	0.011	0.028	0.042	0.026	-0.729	-0.726	0.061	0.053	-0.725	-0.724	0.029	0.030	0.008	0.013	-	-	-
5_{eq}	0.632	1.269	0.045	1.260	0.041	0.055	-1.242	0.586	0.038	0.026	0.009	0.002	-0.728	-0.726	0.068	0.036	-0.726	-0.725	0.036	0.004	0.014	0.027	-	-	-
6_{ax}	0.640	1.272	0.043	0.044	0.043	1.267	-1.245	0.575	0.038	0.032	0.022	0.051	-0.726	-0.725	0.029	0.027	0.002	0.011	0.029	0.025	-0.728	-0.726	-	-	-
6_{eq}	0.669	1.272	0.044	0.043	0.044	1.282	-1.241	0.583	0.035	0.034	0.012	0.025	-0.727	-0.725	0.035	0.002	0.004	0.018	0.035	0.002	-0.723	-0.724	-	-	-
7_{ax}	0.604	0.047	1.258	0.049	1.268	0.056	-1.229	0.591	0.002	0.032	0.023	-0.002	0.027	0.011	-0.723	-0.724	0.067	0.034	-0.722	-0.722	0.048	0.004	-	-	-
7_{eq}	0.590	0.054	1.255	0.046	1.251	0.058	-1.232	0.591	0.031	0.016	0.009	0.015	0.025	0.015	-0.724	-0.723	0.068	0.039	-0.723	-0.722	0.043	0.017	-	-	-
8_{ax}	0.640	1.286	0.045	1.272	0.047	1.291	-1.245	0.567	0.026	0.037	0.040	0.059	-0.722	-0.720	0.069	0.059	-0.720	-0.719	0.069	0.060	-0.721	-0.719	-	-	-
8_{eq}	0.677	1.291	0.046	1.278	0.045	1.301	-1.239	0.576	0.037	0.039	0.014	0.026	-0.721	-0.719	0.075	0.037	-0.720	-0.719	0.075	0.037	-0.718	-0.718	-	-	-
9_{ax}	0.604	1.282	0.636	0.048	0.604	0.053	-1.241	0.575	0.030	0.044	0.013	0.032	-0.729	-0.730	-0.714	0.066	0.031	0.030	-0.717	0.043	0.023	0.017	-	-	-
9_{eq}	0.680	1.333	0.668	1.342	0.668	1.327	-1.236	0.569	0.042	0.035	0.024	0.065	-0.717	-0.718	0.111	-0.714	-0.720	-0.719	0.112	-0.714	-0.719	-0.719	-	-	-
10_{ax}	0.570	0.053	0.640	1.306	0.640	0.047	-1.236	0.589	0.034	0.014	0.011	0.005	0.027	0.017	-0.714	0.068	-0.722	-0.726	-0.715	0.058	0.008	0.026	-	-	-
10_{eq}	0.577	0.051	0.611	0.038	0.607	0.056	-1.237	0.602	0.024	0.013	0.005	0.015	0.001	-0.008	0.023	-0.721	0.032	-0.004	0.023	-0.721	0.020	-0.008	-	-	-
11_{ax}	0.603	1.305	0.677	1.327	0.644	0.050	-1.242	0.568	0.035	0.046	0.016	0.040	-0.725	-0.723	-0.709	0.093	-0.718	-0.720	-0.711	0.073	0.032	0.038	-	-	-
11_{eq}	0.633	1.303	0.668	1.321	0.634	0.049	-1.238	0.579	0.031	0.012	0.040	0.042	-0.726	-0.725	0.104	-0.714	-0.724	-0.723	0.075	-0.717	0.036	0.040	-	-	-
12_{ax}	0.644	1.326	0.683	1.346	0.683	1.331	-1.241	0.555	0.043	0.044	0.031	0.071	-0.718	-0.719	-0.707	0.098	-0.713	-0.716	-0.707	0.100	-0.717	-0.717	-	-	-
12_{eq}	0.624	1.278	0.633	0.038	0.605	0.053	-1.239	0.585	0.027	0.010	0.038	0.041	-0.730	-0.730	0.066	-0.718	0.039	0.021	0.033	-0.720	0.026	0.019	-	-	-
13_{ax}	-1.234	0.595	0.589	0.066	0.043	0.585	-1.247	0.602	0.018	0.022	0.002	-0.011	0.003	-0.032	-0.013	0.011	0.015	-0.017	0.010	-0.008	-	-	-	-	-
13_{eq}	-1.235	0.596	0.586	0.063	0.036	0.586	-1.246	0.601	0.025	0.007	0.009	-0.008	-0.001	-0.014	-0.005	-0.010	0.015	-0.010	0.006	-0.002	-	-	-	-	-
14_{ax}	-1.231	0.582	0.049	0.584	0.044	0.584	-1.245	0.605	0.007	0.024	0.006	-0.014	-0.016	-0.003	0.012	0.001	0.011	0.008	0.005	-0.013	-	-	-	-	-
14_{eq}	-1.234	0.581	0.050	0.590	0.047	0.587	-1.241	0.605	0.007	0.024	0.005	-0.023	-0.016	0.001	0.019	-0.012	0.018	-0.013	0.003	0.004	-	-	-	-	-
15_{ax}	1.147	0.034	0.572	-1.244	1.177	-1.239	-1.258	0.582	0.030	0.026	0.013	0.023	0.017	0.010	0.022	0.013	0.046	0.029	-	-	-	-	-	-	-
15_{eq}	1.160	0.034	0.574	-1.245	1.187	-1.228	-1.265	0.582	0.026	0.041	0.007	-0.002	0.012	0.031	0.029	-0.007	0.052	0.012	-	-	-	-	-	-	-
16_{ax}	1.777	-1.245	0.573	0.023	0.571	-1.235	-1.255	0.577	0.029	0.030	0.017	0.054	0.021	0.022	0.004	0.011	0.021	0.009	-	-	-	-	-	-	-
16_{eq}	1.789	-1.227	0.581	0.019	0.581	-1.227	-1.285	0.566	0.024	0.038	0.038	0.039	0.026	-0.004	0.006	0.014	0.026	-0.004	-	-	-	-	-	-	-
17_{ax}	0.602	0.569	-1.247	1.193	-1.247	0.569	-1.243	0.577	0.027	0.017	0.027	0.018	0.038	0.000	0.051	0.011	0.038	0.000	-	-	-	-	-	-	-
17_{eq}	0.590	0.585	-1.244	1.191	-1.246	0.584	-1.255	0.594	0.030	0.014	0.010	0.014	0.016	0.005	0.052	0.015	0.035	0.008	-	-	-	-	-	-	-
18_{ax}	1.760	-1.248	1.150	-1.251	1.155	-1.239	-1.258	0.569	0.033	0.035	0.020	0.066	0.061	0.048	0.060	0.039	-	-	-	-	-	-	-	-	-
18_{eq}	1.780	-1.232	1.165	-1.253	1.165	-1.232	-1.291	0.557	0.028	0.042	0.042	0.050	0.065	0.024	0.065	0.024	-	-	-	-	-	-	-	-	-

Table S60. Atomic charges obtained from the Natural Population Analysis (NPA) at the M06-2X/aug-cc-pVTZ level for molecules 1-18.

Atomic Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
1_{ax}	-0.593	0.43	-0.425	-0.392	-0.417	-0.044	-0.596	-0.223	0.173	0.186	0.164	0.156	0.215	0.203	0.204	0.204	0.206	0.196	0.187	0.165	-	-	-	-	-
1_{eq}	-0.594	0.441	-0.426	-0.391	-0.419	-0.038	-0.57	-0.223	0.186	0.181	0.16	0.119	0.213	0.211	0.208	0.191	0.206	0.201	0.189	0.153	-	-	-	-	-
2_{ax}	0.072	0.744	-0.458	-0.391	-0.394	-0.406	-0.591	-0.217	0.187	0.162	0.181	0.187	-0.384	-0.389	0.223	0.224	0.209	0.201	0.207	0.206	0.214	0.21	-	-	-
2_{eq}	0.079	0.737	-0.453	-0.393	-0.39	-0.405	-0.572	-0.216	0.184	0.179	0.161	0.171	-0.386	-0.381	0.227	0.212	0.209	0.206	0.211	0.191	0.216	0.214	-	-	-
3_{ax}	0.137	-0.49	0.763	-0.451	-0.398	-0.401	-0.588	-0.221	0.158	0.191	0.171	0.17	0.227	0.225	-0.385	-0.387	0.226	0.21	0.208	0.22	0.219	0.197	-	-	-
3_{eq}	0.135	-0.466	0.762	-0.45	-0.394	-0.42	-0.58	-0.218	0.191	0.161	0.163	0.167	0.232	0.222	-0.379	-0.393	0.226	0.213	0.212	0.206	0.21	0.201	-	-	-
4_{ax}	0.137	-0.426	-0.458	0.763	-0.456	-0.405	-0.597	-0.219	0.163	0.191	0.16	0.172	0.21	0.218	0.225	0.221	-0.382	-0.396	0.224	0.227	0.217	0.211	-	-	-
4_{eq}	0.139	-0.424	-0.451	0.762	-0.452	-0.406	-0.579	-0.219	0.162	0.191	0.16	0.153	0.209	0.215	0.228	0.213	-0.382	-0.391	0.228	0.212	0.217	0.215	-	-	-
5_{ax}	0.073	0.744	-0.524	0.763	-0.457	-0.412	-0.592	-0.217	0.164	0.191	0.182	0.195	-0.377	-0.374	0.245	0.247	-0.376	-0.381	0.230	0.230	0.222	0.226	-	-	-
5_{eq}	0.081	0.737	-0.52	0.762	-0.453	-0.412	-0.568	-0.218	0.180	0.187	0.163	0.172	-0.381	-0.366	0.248	0.236	-0.376	-0.376	0.234	0.214	0.225	0.229	-	-	-
6_{ax}	0.009	0.749	-0.458	-0.398	-0.458	0.745	-0.579	-0.215	0.179	0.193	0.171	0.207	-0.369	-0.375	0.23	0.228	0.216	0.217	0.23	0.227	-0.376	-0.373	-	-	-
6_{eq}	0.014	0.740	-0.453	-0.400	-0.452	0.746	-0.556	-0.216	0.178	0.195	0.164	0.194	-0.38	-0.366	0.233	0.213	0.217	0.222	0.233	0.213	-0.372	-0.366	-	-	-
7_{ax}	0.136	-0.489	0.762	-0.518	0.763	-0.467	-0.576	-0.223	0.159	0.196	0.171	0.175	0.234	0.227	-0.379	-0.372	0.248	0.235	-0.38	-0.365	0.243	0.222	-	-	-
7_{eq}	0.130	-0.483	0.762	-0.517	0.761	-0.465	-0.576	-0.22	0.194	0.167	0.162	0.183	0.232	0.224	-0.374	-0.377	0.248	0.237	-0.373	-0.377	0.239	0.224	-	-	-
8_{ax}	0.010	0.745	-0.524	0.762	-0.524	0.748	-0.58	-0.215	0.173	0.195	0.18	0.214	-0.37	-0.359	0.251	0.25	-0.371	-0.366	0.251	0.251	-0.363	-0.36	-	-	-
8_{eq}	0.017	0.739	-0.52	0.761	-0.518	0.746	-0.552	-0.217	0.179	0.198	0.166	0.195	-0.374	-0.352	0.254	0.237	-0.371	-0.361	0.254	0.237	-0.367	-0.351	-	-	-
9_{ax}	0.074	0.704	0.184	-0.46	0.241	-0.442	-0.592	-0.218	0.192	0.183	0.166	0.196	-0.367	-0.371	-0.368	0.187	0.228	0.225	-0.388	0.172	0.228	0.226	-	-	-
9_{eq}	0.065	0.704	0.185	-0.469	0.241	-0.443	-0.571	-0.218	0.190	0.164	0.180	0.202	-0.366	-0.374	0.185	-0.375	0.234	0.232	0.173	-0.396	0.230	0.228	-	-	-
10_{ax}	0.134	-0.442	0.186	0.686	0.186	-0.462	-0.596	-0.221	0.196	0.166	0.163	0.182	0.23	0.227	-0.368	0.188	-0.356	-0.366	-0.368	0.183	0.222	0.232	-	-	-
10_{eq}	0.127	-0.461	0.189	0.692	0.187	-0.444	-0.578	-0.218	0.192	0.166	0.160	0.182	0.223	0.227	0.185	-0.374	-0.351	-0.374	0.186	-0.374	0.231	0.226	-	-	-
11_{ax}	0.073	0.704	0.123	0.688	0.184	-0.449	-0.593	-0.219	0.194	0.184	0.168	0.203	-0.363	-0.356	-0.343	0.204	-0.353	-0.351	-0.362	0.191	0.234	0.240	-	-	-
11_{eq}	0.067	0.703	0.127	0.691	0.186	-0.451	-0.568	-0.218	0.192	0.165	0.181	0.201	-0.361	-0.359	0.202	-0.352	-0.346	-0.359	0.192	-0.372	0.237	0.242	-	-	-
12_{ax}	0.011	0.706	0.124	0.688	0.123	0.709	-0.583	-0.216	0.199	0.183	0.176	0.22	-0.357	-0.342	-0.338	0.207	-0.35	-0.337	-0.338	0.208	-0.35	-0.343	-	-	-
12_{eq}	0.004	0.709	0.128	0.690	0.127	0.705	-0.553	-0.216	0.199	0.178	0.171	0.221	-0.349	-0.344	0.208	-0.350	-0.341	-0.345	0.207	-0.350	-0.354	-0.344	-	-	-
13_{ax}	-0.574	-0.068	0.105	-0.401	-0.423	-0.033	-0.587	-0.22	0.167	0.189	0.158	0.167	0.215	0.197	0.205	0.214	0.188	0.15	0.189	0.163	-	-	-	-	-
13_{eq}	-0.573	-0.061	0.107	-0.403	-0.42	-0.034	-0.58	-0.218	0.189	0.16	0.162	0.16	0.213	0.201	0.209	0.2	0.188	0.154	0.186	0.16	-	-	-	-	-
14_{ax}	-0.577	-0.038	-0.433	0.136	-0.452	-0.039	-0.596	-0.218	0.161	0.19	0.16	0.168	0.207	0.21	0.186	0.163	0.186	0.168	0.215	0.205	-	-	-	-	-
14_{eq}	-0.572	-0.035	-0.433	0.136	-0.452	-0.034	-0.58	-0.219	0.161	0.19	0.16	0.153	0.207	0.209	0.19	0.153	0.191	0.153	0.214	0.21	-	-	-	-	-
15_{ax}	0.426	-0.456	-0.042	-0.571	0.261	-0.593	-0.594	-0.224	0.175	0.188	0.165	0.160	0.220	0.213	0.190	0.170	0.177	0.136	-	-	-	-	-	-	-
15_{eq}	0.436	-0.457	-0.041	-0.569	0.264	-0.592	-0.566	-0.225	0.189	0.183	0.161	0.124	0.216	0.222	0.195	0.157	0.180	0.124	-	-	-	-	-	-	-
16_{ax}	0.692	-0.566	-0.046	-0.449	-0.047	-0.587	-0.594	-0.228	0.174	0.189	0.167	0.152	0.190	0.177	0.211	0.206	0.191	0.168	-	-	-	-	-	-	-
16_{eq}	0.700	-0.588	-0.041	-0.450	-0.041	-0.588	-0.556	-0.235	0.186	0.181	0.181	0.127	0.194	0.158	0.211	0.209	0.194	0.158	-	-	-	-	-	-	-
17_{ax}	0.072	-0.077	-0.576	0.268	-0.576	-0.077	-0.577	-0.231	0.174	0.183	0.174	0.195	0.204	0.170	0.180	0.123	0.204	0.170	-	-	-	-	-	-	-
17_{eq}	0.077	-0.069	-0.569	0.267	-0.568	-0.051	-0.578	-0.217	0.191	0.165	0.161	0.169	0.191	0.165	0.179	0.125	0.197	0.165	-	-	-	-	-	-	-
18_{ax}	0.686	-0.566	0.254	-0.568	0.254	-0.588	-0.590	-0.229	0.176	0.192	0.168	0.157	0.182	0.149	0.182	0.141	-	-	-	-	-	-	-	-	-
18_{eq}	0.693	-0.587	0.257	-0.567	0.257	-0.587	-0.553	-0.236	0.188	0.184	0.184	0.134	0.185	0.131	0.185	0.131	-	-	-	-	-	-	-	-	-

Table S61. Atomic charges obtained from the CHelp analysis at the M06-2X/aug-cc-pVTZ level for molecules 1-18.

Atomic Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1_{ax}	-0.679	0.853	-0.251	0.593	-0.433	0.795	-0.512	0.346	-0.030	-0.032	-0.061	-0.108	-0.011	0.004	-0.125	-0.172	0.050	0.061	-0.141	-0.146	-	-
1_{eq}	-0.593	0.851	-0.011	0.042	-0.003	0.431	-0.598	0.512	-0.067	-0.065	-0.108	-0.127	-0.044	-0.010	0.005	-0.049	-0.031	-0.009	-0.045	-0.081	-	-
2_{ax}	0.546	0.344	0.165	0.144	-0.031	-0.182	-0.474	0.429	-0.053	-0.080	-0.062	-0.089	-0.264	-0.269	-0.033	-0.072	-0.052	-0.048	0.031	-0.002	0.031	0.021
2_{eq}	0.454	0.506	-0.085	0.213	-0.085	0.051	-0.517	0.449	-0.063	-0.061	-0.071	-0.085	-0.302	-0.288	0.044	-0.023	-0.045	-0.055	0.025	-0.014	-0.019	-0.027
3_{ax}	0.707	-0.151	0.835	-0.301	0.428	-0.552	-0.489	0.225	-0.060	0.022	-0.011	-0.097	0.025	-0.039	-0.351	-0.336	0.046	0.040	-0.043	-0.106	0.113	0.097
3_{eq}	0.495	-0.192	0.619	-0.060	0.221	-0.243	-0.503	0.371	-0.031	-0.049	-0.060	-0.046	0.039	0.053	-0.309	-0.306	0.026	-0.005	-0.040	-0.076	0.057	0.038
4_{ax}	0.428	0.063	0.146	0.655	-0.070	-0.076	-0.520	0.439	-0.096	-0.041	-0.047	-0.078	-0.026	-0.070	-0.038	-0.086	-0.336	-0.326	0.030	0.014	0.026	0.010
4_{eq}	0.462	-0.081	-0.228	0.922	-0.265	0.184	-0.582	0.520	-0.094	-0.069	-0.089	-0.071	0.033	0.022	0.078	0.016	-0.384	-0.371	0.063	0.013	-0.033	-0.047
5_{ax}	0.337	0.621	-0.035	0.590	0.204	-0.025	-0.450	0.226	-0.010	0.000	0.004	-0.056	-0.305	-0.319	0.035	-0.038	-0.304	-0.332	-0.042	-0.082	0.013	-0.034
5_{eq}	0.166	0.773	-0.467	0.991	-0.471	0.302	-0.471	0.409	-0.044	-0.042	-0.066	-0.021	-0.321	-0.318	0.146	0.061	-0.359	-0.365	0.130	0.067	-0.021	-0.079
6_{ax}	0.414	0.598	-0.071	0.131	-0.162	0.417	-0.538	0.466	-0.056	-0.039	-0.078	-0.041	-0.314	-0.324	0.041	0.002	-0.014	-0.027	0.083	0.046	-0.261	-0.274
6_{eq}	0.286	0.616	-0.128	0.219	-0.201	0.658	-0.394	0.157	0.023	0.022	0.006	-0.068	-0.291	-0.321	0.034	-0.008	-0.024	-0.032	0.063	0.016	-0.318	-0.315
7_{ax}	0.666	-0.339	0.673	-0.221	0.886	-0.493	-0.473	0.142	0.003	0.036	0.014	-0.087	0.084	0.063	-0.313	-0.263	0.057	0.040	-0.340	-0.347	0.134	0.080
7_{eq}	0.658	-0.467	0.863	-0.209	0.576	-0.095	-0.560	0.581	-0.073	-0.108	-0.122	-0.112	0.130	0.075	-0.334	-0.368	0.085	0.028	-0.272	-0.299	0.019	0.003
8_{ax}	0.263	0.555	-0.174	0.599	-0.133	0.552	-0.489	0.526	-0.082	-0.075	-0.076	-0.012	-0.268	-0.291	0.103	0.018	-0.277	-0.287	0.071	0.033	-0.266	-0.290
8_{eq}	0.101	0.814	-0.589	0.991	-0.472	0.774	-0.387	0.350	-0.020	-0.051	-0.025	-0.036	-0.312	-0.340	0.184	0.101	-0.347	-0.340	0.129	0.087	-0.308	-0.304
9_{ax}	0.498	0.382	0.453	-0.257	0.567	-0.174	-0.572	0.369	-0.006	-0.064	-0.045	-0.044	-0.234	-0.287	-0.305	-0.045	0.062	0.072	-0.336	-0.081	0.049	-0.003
9_{eq}	0.727	0.261	0.353	0.144	0.270	-0.219	-0.513	0.218	0.023	-0.025	-0.003	-0.131	-0.223	-0.266	-0.010	-0.315	-0.019	-0.057	0.008	-0.309	0.070	0.016
10_{ax}	0.317	-0.085	0.449	0.442	0.562	-0.362	-0.527	0.465	-0.040	-0.080	-0.076	0.017	0.048	0.004	-0.315	-0.067	-0.278	-0.267	-0.334	-0.063	0.111	0.077
10_{eq}	0.743	-0.408	0.401	0.565	0.284	-0.185	-0.566	0.347	0.001	-0.062	-0.056	-0.101	0.120	0.061	-0.004	-0.323	-0.295	-0.315	0.027	-0.301	0.046	0.022
11_{ax}	0.402	0.450	0.069	0.660	0.438	-0.158	-0.434	0.163	0.035	0.005	-0.002	-0.025	-0.225	-0.256	-0.204	0.025	-0.314	-0.277	-0.308	-0.094	0.073	-0.022
11_{eq}	0.522	0.402	0.274	0.593	0.116	-0.128	-0.482	0.261	0.002	-0.019	-0.006	-0.076	-0.263	-0.272	0.041	-0.293	-0.278	-0.305	0.073	-0.250	0.065	0.024
12_{ax}	0.246	0.454	-0.133	0.515	0.098	0.574	-0.504	0.498	-0.043	-0.081	-0.075	0.015	-0.194	-0.223	-0.140	0.113	-0.221	-0.210	-0.208	0.050	-0.255	-0.277
12_{eq}	0.453	0.504	0.009	0.659	0.309	0.341	-0.489	0.434	-0.036	-0.074	-0.042	-0.072	-0.249	-0.278	0.120	-0.244	-0.275	-0.324	0.024	-0.302	-0.212	-0.255
13_{ax}	-0.503	0.393	0.487	0.020	0.010	0.364	-0.487	0.313	-0.024	-0.018	-0.063	-0.131	-0.007	-0.050	-0.022	-0.032	-0.024	-0.071	-0.072	-0.082	-	-
13_{eq}	-0.544	0.047	0.521	0.182	-0.274	0.643	-0.627	0.596	-0.055	-0.151	-0.118	-0.096	-0.037	-0.053	0.028	0.038	-0.094	-0.109	0.092	0.011	-	-
14_{ax}	-0.616	0.658	-0.057	0.487	-0.120	0.492	-0.514	0.493	-0.101	-0.072	-0.082	-0.079	-0.013	-0.013	-0.054	-0.073	-0.103	-0.164	-0.035	-0.034	-	-
14_{eq}	-0.519	0.340	-0.072	0.741	-0.416	0.467	-0.574	0.395	-0.056	-0.028	-0.073	-0.147	0.076	0.079	-0.030	-0.085	-0.014	-0.052	-0.032	-	-	-
15_{ax}	0.445	-0.032	0.697	-0.660	0.903	-0.588	-0.473	0.454	-0.071	-0.053	-0.080	0.024	-0.033	-0.025	-0.114	-0.163	-0.103	-0.128	-	-	-	-
15_{eq}	0.935	-0.197	0.484	-0.580	0.719	-0.616	-0.572	0.431	-0.026	-0.067	-0.090	-0.146	-0.029	0.042	-0.024	-0.106	-0.043	-0.112	-	-	-	-
16_{ax}	1.068	-0.702	0.687	-0.365	0.861	-0.687	-0.470	0.122	0.016	0.045	-0.013	-0.088	-0.076	-0.141	0.018	0.052	-0.152	-0.173	-	-	-	-
16_{eq}	1.050	-0.538	0.245	0.230	0.245	-0.538	-0.653	0.727	-0.103	-0.144	-0.144	-0.131	0.027	-0.056	-0.097	-0.091	0.027	-0.056	-	-	-	-
17_{ax}	0.224	0.604	-0.616	0.744	-0.628	0.681	-0.600	0.568	-0.104	-0.078	-0.093	-0.036	-0.067	-0.162	-0.049	-0.111	-0.095	-0.183	-	-	-	-
17_{eq}	0.372	0.216	-0.585	0.846	-0.628	0.482	-0.620	0.627	-0.060	-0.130	-0.145	-0.053	0.046	-0.029	-0.073	-0.127	-0.054	-0.084	-	-	-	-
18_{ax}	1.040	-0.681	1.032	-0.658	0.721	-0.645	-0.533	0.377	-0.064	-0.016	-0.065	-0.069	-0.130	-0.199	-0.029	-0.079	-	-	-	-	-	-
18_{eq}	1.219	-0.619	0.691	-0.564	0.691	-0.619	-0.671	0.763	-0.104	-0.155	-0.155	-0.213	-0.027	-0.106	-0.027	-0.106	-	-	-	-	-	-

Table S62. Atomic charges obtained from the CHelpG analysis at the M06-2X/aug-cc-pVTZ level for molecules 1-18.

Atomic Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1_{ax}	-0.465	0.338	-0.249	0.190	-0.210	0.262	-0.347	0.031	0.041	0.063	0.031	0.067	0.060	0.078	-0.015	-0.017	0.029	0.073	0.019	0.018	-	-
1_{eq}	-0.371	0.392	-0.223	0.100	-0.096	0.108	-0.410	0.112	0.059	0.020	0.000	0.041	0.057	0.093	0.001	-0.013	0.020	0.048	0.056	0.006	-	-
2_{ax}	0.240	0.434	-0.052	-0.078	0.093	-0.242	-0.322	-0.075	0.089	0.061	0.067	0.031	-0.266	-0.272	0.051	0.041	0.026	0.037	0.006	-0.014	0.077	0.068
2_{eq}	0.219	0.461	-0.183	-0.009	0.029	-0.172	-0.403	0.076	0.055	0.053	0.012	0.047	-0.285	-0.232	0.089	0.053	0.024	0.023	0.016	-0.004	0.064	0.068
3_{ax}	0.263	-0.212	0.694	-0.243	0.157	-0.244	-0.342	-0.022	0.035	0.082	0.056	0.024	0.070	0.051	-0.337	-0.281	0.069	0.067	0.003	-0.017	0.065	0.060
3_{eq}	0.377	-0.434	0.680	-0.175	0.016	-0.201	-0.416	0.042	0.077	0.027	0.022	0.027	0.143	0.123	-0.311	-0.300	0.067	0.056	0.035	0.009	0.057	0.078
4_{ax}	0.196	-0.115	-0.048	0.519	-0.005	-0.208	-0.326	-0.025	0.043	0.077	0.054	0.034	0.040	0.044	0.049	0.045	-0.311	-0.275	0.050	0.018	0.075	0.067
4_{eq}	0.280	-0.126	-0.229	0.585	-0.123	-0.129	-0.438	0.108	0.008	0.064	0.003	0.031	0.067	0.079	0.103	0.064	-0.305	-0.277	0.075	0.040	0.061	0.061
5_{ax}	0.186	0.436	-0.268	0.526	-0.055	-0.217	-0.307	-0.073	0.063	0.093	0.068	0.052	-0.238	-0.251	0.142	0.105	-0.283	-0.255	0.073	0.029	0.097	0.077
5_{eq}	0.144	0.546	-0.425	0.628	-0.174	-0.069	-0.390	0.060	0.055	0.066	0.021	0.056	-0.275	-0.232	0.176	0.118	-0.290	-0.272	0.088	0.049	0.067	0.054
6_{ax}	0.132	0.444	-0.137	0.000	-0.131	0.422	-0.322	-0.074	0.069	0.102	0.073	0.079	-0.252	-0.253	0.081	0.053	0.037	0.034	0.078	0.059	-0.241	-0.252
6_{eq}	0.036	0.444	-0.248	0.090	-0.223	0.469	-0.306	0.032	0.043	0.080	0.038	0.077	-0.239	-0.216	0.106	0.076	0.028	0.023	0.098	0.071	-0.248	-0.231
7_{ax}	0.423	-0.312	0.785	-0.443	0.789	-0.453	-0.389	0.008	0.021	0.089	0.050	0.010	0.087	0.065	-0.328	-0.291	0.142	0.117	-0.314	-0.302	0.138	0.108
7_{eq}	0.469	-0.401	0.656	-0.412	0.732	-0.470	-0.419	0.043	0.081	0.026	0.031	0.015	0.130	0.125	-0.283	-0.287	0.157	0.121	-0.296	-0.296	0.148	0.130
8_{ax}	0.093	0.464	-0.300	0.602	-0.319	0.477	-0.319	-0.067	0.074	0.105	0.069	0.089	-0.228	-0.245	0.149	0.105	-0.275	-0.256	0.158	0.104	-0.236	-0.245
8_{eq}	0.052	0.539	-0.457	0.698	-0.394	0.547	-0.326	0.034	0.042	0.087	0.040	0.059	-0.239	-0.229	0.183	0.126	-0.285	-0.267	0.164	0.113	-0.247	-0.240
9_{ax}	0.264	0.253	0.360	-0.408	0.497	-0.430	-0.366	-0.012	0.088	0.047	0.051	0.068	-0.196	-0.216	-0.267	0.034	0.130	0.151	-0.313	-0.013	0.146	0.130
9_{eq}	0.480	0.218	0.321	-0.332	0.486	-0.426	-0.406	0.008	0.086	0.028	0.052	0.024	-0.211	-0.213	0.060	-0.285	0.122	0.079	0.002	-0.319	0.121	0.106
10_{ax}	0.268	-0.391	0.384	0.233	0.376	-0.342	-0.367	-0.001	0.086	0.039	0.047	0.062	0.138	0.123	-0.264	0.015	-0.218	-0.175	-0.272	0.034	0.116	0.108
10_{eq}	0.477	-0.445	0.210	0.319	0.348	-0.459	-0.428	0.065	0.076	0.014	0.021	0.047	0.153	0.145	0.100	-0.250	-0.211	-0.243	0.059	-0.275	0.142	0.134
11_{ax}	0.241	0.310	0.214	0.314	0.354	-0.322	-0.369	-0.032	0.098	0.054	0.061	0.064	-0.196	-0.219	-0.210	0.058	-0.220	-0.182	-0.261	0.008	0.133	0.103
11_{eq}	0.415	0.268	0.114	0.352	0.340	-0.409	-0.387	-0.016	0.094	0.037	0.064	0.038	-0.203	-0.201	0.139	-0.231	-0.207	-0.243	0.059	-0.279	0.140	0.117
12_{ax}	0.046	0.311	0.135	0.310	0.138	0.361	-0.346	-0.031	0.107	0.062	0.072	0.137	-0.171	-0.192	-0.182	0.089	-0.193	-0.156	-0.182	0.080	-0.190	-0.203
12_{eq}	0.251	0.241	0.097	0.340	0.084	0.207	-0.317	0.023	0.091	0.042	0.042	0.078	-0.174	-0.182	0.154	-0.208	-0.179	-0.210	0.160	-0.208	-0.159	-0.172
13_{ax}	-0.354	0.044	0.155	-0.120	0.042	0.090	-0.314	-0.011	0.061	0.068	0.035	0.026	0.045	0.041	-0.003	0.026	0.045	0.029	0.060	0.037	-	-
13_{eq}	-0.461	0.085	0.266	0.007	-0.128	0.216	-0.471	0.132	0.060	-0.009	0.007	0.025	0.021	0.015	0.030	0.041	0.035	0.004	0.073	0.051	-	-
14_{ax}	-0.486	0.281	-0.279	0.301	-0.182	0.283	-0.348	0.018	0.031	0.063	0.040	0.007	0.027	0.060	0.014	0.002	0.030	-0.015	0.061	0.091	-	-
14_{eq}	-0.449	0.260	-0.302	0.449	-0.237	0.176	-0.462	0.107	0.013	0.060	0.001	-0.005	0.044	0.102	0.053	0.003	0.036	-0.014	0.066	0.101	-	-
15_{ax}	0.421	-0.245	0.328	-0.481	0.373	-0.463	-0.364	0.054	0.032	0.063	0.025	0.041	0.046	0.095	0.022	-0.025	0.061	0.017	-	-	-	-
15_{eq}	0.456	-0.247	0.260	-0.419	0.211	-0.371	-0.415	0.105	0.068	0.017	0.002	0.023	0.051	0.117	0.034	-0.012	0.105	0.014	-	-	-	-
16_{ax}	0.476	-0.477	0.325	-0.243	0.304	-0.468	-0.350	0.049	0.031	0.068	0.024	0.096	0.023	-0.015	0.033	0.097	0.016	0.011	-	-	-	-
16_{eq}	0.365	-0.338	0.128	-0.059	0.128	-0.338	-0.390	0.138	0.048	0.020	0.020	0.083	0.050	0.012	0.013	0.057	0.050	0.012	-	-	-	-
17_{ax}	0.233	0.087	-0.379	0.222	-0.379	0.085	-0.433	0.104	0.038	0.037	0.038	0.009	0.081	0.021	0.090	0.042	0.082	0.021	-	-	-	-
17_{eq}	0.254	0.106	-0.446	0.299	-0.424	0.089	-0.486	0.168	0.057	-0.004	-0.014	0.053	0.073	0.049	0.088	0.021	0.075	0.042	-	-	-	-
18_{ax}	0.550	-0.471	0.420	-0.467	0.420	-0.455	-0.364	0.053	0.027	0.077	0.020	0.079	0.073	-0.020	0.053	0.006	-	-	-	-	-	-
18_{eq}	0.410	-0.339	0.259	-0.382	0.259	-0.339	-0.399	0.141	0.046	0.030	0.030	0.073	0.092	0.013	0.092	0.013	-	-	-	-	-	-

Table S63. Atomic charges obtained from the Hirshfeld (CM5) analysis at the M06-2X/aug-cc-pVTZ level for molecules 1-18.

Atomic Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1_{ax}	-0.275	0.102	-0.162	-0.161	-0.165	-0.061	-0.271	-0.130	0.091	0.101	0.090	0.108	0.095	0.092	0.086	0.088	0.089	0.087	0.102	0.092	-	-
1_{eq}	-0.269	0.102	-0.164	-0.160	-0.165	-0.059	-0.265	-0.129	0.102	0.094	0.088	0.093	0.094	0.097	0.089	0.083	0.089	0.090	0.104	0.087	-	-
2_{ax}	0.008	0.211	-0.163	-0.158	-0.160	-0.159	-0.263	-0.129	0.103	0.089	0.089	0.105	-0.153	-0.157	0.099	0.101	0.090	0.087	0.088	0.089	0.095	0.091
2_{eq}	0.007	0.210	-0.162	-0.158	-0.159	-0.158	-0.266	-0.131	0.101	0.090	0.088	0.100	-0.155	-0.151	0.101	0.097	0.091	0.090	0.091	0.084	0.096	0.096
3_{ax}	0.012	-0.166	0.213	-0.162	-0.158	-0.159	-0.268	-0.129	0.087	0.103	0.089	0.094	0.100	0.102	-0.168	-0.154	0.100	0.096	0.090	0.094	0.096	0.088
3_{eq}	0.010	-0.161	0.213	-0.163	-0.156	-0.165	-0.273	-0.128	0.104	0.088	0.089	0.095	0.106	0.105	-0.163	-0.162	0.101	0.098	0.093	0.090	0.090	0.091
4_{ax}	0.009	-0.162	-0.163	0.212	-0.162	-0.156	-0.270	-0.128	0.089	0.103	0.088	0.095	0.091	0.094	0.099	0.100	-0.165	-0.164	0.099	0.101	0.097	0.093
4_{eq}	0.008	-0.162	-0.161	0.211	-0.161	-0.157	-0.273	-0.129	0.088	0.103	0.087	0.090	0.091	0.095	0.102	0.097	-0.164	-0.159	0.102	0.097	0.097	0.096
5_{ax}	0.008	0.215	-0.162	0.216	-0.161	-0.155	-0.263	-0.127	0.092	0.106	0.091	0.110	-0.147	-0.148	0.115	0.115	-0.158	-0.155	0.104	0.104	0.102	0.098
5_{eq}	0.008	0.215	-0.162	0.215	-0.160	-0.154	-0.262	-0.129	0.092	0.104	0.090	0.101	-0.150	-0.141	0.117	0.112	-0.158	-0.150	0.107	0.100	0.103	0.102
6_{ax}	0.006	0.215	-0.161	-0.154	-0.162	0.214	-0.258	-0.122	0.093	0.108	0.096	0.118	-0.152	-0.150	0.104	0.104	0.098	0.094	0.104	0.103	-0.150	-0.150
6_{eq}	0.007	0.213	-0.161	-0.154	-0.161	0.215	-0.255	-0.123	0.091	0.110	0.092	0.114	-0.152	-0.143	0.106	0.099	0.098	0.097	0.106	0.099	-0.155	-0.142
7_{ax}	0.016	-0.165	0.217	-0.162	0.218	-0.158	-0.265	-0.127	0.088	0.108	0.090	0.099	0.105	0.105	-0.161	-0.145	0.116	0.111	-0.162	-0.147	0.112	0.104
7_{eq}	0.013	-0.166	0.217	-0.162	0.218	-0.160	-0.270	-0.126	0.107	0.093	0.090	0.101	0.105	0.106	-0.157	-0.152	0.116	0.114	-0.156	-0.152	0.111	0.107
8_{ax}	0.007	0.218	-0.161	0.221	-0.161	0.220	-0.257	-0.120	0.098	0.111	0.095	0.123	-0.143	-0.141	0.119	0.117	-0.152	-0.146	0.120	0.119	-0.145	-0.141
8_{eq}	0.007	0.217	-0.161	0.220	-0.161	0.220	-0.252	-0.121	0.093	0.112	0.094	0.115	-0.145	-0.134	0.121	0.114	-0.152	-0.142	0.122	0.114	-0.148	-0.134
9_{ax}	0.013	0.211	0.035	-0.161	0.037	-0.159	-0.262	-0.126	0.107	0.092	0.093	0.112	-0.140	-0.141	-0.164	0.112	0.106	0.103	-0.178	0.103	0.105	0.102
9_{eq}	0.008	0.211	0.035	-0.158	0.038	-0.159	-0.265	-0.127	0.105	0.092	0.091	0.111	-0.139	-0.143	0.112	-0.160	0.108	0.107	0.104	-0.178	0.106	0.104
10_{ax}	0.016	-0.157	0.034	0.211	0.033	-0.164	-0.269	-0.125	0.108	0.093	0.091	0.103	0.107	0.103	-0.163	0.113	-0.144	-0.140	-0.163	0.111	0.100	0.104
10_{eq}	0.010	-0.163	0.036	0.213	0.036	-0.158	-0.271	-0.127	0.105	0.092	0.089	0.100	0.101	0.103	0.112	-0.160	-0.139	-0.142	0.112	-0.160	0.107	0.104
11_{ax}	0.013	0.214	0.034	0.214	0.034	-0.156	-0.262	-0.124	0.109	0.094	0.095	0.117	-0.135	-0.134	-0.143	0.123	-0.140	-0.132	-0.157	0.114	0.112	0.108
11_{eq}	0.008	0.214	0.036	0.216	0.037	-0.156	-0.261	-0.126	0.107	0.094	0.092	0.111	-0.134	-0.135	0.125	-0.142	-0.134	-0.134	0.117	-0.157	0.112	0.110
12_{ax}	0.010	0.217	0.035	0.217	0.035	0.218	-0.257	-0.117	0.114	0.098	0.101	0.129	-0.132	-0.127	-0.137	0.125	-0.135	-0.124	-0.137	0.126	-0.134	-0.128
12_{eq}	0.006	0.218	0.037	0.219	0.037	0.216	-0.252	-0.118	0.114	0.096	0.098	0.123	-0.133	-0.127	0.129	-0.139	-0.128	-0.126	0.129	-0.139	-0.132	-0.128
13_{ax}	-0.276	-0.064	0.004	-0.159	-0.165	-0.059	-0.268	-0.129	0.091	0.102	0.086	0.092	0.094	0.086	0.089	0.093	0.104	0.086	0.103	0.091	-	-
13_{eq}	-0.278	-0.064	0.003	-0.161	-0.164	-0.059	-0.273	-0.129	0.103	0.088	0.089	0.095	0.092	0.090	0.091	0.089	0.104	0.089	0.103	0.092	-	-
14_{ax}	-0.283	-0.060	-0.163	0.009	-0.169	-0.060	-0.272	-0.129	0.088	0.102	0.086	0.092	0.090	0.094	0.102	0.091	0.102	0.093	0.095	0.093	-	-
14_{eq}	-0.280	-0.058	-0.164	0.007	-0.169	-0.058	-0.275	-0.130	0.087	0.102	0.087	0.089	0.090	0.096	0.105	0.087	0.105	0.087	0.095	0.097	-	-
15_{ax}	0.104	-0.165	-0.056	-0.276	0.038	-0.272	-0.270	-0.128	0.093	0.103	0.091	0.112	0.101	0.099	0.107	0.096	0.123	0.101	-	-	-	-
15_{eq}	0.102	-0.166	-0.056	-0.275	0.040	-0.267	-0.261	-0.127	0.105	0.095	0.089	0.096	0.100	0.105	0.109	0.090	0.125	0.095	-	-	-	-
16_{ax}	0.196	-0.262	-0.056	-0.167	-0.058	-0.269	-0.270	-0.128	0.092	0.104	0.093	0.128	0.107	0.097	0.096	0.095	0.106	0.094	-	-	-	-
16_{eq}	0.196	-0.264	-0.056	-0.168	-0.056	-0.264	-0.260	-0.128	0.103	0.095	0.095	0.116	0.109	0.091	0.096	0.097	0.109	0.091	-	-	-	-
17_{ax}	0.003	-0.058	-0.271	0.041	-0.271	-0.058	-0.281	-0.135	0.091	0.098	0.091	0.112	0.114	0.094	0.125	0.096	0.114	0.094	-	-	-	-
17_{eq}	0.000	-0.062	-0.273	0.040	-0.273	-0.056	-0.270	-0.126	0.105	0.091	0.090	0.102	0.107	0.095	0.125	0.098	0.112	0.097	-	-	-	-
18_{ax}	0.199	-0.258	0.046	-0.270	0.043	-0.267	-0.269	-0.125	0.094	0.107	0.095	0.133	0.130	0.108	0.128	0.105	-	-	-	-	-	-
18_{eq}	0.198	-0.260	0.045	-0.270	0.045	-0.260	-0.256	-0.126	0.105	0.098	0.098	0.120	0.131	0.101	0.131	0.101	-	-	-	-	-	-

Table S64. Atomic charges obtained from the MK analysis at the M06-2X/aug-cc-pVTZ level for molecules 1-18.

Atomic Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1_{ax}	-0.454	0.298	-0.341	0.217	-0.234	0.265	-0.292	-0.151	0.084	0.112	0.080	0.087	0.087	0.111	-0.015	-0.014	0.033	0.081	0.022	0.023	-	-
1_{eq}	-0.336	0.326	-0.286	0.093	-0.136	0.048	-0.372	0.040	0.077	0.039	0.018	0.068	0.082	0.119	0.011	0.002	0.038	0.070	0.075	0.027	-	-
2_{ax}	0.168	0.402	-0.099	-0.091	0.068	-0.317	-0.250	-0.240	0.129	0.102	0.112	0.065	-0.253	-0.251	0.069	0.065	0.036	0.051	0.022	0.002	0.106	0.101
2_{eq}	0.183	0.422	-0.222	-0.037	0.006	-0.222	-0.361	-0.066	0.093	0.092	0.047	0.074	-0.272	-0.211	0.105	0.075	0.037	0.042	0.029	0.013	0.084	0.088
3_{ax}	0.213	-0.370	0.652	-0.370	0.163	-0.338	-0.287	-0.117	0.058	0.106	0.082	0.064	0.125	0.116	-0.307	-0.245	0.113	0.118	0.020	0.007	0.095	0.104
3_{eq}	0.319	-0.585	0.666	-0.291	0.046	-0.357	-0.357	-0.068	0.105	0.056	0.048	0.081	0.194	0.182	-0.289	-0.275	0.102	0.104	0.046	0.027	0.108	0.138
4_{ax}	0.133	-0.096	-0.139	0.513	-0.124	-0.254	-0.264	-0.186	0.086	0.117	0.096	0.056	0.046	0.055	0.076	0.081	-0.296	-0.256	0.091	0.063	0.104	0.097
4_{eq}	0.259	-0.185	-0.294	0.526	-0.156	-0.192	-0.413	0.047	0.025	0.080	0.017	0.056	0.089	0.111	0.133	0.099	-0.285	-0.250	0.096	0.064	0.084	0.089
5_{ax}	0.231	0.424	-0.333	0.503	-0.098	-0.285	-0.259	-0.250	0.108	0.136	0.114	0.044	-0.236	-0.242	0.166	0.131	-0.271	-0.239	0.095	0.046	0.116	0.099
5_{eq}	0.121	0.417	-0.495	0.496	-0.139	-0.198	-0.343	-0.049	0.085	0.094	0.046	0.100	-0.238	-0.180	0.221	0.167	-0.254	-0.224	0.100	0.067	0.104	0.102
6_{ax}	0.090	0.429	-0.179	-0.022	-0.165	0.450	-0.266	-0.258	0.119	0.147	0.120	0.093	-0.242	-0.243	0.097	0.068	0.051	0.046	0.086	0.074	-0.246	-0.251
6_{eq}	0.081	0.373	-0.317	0.090	-0.270	0.444	-0.297	-0.053	0.064	0.105	0.059	0.081	-0.218	-0.191	0.133	0.104	0.036	0.034	0.115	0.090	-0.241	-0.221
7_{ax}	0.317	-0.483	0.717	-0.623	0.762	-0.594	-0.304	-0.080	0.043	0.107	0.077	0.071	0.153	0.146	-0.288	-0.239	0.208	0.196	-0.289	-0.261	0.189	0.177
7_{eq}	0.371	-0.589	0.603	-0.546	0.697	-0.615	-0.344	-0.097	0.116	0.061	0.070	0.090	0.199	0.210	-0.250	-0.241	0.208	0.185	-0.268	-0.260	0.204	0.197
8_{ax}	-0.088	0.489	-0.412	0.573	-0.442	0.471	-0.234	-0.226	0.117	0.143	0.116	0.148	-0.218	-0.225	0.184	0.155	-0.251	-0.228	0.199	0.156	-0.212	-0.217
8_{eq}	-0.051	0.438	-0.571	0.661	-0.508	0.556	-0.280	-0.026	0.057	0.104	0.054	0.115	-0.197	-0.178	0.229	0.184	-0.261	-0.234	0.203	0.161	-0.236	-0.220
9_{ax}	0.253	0.257	0.332	-0.464	0.493	-0.486	-0.306	-0.201	0.132	0.098	0.100	0.076	-0.198	-0.209	-0.258	0.053	0.150	0.172	-0.304	-0.005	0.164	0.149
9_{eq}	0.382	0.129	0.220	-0.412	0.466	-0.509	-0.355	-0.043	0.099	0.041	0.065	0.082	-0.174	-0.168	0.109	-0.242	0.157	0.123	0.021	-0.296	0.156	0.149
10_{ax}	0.249	-0.499	0.379	0.222	0.301	-0.450	-0.311	-0.133	0.118	0.072	0.083	0.088	0.171	0.165	-0.253	0.030	-0.209	-0.161	-0.243	0.072	0.154	0.155
10_{eq}	0.495	-0.500	0.193	0.250	0.312	-0.519	-0.393	-0.095	0.119	0.054	0.063	0.059	0.168	0.170	0.117	-0.233	-0.189	-0.218	0.084	-0.256	0.162	0.157
11_{ax}	0.209	0.247	0.133	0.268	0.317	-0.414	-0.323	-0.148	0.128	0.084	0.090	0.093	-0.170	-0.188	-0.179	0.101	-0.200	-0.155	-0.242	0.036	0.171	0.141
11_{eq}	0.281	0.215	-0.013	0.357	0.298	-0.504	-0.318	-0.116	0.117	0.062	0.093	0.105	-0.171	-0.161	0.187	-0.188	-0.195	-0.225	0.082	-0.256	0.186	0.162
12_{ax}	-0.119	0.288	0.077	0.271	0.117	0.365	-0.278	-0.143	0.134	0.095	0.103	0.194	-0.151	-0.165	-0.162	0.124	-0.177	-0.135	-0.175	0.099	-0.177	-0.185
12_{eq}	0.072	0.212	0.003	0.324	-0.028	0.245	-0.244	-0.108	0.124	0.079	0.077	0.144	-0.145	-0.150	0.189	-0.172	-0.157	-0.186	0.195	-0.171	-0.147	-0.155
13_{ax}	-0.303	-0.087	0.142	-0.192	0.042	0.006	-0.280	-0.097	0.086	0.090	0.057	0.049	0.065	0.072	0.009	0.042	0.067	0.057	0.098	0.078	-	-
13_{eq}	-0.402	-0.018	0.167	-0.141	-0.093	0.090	-0.397	-0.005	0.092	0.033	0.039	0.087	0.069	0.070	0.042	0.057	0.065	0.046	0.103	0.096	-	-
14_{ax}	-0.459	0.221	-0.325	0.258	-0.237	0.223	-0.293	-0.134	0.070	0.102	0.079	0.029	0.050	0.091	0.035	0.031	0.053	0.007	0.082	0.117	-	-
14_{eq}	-0.415	0.182	-0.301	0.341	-0.257	0.105	-0.416	0.013	0.036	0.085	0.027	0.038	0.062	0.130	0.074	0.030	0.058	0.012	0.080	0.117	-	-
15_{ax}	0.391	-0.277	0.279	-0.471	0.367	-0.450	-0.317	-0.126	0.076	0.111	0.074	0.053	0.061	0.112	0.040	-0.007	0.064	0.019	-	-	-	-
15_{eq}	0.411	-0.249	0.195	-0.390	0.155	-0.341	-0.392	0.028	0.089	0.037	0.023	0.040	0.061	0.126	0.052	0.009	0.118	0.027	-	-	-	-
16_{ax}	0.385	-0.450	0.280	-0.251	0.298	-0.444	-0.305	-0.095	0.065	0.108	0.064	0.127	0.037	0.001	0.040	0.104	0.018	0.019	-	-	-	-
16_{eq}	0.329	-0.323	0.110	-0.081	0.110	-0.323	-0.373	0.068	0.070	0.039	0.039	0.093	0.056	0.020	0.022	0.067	0.056	0.020	-	-	-	-
17_{ax}	0.220	-0.079	-0.331	0.158	-0.331	-0.079	-0.395	-0.037	0.084	0.074	0.084	0.042	0.134	0.075	0.107	0.067	0.134	0.075	-	-	-	-
17_{eq}	0.269	-0.018	-0.408	0.272	-0.385	-0.034	-0.443	0.040	0.090	0.026	0.020	0.076	0.104	0.088	0.090	0.033	0.106	0.077	-	-	-	-
18_{ax}	0.482	-0.442	0.362	-0.445	0.386	-0.429	-0.327	-0.086	0.061	0.115	0.059	0.099	0.088	-0.003	0.060	0.019	-	-	-	-	-	-
18_{eq}	0.392	-0.304	0.146	-0.335	0.146	-0.304	-0.395	0.101	0.060	0.040	0.040	0.078	0.122	0.046	0.122	0.046	-	-	-	-	-	-

Table S65. Atomic charges obtained from the Mülliken analysis at the M06-2X/aug-cc-pVTZ level for molecules 1-18.

Atomic Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1_{ax}	-0.622	0.178	-0.728	-0.364	-0.455	-0.491	-0.416	-1.038	0.399	0.305	0.283	0.844	0.304	0.197	0.311	0.198	0.354	0.118	0.363	0.257	-	-
1_{eq}	-0.628	0.492	-0.577	-0.321	-0.475	-0.504	-0.533	-1.032	0.302	0.370	0.312	0.482	0.366	0.168	0.263	0.161	0.325	0.148	0.429	0.249	-	-
2_{ax}	-0.048	0.958	-0.620	-0.441	-0.463	-0.724	-0.433	-1.039	0.277	0.332	0.395	0.858	-0.447	-0.482	0.406	0.159	0.323	0.079	0.383	0.090	0.282	0.156
2_{eq}	0.249	1.107	-0.726	-0.439	-0.474	-0.574	-0.543	-1.020	0.271	0.363	0.341	0.464	-0.437	-0.510	0.403	0.184	0.337	0.087	0.314	0.071	0.357	0.175
3_{ax}	0.188	-0.575	1.088	-0.704	-0.463	-0.659	-0.486	-1.002	0.333	0.293	0.352	0.570	0.165	0.356	-0.442	-0.456	0.396	0.143	0.370	0.087	0.288	0.157
3_{eq}	0.507	-0.813	0.993	-0.731	-0.497	-0.489	-0.600	-1.016	0.295	0.317	0.312	0.398	0.415	0.215	-0.426	-0.462	0.393	0.165	0.326	0.097	0.420	0.181
4_{ax}	0.191	-0.421	-0.678	1.000	-0.734	-0.702	-0.477	-0.969	0.334	0.299	0.328	0.624	0.150	0.326	0.425	0.167	-0.435	-0.474	0.446	0.156	0.282	0.163
4_{eq}	0.496	-0.474	-0.809	1.066	-0.747	-0.542	-0.601	-1.019	0.308	0.300	0.322	0.343	0.444	0.201	0.389	0.150	-0.431	-0.463	0.394	0.153	0.356	0.165
5_{ax}	-0.014	0.934	-0.767	0.983	-0.737	-0.703	-0.435	-1.039	0.339	0.286	0.394	0.826	-0.428	-0.473	0.414	0.238	-0.423	-0.458	0.420	0.169	0.288	0.187
5_{eq}	0.241	1.066	-0.864	1.032	-0.749	-0.527	-0.549	-1.028	0.358	0.274	0.350	0.451	-0.421	-0.501	0.394	0.261	-0.417	-0.456	0.363	0.164	0.354	0.206
6_{ax}	-0.071	0.801	-0.674	-0.427	-0.602	0.930	-0.460	-1.075	0.396	0.298	0.365	0.783	-0.433	-0.473	0.425	0.143	0.323	0.100	0.406	0.157	-0.434	-0.478
6_{eq}	0.218	1.028	-0.724	-0.421	-0.712	0.896	-0.578	-1.082	0.389	0.293	0.335	0.633	-0.431	-0.487	0.382	0.181	0.335	0.115	0.389	0.163	-0.454	-0.468
7_{ax}	0.261	-0.580	1.048	-0.839	0.967	-0.875	-0.550	-0.992	0.335	0.299	0.351	0.579	0.170	0.339	-0.429	-0.449	0.400	0.233	-0.417	-0.449	0.340	0.258
7_{eq}	0.526	-0.750	0.960	-0.867	0.956	-0.802	-0.596	-1.020	0.297	0.316	0.329	0.458	0.432	0.256	-0.424	-0.455	0.405	0.235	-0.413	-0.458	0.388	0.227
8_{ax}	-0.079	0.902	-0.745	0.944	-0.819	0.789	-0.472	-1.077	0.376	0.307	0.396	0.790	-0.417	-0.464	0.419	0.236	-0.415	-0.449	0.433	0.225	-0.419	-0.461
8_{eq}	0.161	1.006	-0.850	0.982	-0.844	0.892	-0.586	-1.064	0.390	0.297	0.336	0.638	-0.419	-0.477	0.391	0.257	-0.406	-0.449	0.389	0.249	-0.437	-0.457
9_{ax}	0.022	0.968	0.069	-0.634	0.155	-0.843	-0.456	-1.020	0.289	0.395	0.326	0.836	-0.441	-0.469	-0.492	0.379	0.341	0.189	-0.490	0.346	0.314	0.215
9_{eq}	0.248	0.996	-0.209	-0.570	0.006	-0.661	-0.578	-1.057	0.287	0.311	0.392	0.630	-0.413	-0.473	0.543	-0.521	0.314	0.202	0.492	-0.542	0.333	0.270
10_{ax}	0.167	-0.833	0.021	0.914	0.148	-0.563	-0.463	-0.970	0.297	0.327	0.345	0.657	0.293	0.238	-0.467	0.389	-0.443	-0.453	-0.482	0.366	0.177	0.333
10_{eq}	0.491	-0.507	-0.253	0.889	-0.216	-0.536	-0.606	-1.025	0.298	0.310	0.328	0.432	0.404	0.246	0.518	-0.519	-0.389	-0.426	0.524	-0.525	0.328	0.232
11_{ax}	-0.003	0.935	-0.015	0.901	0.011	-0.831	-0.452	-1.021	0.293	0.397	0.337	0.813	-0.436	-0.463	-0.462	0.423	-0.433	-0.448	-0.463	0.390	0.292	0.236
11_{eq}	0.224	1.011	-0.283	0.903	-0.214	-0.555	-0.578	-1.038	0.288	0.309	0.393	0.583	-0.403	-0.469	0.538	-0.507	-0.378	-0.420	0.512	-0.522	0.324	0.282
12_{ax}	-0.054	0.885	-0.009	0.871	-0.056	0.764	-0.486	-1.068	0.311	0.399	0.375	0.777	-0.420	-0.460	-0.455	0.422	-0.430	-0.441	-0.451	0.406	-0.424	-0.457
12_{eq}	0.142	0.921	-0.287	0.904	-0.277	0.989	-0.608	-1.097	0.332	0.375	0.350	0.687	-0.416	-0.439	0.541	-0.511	-0.371	-0.411	0.545	-0.511	-0.406	-0.452
13_{ax}	-0.664	-0.419	0.078	-0.521	-0.469	-0.447	-0.443	-0.974	0.316	0.297	0.341	0.541	0.267	0.218	0.377	0.140	0.407	0.175	0.439	0.343	-	-
13_{eq}	-0.696	-0.443	0.402	-0.482	-0.497	-0.438	-0.522	-1.034	0.283	0.344	0.330	0.409	0.321	0.176	0.368	0.122	0.428	0.183	0.436	0.309	-	-
14_{ax}	-0.673	-0.457	-0.690	0.176	-0.501	-0.335	-0.458	-0.946	0.334	0.287	0.341	0.603	0.215	0.269	0.423	0.250	0.411	0.234	0.327	0.190	-	-
14_{eq}	-0.641	-0.441	-0.585	0.469	-0.495	-0.518	-0.564	-1.017	0.297	0.301	0.325	0.411	0.450	0.268	0.367	0.202	0.397	0.200	0.367	0.209	-	-
15_{ax}	0.196	-0.659	-0.361	-0.584	-0.511	-0.577	-0.402	-1.007	0.395	0.297	0.294	0.789	0.291	0.245	0.391	0.286	0.558	0.360	-	-	-	-
15_{eq}	0.538	-0.581	-0.334	-0.597	-0.543	-0.584	-0.516	-1.011	0.297	0.376	0.317	0.490	0.307	0.270	0.382	0.242	0.608	0.339	-	-	-	-
16_{ax}	0.105	-0.642	-0.442	-0.450	-0.373	-0.568	-0.416	-1.002	0.394	0.309	0.322	0.939	0.377	0.289	0.285	0.231	0.342	0.300	-	-	-	-
16_{eq}	0.203	-0.516	-0.439	-0.428	-0.439	-0.516	-0.494	-0.942	0.272	0.363	0.364	0.686	0.405	0.289	0.313	0.186	0.405	0.289	-	-	-	-
17_{ax}	0.185	-0.547	-0.538	-0.479	-0.538	-0.547	-0.669	-0.771	0.290	0.285	0.290	0.656	0.452	0.307	0.538	0.326	0.452	0.307	-	-	-	-
17_{eq}	0.308	-0.363	-0.620	-0.533	-0.601	-0.453	-0.528	-0.980	0.296	0.329	0.337	0.537	0.388	0.340	0.585	0.311	0.397	0.251	-	-	-	-
18_{ax}	0.222	-0.639	-0.488	-0.536	-0.413	-0.536	-0.397	-0.964	0.392	0.299	0.313	0.899	0.558	0.384	0.544	0.362	-	-	-	-	-	-
18_{eq}	0.235	-0.500	-0.452	-0.564	-0.452	-0.500	-0.461	-0.942	0.267	0.380	0.380	0.717	0.583	0.364	0.583	0.364	-	-	-	-	-	-

Table S66. Cremer-Pople puckering coordinates parameters[a] for compounds 1-18. The meridian (φ) and azimuthal (θ) angles are given in degrees alongside the radius Q.

Compound	φ	θ	Q	Conformation
$\mathbf{1}_{ax}$	59.154	177.859	0.554	$^1C_4$
$\mathbf{1}_{eq}$	180.364	177.973	0.565	$^1C_4$
$\mathbf{2}_{ax}$	332.808	177.825	0.572	$^1C_4$
$\mathbf{2}_{eq}$	25.202	177.093	0.562	$^1C_4$
$\mathbf{3}_{ax}$	319.703	173.967	0.554	$^1C_4$
$\mathbf{3}_{eq}$	310.656	176.626	0.559	$^1C_4$
$\mathbf{4}_{ax}$	256.341	176.577	0.567	$^1C_4$
$\mathbf{4}_{eq}$	243.759	176.883	0.561	$^1C_4$
$\mathbf{5}_{ax}$	286.921	172.613	0.555	$^1C_4$
$\mathbf{5}_{eq}$	304.260	173.719	0.542	$^1C_4$
$\mathbf{6}_{ax}$	51.691	176.524	0.559	$^1C_4$
$\mathbf{6}_{eq}$	56.758	174.187	0.554	$^1C_4$
$\mathbf{7}_{ax}$	259.774	175.002	0.512	$^1C_4$
$\mathbf{7}_{eq}$	240.463	173.199	0.536	$^1C_4$
$\mathbf{8}_{ax}$	231.207	175.694	0.521	$^1C_4$
$\mathbf{8}_{eq}$	250.453	178.248	0.515	$^1C_4$
$\mathbf{9}_{ax}$	176.099	178.847	0.582	$^1C_4$
$\mathbf{9}_{eq}$	72.750	178.041	0.574	$^1C_4$
$\mathbf{10}_{ax}$	195.514	179.016	0.583	$^1C_4$
$\mathbf{10}_{eq}$	312.119	179.581	0.578	$^1C_4$
$\mathbf{11}_{ax}$	187.659	174.752	0.577	$^1C_4$
$\mathbf{11}_{eq}$	222.355	172.237	0.549	$^1C_4$
$\mathbf{12}_{ax}$	228.770	177.654	0.555	$^1C_4$
$\mathbf{12}_{eq}$	143.465	179.716	0.545	$^1C_4$
$\mathbf{13}_{ax}$	129.935	179.298	0.563	$^1C_4$
$\mathbf{13}_{eq}$	135.953	178.154	0.565	$^1C_4$
$\mathbf{14}_{ax}$	47.088	177.892	0.568	$^1C_4$
$\mathbf{14}_{eq}$	56.164	178.820	0.563	$^1C_4$
$\mathbf{15}_{ax}$	51.857	175.910	0.547	$^1C_4$
$\mathbf{15}_{eq}$	150.821	178.773	0.555	$^1C_4$
$\mathbf{16}_{ax}$	65.561	177.094	0.537	$^1C_4$
$\mathbf{16}_{eq}$	240.054	179.048	0.556	$^1C_4$
$\mathbf{17}_{ax}$	60.003	171.263	0.522	$^1C_4$
$\mathbf{17}_{eq}$	51.683	179.090	0.557	$^1C_4$
$\mathbf{18}_{ax}$	61.017	175.093	0.525	$^1C_4$
$\mathbf{18}_{eq}$	60.000	179.600	0.542	$^1C_4$

[a] Since the Cremer-Pople parameters are meant to describe only pyranose rings, all six-membered rings in this work were renumbered accordingly with the Figure below.

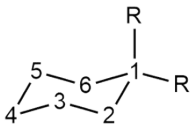

Table S67. Cartesian coordinates of the optimized geometries for the axial and equatorial geometries of compounds 1-18 obtained at the M06-2X/aug-cc-pVTZ level in the gas phase.

1_{ax} Energy (hartrees) = -386.281995221 No negative frequencies				1_{eq} Energy (hartrees) = -386.279773361 No negative frequencies			
O	-0.14983000	0.87073000	0.91441000	O	-0.16513000	-0.97637000	-0.31342000
C	-0.55466000	-0.45149000	0.65297000	C	-0.55511000	0.27338000	0.22226000
C	0.63122000	-1.38268000	0.46904000	C	0.42259000	1.36137000	-0.16974000
C	1.57502000	-0.84915000	-0.60557000	C	1.83186000	0.98411000	0.28195000
C	1.94813000	0.59564000	-0.28360000	C	2.18863000	-0.41016000	-0.22715000
C	0.68663000	1.42127000	-0.09643000	C	1.09866000	-1.39457000	0.16703000
O	-1.34377000	-0.53327000	-0.50262000	O	-1.80734000	0.59203000	-0.26765000
C	-2.52869000	0.22915000	-0.42518000	C	-2.82116000	-0.30821000	0.13167000
H	-2.31276000	1.29788000	-0.37292000	H	-3.76483000	0.10409000	-0.21497000
H	-3.10559000	0.01675000	-1.32142000	H	-2.66715000	-1.29427000	-0.30593000
H	-3.11361000	-0.05194000	0.45645000	H	-2.84682000	-0.40023000	1.22252000
H	-1.15423000	-0.72933000	1.52622000	H	-0.59494000	0.16819000	1.32296000
H	0.26111000	-2.37625000	0.21928000	H	0.09919000	2.30491000	0.26894000
H	1.15343000	-1.44455000	1.42574000	H	0.37897000	1.45893000	-1.25623000
H	2.46473000	-1.47517000	-0.67110000	H	2.55341000	1.72282000	-0.06561000
H	1.07498000	-0.88894000	-1.57517000	H	1.87495000	0.98848000	1.37540000
H	2.55454000	1.03266000	-1.07813000	H	3.14670000	-0.74222000	0.17530000
H	2.53344000	0.63108000	0.63864000	H	2.27048000	-0.39737000	-1.31613000
H	0.91320000	2.43396000	0.23095000	H	1.27437000	-2.38210000	-0.25497000
H	0.13366000	1.47764000	-1.04023000	H	1.06259000	-1.49211000	1.26123000

2_{ax} Energy (hartrees) = -548.886221437 No negative frequencies				2_{eq} Energy (hartrees) = -548.884058618 No negative frequencies			
C	-0.54007000	-0.38577000	0.63355000	C	0.44035000	0.64485000	-0.29449000
C	0.01381000	0.93229000	0.09807000	C	0.04510000	-0.79884000	0.01497000
C	0.96290000	0.76635000	-1.06067000	C	-1.33600000	-1.16560000	-0.47723000
C	2.10359000	-0.17925000	-0.68473000	C	-2.38541000	-0.19936000	0.06221000
C	1.55985000	-1.51366000	-0.17743000	C	-2.02146000	1.23647000	-0.30499000
C	0.61900000	-1.30252000	1.00788000	C	-0.63411000	1.59444000	0.21907000
O	-1.31105000	-1.02259000	-0.35909000	O	1.64923000	1.02646000	0.29799000
C	-2.69117000	-0.71696000	-0.33711000	C	2.82652000	0.46955000	-0.25250000
H	-3.16270000	-1.34271000	-1.09070000	H	3.64989000	1.10481000	0.06552000
H	-3.12167000	-0.95196000	0.64091000	H	2.99583000	-0.54741000	0.10036000
H	-2.87925000	0.33188000	-0.56731000	H	2.78080000	0.46070000	-1.34569000
H	-1.15465000	-0.15507000	1.51090000	H	0.51354000	0.71215000	-1.39019000
F	-1.01675000	1.75640000	-0.25915000	F	0.95439000	-1.65962000	-0.54367000
F	0.65024000	1.56737000	1.13285000	F	0.12045000	-1.00399000	1.36141000
H	1.32454000	1.75449000	-1.34445000	H	-1.52730000	-2.19568000	-0.17646000
H	0.38598000	0.35652000	-1.89051000	H	-1.31449000	-1.13380000	-1.56861000
H	2.74863000	-0.33174000	-1.54937000	H	-3.36564000	-0.46452000	-0.33256000
H	2.71307000	0.28669000	0.09292000	H	-2.43769000	-0.29609000	1.14872000
H	2.38109000	-2.16708000	0.11667000	H	-2.75787000	1.93062000	0.09925000
H	1.01578000	-2.01649000	-0.97931000	H	-2.04403000	1.34864000	-1.39326000
H	0.20467000	-2.24918000	1.35295000	H	-0.35002000	2.60729000	-0.06295000
H	1.16399000	-0.85154000	1.83944000	H	-0.62029000	1.54496000	1.31014000

3_{ax} Energy (hartrees) = -548.886899526 No negative frequencies				3_{eq} Energy (hartrees) = -548.888171180 No negative frequencies			
C	1.10890600	0.44603600	0.73836900	C	-1.02437000	-0.16888000	0.12649000
C	-0.03501000	-0.51245600	1.08866500	C	0.14142000	-0.98977000	-0.40647000
C	-1.13038000	-0.51051700	0.04646100	C	1.46490000	-0.38316000	-0.00843000
C	-1.62988400	0.86652000	-0.32039100	C	1.61288000	1.07131000	-0.38493000
C	-0.46749300	1.78495000	-0.69039700	C	0.43755000	1.87883000	0.16022000
C	0.56473000	1.83576700	0.43433300	C	-0.89670000	1.29183000	-0.29905000
O	1.84662000	0.05223700	-0.39921700	O	-2.19496000	-0.78463000	-0.36629000
C	2.46886000	-1.20513200	-0.29952100	C	-3.38406000	-0.33715000	0.23802000
H	2.98547100	-1.31520400	0.66090100	H	-4.18225000	-0.99319000	-0.10020000
H	3.20050400	-1.26479300	-1.10157400	H	-3.62973000	0.68905000	-0.04751000
H	1.75241900	-2.02148700	-0.41716000	H	-3.31503000	-0.39306000	1.32967000
H	1.78721800	0.48860300	1.60051000	H	-1.02525000	-0.21929000	1.22448000
H	0.31253300	-1.53581300	1.22727400	H	0.09313000	-2.01281000	-0.03615000
H	-0.47947700	-0.18708000	2.03042200	H	0.08747000	-1.01435000	-1.49612000
F	-2.17721600	-1.26825000	0.50213900	F	2.48322000	-1.10909000	-0.55636000
F	-0.68698700	-1.14913800	-1.08069400	F	1.61688000	-0.50421000	1.35198000
H	-2.34451600	0.75949400	-1.13605600	H	2.56742000	1.42759000	0.00123000
H	-2.16388000	1.25787800	0.54817800	H	1.64333000	1.12690000	-1.47455000
H	-0.84511700	2.78450100	-0.90215200	H	0.52351000	2.91601000	-0.16045000

H	0.01198200	1.41683900	-1.59762600	H	0.48014000	1.87874000	1.25153000
H	1.39839800	2.48168600	0.16112200	H	-1.71858000	1.87778000	0.11224000
H	0.11096200	2.24296900	1.34177700	H	-0.97523000	1.33524000	-1.38955000
4_{ax} Energy (hartrees) = -548.890030684 No negative frequencies				**4_{eq} Energy (hartrees) = -548.888314078 No negative frequencies**			
C	-1.26523000	0.53962000	0.57865000	C	-1.21754000	0.22801000	-0.27729000
C	-0.58093000	-0.69928000	1.15887000	C	-0.60783000	-1.08645000	0.20866000
C	0.45755000	-1.25358000	0.18654000	C	0.79784000	-1.27627000	-0.35681000
C	1.45240000	-0.17788000	-0.18083000	C	1.67064000	-0.08658000	-0.03340000
C	0.82182000	1.08346000	-0.71901000	C	1.08135000	1.23506000	-0.46587000
C	-0.23554000	1.61197000	0.24960000	C	-0.32683000	1.40303000	0.09641000
O	-1.95255000	0.25857000	-0.62926000	O	-2.48506000	0.48117000	0.28774000
C	-3.03702000	-0.62518000	-0.49190000	C	-3.49670000	-0.40437000	-0.12491000
H	-3.68393000	-0.32986000	0.34150000	H	-3.37483000	-1.40000000	0.30952000
H	-3.60840000	-0.58179000	-1.41598000	H	-4.44355000	0.00892000	0.21379000
H	-2.70897000	-1.65647000	-0.33185000	H	-3.51873000	-0.49624000	-1.21658000
H	-1.98399000	0.92975000	1.31017000	H	-1.31758000	0.18552000	-1.37415000
H	-1.31387000	-1.46627000	1.40714000	H	-1.22916000	-1.93196000	-0.08455000
H	-0.09588000	-0.41334000	2.09376000	H	-0.57350000	-1.06357000	1.30019000
H	1.00400000	-2.09349000	0.61414000	H	1.27557000	-2.16980000	0.04346000
H	-0.02218000	-1.58609000	-0.73476000	H	0.76587000	-1.37103000	-1.44401000
F	2.34876000	-0.66996000	-1.08653000	F	2.90098000	-0.25189000	-0.60422000
F	2.19348000	0.13544000	0.93480000	F	1.89279000	-0.05403000	1.31997000
H	1.61205000	1.81436000	-0.88740000	H	1.74529000	2.03145000	-0.13180000
H	0.36380000	0.84121000	-1.67738000	H	1.06688000	1.24436000	-1.55742000
H	-0.74115000	2.47207000	-0.18703000	H	-0.77656000	2.32520000	-0.26850000
H	0.24056000	1.93720000	1.17588000	H	-0.28865000	1.46653000	1.18559000
5_{ax} Energy (hartrees) = -747.405765518 No negative frequencies				**5_{eq} Energy (hartrees) = -747.402125365 No negative frequencies**			
C	-1.11286000	-0.28678000	0.67619000	C	-1.00417000	-0.64912000	-0.33420000
C	-0.52030000	0.96453000	0.03080000	C	-0.52255000	0.77059000	-0.02151000
C	0.61023000	0.67155000	-0.93058000	C	0.88459000	1.05705000	-0.50887000
C	1.65615000	-0.23081000	-0.30542000	C	1.86986000	-0.01747000	-0.09874000
C	1.08452000	-1.46062000	0.35911000	C	1.40162000	-1.41609000	-0.42243000
C	0.00076000	-1.06957000	1.36217000	C	0.01823000	-1.66050000	0.16831000
O	-1.69256000	-1.10569000	-0.31048000	O	-2.22209000	-0.96077000	0.27207000
C	-3.07399000	-0.89223000	-0.53477000	C	-3.36667000	-0.29344000	-0.22655000
H	-3.63837000	-1.03377000	0.39123000	H	-3.44355000	0.72020000	0.16561000
H	-3.39104000	-1.63589000	-1.26104000	H	-4.22781000	-0.87311000	0.09590000
H	-3.27080000	0.10548000	-0.92684000	H	-3.34858000	-0.25062000	-1.31940000
H	-1.86202000	0.04212000	1.40390000	H	-1.09139000	-0.70764000	-1.42987000
F	-1.49406000	1.65084000	-0.63457000	F	-1.35592000	1.68435000	-0.60954000
F	-0.09432000	1.79074000	1.02676000	F	-0.60970000	0.98938000	1.31404000
H	1.07034000	1.60512000	-1.25047000	H	1.20579000	2.02334000	-0.12254000
H	0.18908000	0.15625000	-1.79219000	H	0.86574000	1.10047000	-1.59748000
F	2.54590000	-0.59663000	-1.27266000	F	3.06187000	0.22848000	-0.71533000
F	2.37704000	0.48176000	0.61154000	F	2.11410000	0.07684000	1.23977000
H	1.90265000	-1.99247000	0.84237000	H	2.13426000	-2.11807000	-0.02709000
H	0.66552000	-2.09807000	-0.41881000	H	1.38742000	-1.51785000	-1.50921000
H	-0.43163000	-1.96060000	1.81310000	H	-0.33772000	-2.65663000	-0.08548000
H	0.42867000	-0.45959000	2.15793000	H	0.05403000	-1.59157000	1.25634000
6_{ax} Energy (hartrees) = -747.401653181 No negative frequencies				**6_{eq} Energy (hartrees) = -747.396931135 No negative frequencies**			
C	-0.43292000	0.46857000	-0.35764000	C	0.53677000	-0.24959000	-0.32391000
C	1.05906000	0.77370000	-0.21699000	C	0.24123000	1.21340000	0.01734000
C	1.67145000	0.18027000	1.02719000	C	-1.05213000	1.72435000	-0.57385000
C	1.42528000	-1.32831000	1.06864000	C	-2.21606000	0.82876000	-0.15810000
C	-0.06877000	-1.64452000	0.99918000	C	-1.96565000	-0.61099000	-0.59788000
C	-0.68044000	-1.03770000	-0.23946000	C	-0.67186000	-1.13262000	-0.01361000
O	-1.09345000	1.11713000	0.69209000	O	1.64601000	-0.73041000	0.35960000
C	-2.28883000	1.77669000	0.31537000	C	2.85578000	-0.70339000	-0.37463000
H	-3.01501000	1.07191000	-0.09244000	H	3.14074000	0.31646000	-0.63652000
H	-2.69181000	2.23198000	1.21559000	H	3.61711000	-1.13813000	0.26660000
H	-2.07836000	2.55682000	-0.42018000	H	2.76627000	-1.30504000	-1.28362000
H	-0.76885000	0.81215000	-1.34076000	H	0.67993000	-0.29667000	-1.41086000
F	1.22345000	2.12224000	-0.23664000	F	1.28660000	1.97234000	-0.43152000
F	1.70288000	0.29842000	-1.32120000	F	0.21618000	1.36957000	1.36482000
H	2.73457000	0.41737000	1.02294000	H	-1.18492000	2.75130000	-0.23538000
H	1.20820000	0.67293000	1.88267000	H	-0.94379000	1.73743000	-1.66021000
H	1.84372000	-1.74250000	1.98377000	H	-3.14186000	1.19515000	-0.59724000
H	1.93861000	-1.80459000	0.23262000	H	-2.33278000	0.86389000	0.92557000
H	-0.25493000	-2.71743000	0.97254000	H	-2.76173000	-1.28063000	-0.27466000
H	-0.59196000	-1.22187000	1.85728000	H	-1.89172000	-0.67458000	-1.68529000
F	-2.02838000	-1.24663000	-0.24933000	F	-0.41823000	-2.37916000	-0.50140000

F	-0.19636000	-1.65693000	-1.35154000	F	-0.80497000	-1.26780000	1.33062000
7_{ax}				**7_{eq}**			
Energy (hartrees) = -747.401507709				**Energy (hartrees) = -747.405540657**			
No negative frequencies				**No negative frequencies**			
C	-0.84426000	-0.86866000	-0.92551000	C	-1.18622000	-0.40896000	0.07553000
C	-0.97690000	0.65344000	-1.05036000	C	-0.83954000	0.98058000	-0.46354000
C	-0.15681000	1.39204000	-0.01795000	C	0.56874000	1.37254000	-0.08018000
C	1.29779000	0.97265000	0.01981000	C	1.62358000	0.35593000	-0.46587000
C	1.46395000	-0.53405000	0.06486000	C	1.23134000	-1.04341000	-0.03612000
C	0.62215000	-1.28461000	-0.94772000	C	-0.17634000	-1.43469000	-0.41812000
O	-1.40239000	-1.39455000	0.25251000	O	-2.44893000	-0.84246000	-0.36986000
C	-2.78089000	-1.16006000	0.41334000	C	-3.53581000	-0.18859000	0.24472000
H	-3.32886000	-1.37677000	-0.51089000	H	-4.43815000	-0.70510000	-0.07136000
H	-3.12730000	-1.83031000	1.19550000	H	-3.45673000	-0.23858000	1.33509000
H	-2.98236000	-0.13084000	0.71906000	H	-3.60737000	0.85940000	-0.05768000
H	-1.34881000	-1.31631000	-1.79149000	H	-1.16980000	-0.38236000	1.17204000
H	-2.01303000	0.97770000	-0.96565000	H	-1.51043000	1.74592000	-0.07581000
H	-0.61721000	0.95578000	-2.03502000	H	-0.91495000	0.96887000	-1.55245000
F	-0.20878000	2.73301000	-0.28329000	F	0.88423000	2.56733000	-0.65750000
F	-0.71904000	1.23938000	1.21252000	F	0.61663000	1.58513000	1.26800000
H	1.78872000	1.42012000	0.88245000	H	2.57720000	0.62622000	-0.01560000
H	1.77346000	1.33793000	-0.88989000	H	1.72348000	0.36376000	-1.55064000
F	2.78253000	-0.81979000	-0.16967000	F	2.11512000	-1.92828000	-0.57896000
F	1.20870000	-0.98290000	1.31968000	F	1.37325000	-1.15542000	1.31752000
H	0.71041000	-2.35023000	-0.74276000	H	-0.39220000	-2.41594000	0.00097000
H	1.04333000	-1.08247000	-1.93333000	H	-0.23713000	-1.50165000	-1.50568000
8_{ax}				**8_{eq}**			
Energy (hartrees) = -945.913946792				**Energy (hartrees) = -945.907880029**			
No negative frequencies				**No negative frequencies**			
C	-1.12065000	0.13512000	0.28297000	C	-1.02604000	0.11228000	-0.34654000
C	-0.36563000	-1.18762000	0.43702000	C	-0.33436000	-1.20068000	0.03386000
C	0.76597000	-1.33985000	-0.55686000	C	1.06574000	-1.33450000	-0.53016000
C	1.69077000	-0.13711000	-0.55478000	C	1.92231000	-0.12420000	-0.21463000
C	0.97829000	1.19808000	-0.66173000	C	1.26813000	1.19665000	-0.56719000
C	-0.14717000	1.31284000	0.34311000	C	-0.13776000	1.31119000	-0.00970000
O	-1.72670000	0.15920000	-0.97680000	O	-2.24614000	0.25813000	0.29425000
C	-3.12982000	-0.04705000	-0.96049000	C	-3.37455000	-0.13255000	-0.46920000
H	-3.62311000	0.74256000	-0.38933000	H	-3.34552000	-1.19640000	-0.70693000
H	-3.46288000	-0.00588000	-1.99333000	H	-4.24704000	0.07857000	0.14177000
H	-3.37678000	-1.02106000	-0.53585000	H	-3.43223000	0.45077000	-1.39219000
H	-1.83798000	0.23444000	1.10266000	H	-1.13739000	0.10723000	-1.43866000
F	-1.25317000	-2.20417000	0.25457000	F	-1.09329000	-2.23137000	-0.44214000
F	0.09113000	-1.30212000	1.70674000	F	-0.31056000	-1.33389000	1.37641000
H	1.33698000	-2.23700000	-0.32461000	H	1.53306000	-2.22889000	-0.12132000
H	0.32658000	-1.43062000	-1.54869000	H	0.99631000	-1.43261000	-1.61315000
F	2.54943000	-0.25348000	-1.60674000	F	3.08977000	-0.22782000	-0.91090000
F	2.46191000	-0.15573000	0.56391000	F	2.26170000	-0.13288000	1.09826000
H	1.69241000	2.00428000	-0.50393000	H	1.87167000	2.01641000	-0.18102000
H	0.54561000	1.27913000	-1.65759000	H	1.21696000	1.27427000	-1.65281000
F	-0.84249000	2.45489000	0.11196000	F	-0.71869000	2.42398000	-0.53466000
F	0.34676000	1.41107000	1.60174000	F	-0.09421000	1.49047000	1.32766000
9_{ax}				**9_{eq}**			
Energy (hartrees) = -747.386006321				**Energy (hartrees) = -747.384742425**			
No negative frequencies				**No negative frequencies**			
C	0.63827	-0.84488	0.57410	C	0.68641600	-0.61936000	-0.07082600
C	0.69806	0.67253	0.39585	C	0.42351300	0.84455900	0.25979800
C	-0.21334	1.15183	-0.72181	C	-0.99649700	1.27917300	-0.07668500
C	-1.64114	0.70577	-0.47373	C	-2.01691600	0.38774000	0.60613000
C	-1.69952	-0.80283	-0.30195	C	-1.74656100	-1.09528000	0.40209800
C	-0.80184	-1.26977	0.83005	C	-0.30962000	-1.48261800	0.69375700
O	1.08980	-1.48207	-0.59703	O	1.97887300	-1.00813500	0.29972200
C	2.47287	-1.78897	-0.62276	C	2.96893400	-0.84125900	-0.69834400
H	2.64988	-2.35266	-1.53462	H	3.88079600	-1.28534200	-0.30815100
H	3.08689	-0.88870	-0.62601	H	2.68098100	-1.36207100	-1.61611100
H	2.74164	-2.40717	0.23813	H	3.14549500	0.21056900	-0.92230100
H	1.27393	-1.09655	1.42951	H	0.53072700	-0.73410500	-1.14943500
F	1.97350	1.06667	0.14603	F	1.30462500	1.65025400	-0.38503000
F	0.33535	1.26011	1.56803	F	0.60487300	1.06230700	1.59305200
F	-0.15372	2.52475	-0.78496	H	-1.11176600	2.32374600	0.21782100
H	0.17801	0.75088	-1.65853	F	-1.13720600	1.20702200	-1.44772800
H	-2.27066	1.01946	-1.30459	H	-3.01110200	0.63616700	0.23652000
H	-2.00665	1.18433	0.43674	H	-1.99129400	0.59964900	1.67625100
F	-3.00682	-1.16320	-0.01080	H	-2.42745700	-1.68077600	1.02092900
H	-1.42764	-1.30782	-1.23052	F	-2.03016700	-1.42839900	-0.91989100
H	-0.84381	-2.35376	0.91969	H	-0.15065800	-2.52560400	0.42586800
H	-1.15501	-0.82841	1.76315	H	-0.11144800	-1.37553100	1.76163700

10_{ax} **Energy (hartrees) = -747.383058347** **No negative frequencies**				**10_{eq}** **Energy (hartrees) = -747.382105269** **No negative frequencies**			
C	-1.48091	-0.45786	0.71008	C	-1.35306900	0.23283500	-0.07343300
C	-0.37312	-1.50275	0.73489	C	-0.78658500	-1.06032600	0.51766400
C	0.66130	-1.21122	-0.33581	C	0.64489400	-1.28955300	0.07446200
C	1.22688	0.19215	-0.17334	C	1.51093100	-0.07053600	0.36825700
C	0.12058	1.23709	-0.19283	C	0.94003900	1.25673500	-0.11578000
C	-0.90229	0.94758	0.88773	C	-0.49669800	1.42457400	0.33238000
O	-2.14323	-0.60650	-0.53346	O	-2.65606500	0.49447500	0.39600000
C	-3.33251	0.13860	-0.65576	C	-3.65138100	-0.32463500	-0.17178900
H	-3.84128	-0.21364	-1.54915	H	-4.61115800	0.05876500	0.16458200
H	-3.98231	-0.01711	0.21142	H	-3.61308100	-0.28696800	-1.26493900
H	-3.13701	1.20907	-0.76264	H	-3.55901200	-1.36574900	0.14893000
H	-2.18964	-0.65792	1.52115	H	-1.36452900	0.15235100	-1.16696900
H	-0.79299	-2.49236	0.56507	H	-1.37454000	-1.92512600	0.21275700
H	0.12226	-1.49558	1.70655	H	-0.82000500	-0.99428500	1.60701700
F	1.69864	-2.10997	-0.24316	H	1.09908000	-2.14731600	0.57338900
H	0.23032	-1.29126	-1.33478	F	0.67500100	-1.52251500	-1.28494700
F	2.12273	0.44838	-1.15467	F	2.75149900	-0.25235000	-0.12653300
F	1.89977	0.27421	1.00418	F	1.62589900	0.01620500	1.72675100
F	0.68377	2.47581	0.00782	H	1.58430600	2.05358100	0.25920100
H	-0.33378	1.22928	-1.18576	F	1.00150400	1.27184500	-1.49394400
H	-1.68159	1.70745	0.85876	H	-0.90127500	2.33686600	-0.10309600
H	-0.41193	1.01665	1.85980	H	-0.52518400	1.52885200	1.41862800
11_{ax} **Energy (hartrees) = -945.888945531** **No negative frequencies**				**11_{eq}** **Energy (hartrees) = -945.888288243** **No negative frequencies**			
C	1.26564	-0.67453	0.56400	C	-1.14164	0.60920	-0.03515
C	0.88428	0.79659	0.39895	C	-0.70798	-0.84898	0.10320
C	-0.22891	0.99033	-0.62486	C	0.72079	-1.09151	-0.38461
C	-1.43674	0.10955	-0.31367	C	1.70172	-0.11180	0.25957
C	-1.03336	-1.34793	-0.12943	C	1.25416	1.34629	0.22481
C	0.02888	-1.47780	0.94641	C	-0.16471	1.49477	0.73306
O	1.76507	-1.17663	-0.65096	O	-2.41683	0.82066	0.49299
C	3.17420	-1.10827	-0.80030	C	-3.49555	0.58365	-0.39534
H	3.41104	-1.59972	-1.73963	H	-4.38831	0.95796	0.09794
H	3.52649	-0.07766	-0.82861	H	-3.34810	1.12758	-1.33246
H	3.66825	-1.63941	0.01730	H	-3.61782	-0.47723	-0.61027
H	2.01851	-0.72564	1.35672	H	-1.10743	0.85101	-1.10390
F	1.96154	1.52065	0.00198	F	-1.53285	-1.66320	-0.60096
F	0.50560	1.28887	1.60099	F	-0.78461	-1.23785	1.39794
F	-0.61233	2.29708	-0.64780	H	1.02157	-2.11462	-0.15233
H	0.16105	0.70961	-1.60488	F	0.74192	-0.90071	-1.73888
F	-2.32544	0.21898	-1.32836	F	2.90415	-0.24487	-0.33175
F	-2.05360	0.55585	0.80199	F	1.84583	-0.45932	1.56389
F	-2.15115	-2.06051	0.22667	H	1.96445	1.92396	0.81773
H	-0.67470	-1.72793	-1.08725	F	1.32446	1.78472	-1.08049
H	0.30002	-2.52548	1.05643	H	-0.47453	2.53226	0.62682
H	-0.37682	-1.11669	1.89168	H	-0.20610	1.23497	1.79147
12_{ax} **Energy (hartrees) = -1144.387614753** **No negative frequencies**				**12_{eq}** **Energy (hartrees) = -1144.386858533** **No negative frequencies**			
C	-1.32819	0.23831	0.28536	C	1.14046300	0.08097400	-0.22797200
C	-0.68160	-1.13899	0.45642	C	0.33492300	1.30374600	0.20879000
C	0.46772	-1.34584	-0.52578	C	-1.13061100	1.23740900	-0.22711100
C	1.49896	-0.22043	-0.43661	C	-1.78496000	-0.07930400	0.19750500
C	0.86057	1.16245	-0.57371	C	-0.98592500	-1.33002400	-0.17657700
C	-0.28502	1.34994	0.41539	C	0.47471600	-1.20716900	0.25967900
O	-1.86759	0.32113	-1.00114	O	2.43366000	0.18229400	0.25994800
C	-3.28472	0.22856	-1.05872	C	3.44897500	-0.06881600	-0.69954000
H	-3.55844	0.31197	-2.10595	H	4.39662600	0.04900700	-0.18304600
H	-3.62755	-0.72895	-0.66528	H	3.37267500	-1.08329000	-1.09395100
H	-3.73863	1.04775	-0.49770	H	3.38895000	0.65308900	-1.51727800
H	-2.07245	0.37579	1.07529	H	1.10285500	0.06153900	-1.32332200
F	-1.62260	-2.08656	0.22413	F	0.88915000	2.40514600	-0.34175700
F	-0.25620	-1.30362	1.72223	F	0.37496400	1.45640600	1.54712700
F	1.07933	-2.53371	-0.27455	H	-1.68089500	2.07174600	0.21045100
H	0.05101	-1.35607	-1.53455	F	-1.16867800	1.31789100	-1.59110300
F	2.39402	-0.38046	-1.43868	F	-3.00516700	-0.15921700	-0.36427400
F	2.17670	-0.30533	0.72072	F	-1.94469300	-0.06217200	1.53782600
F	1.80876	2.11444	-0.36709	H	-1.43967800	-2.20328800	0.29463300
H	0.45542	1.26263	-1.58255	F	-1.00945800	-1.46875800	-1.53621800
F	-0.88325	2.53685	0.17478	F	1.15882200	-2.26233500	-0.24061300
F	0.18602	1.38881	1.67686	F	0.52780500	-1.29674500	1.60282200
13_{ax}				**13_{eq}**			

Energy (hartrees) = -386.267785525 No negative frequencies				Energy (hartrees) = -386.268344800 No negative frequencies			
O	-0.76484	-1.39214	-0.25026	O	1.26300	-1.34633	0.25529
C	0.04510	-1.01561	0.83718	C	-0.03194	-1.10856	-0.25061
C	0.57034	0.41127	0.70078	C	-0.57208	0.23981	0.22564
C	-0.60365	1.36756	0.54508	C	0.38443	1.34449	-0.18518
C	-1.50763	0.89625	-0.59249	C	1.79874	1.01678	0.28680
C	-1.90118	-0.55662	-0.37646	C	2.19267	-0.37407	-0.18308
O	1.39231	0.59676	-0.43306	O	-1.83312	0.52480	-0.33884
C	2.52375	-0.23516	-0.48695	C	-2.89127	-0.24108	0.18628
H	2.26228	-1.25852	-0.76812	H	-3.81548	0.17383	-0.20854
H	3.18912	0.17559	-1.24270	H	-2.82693	-1.29203	-0.10785
H	3.04902	-0.25362	0.47515	H	-2.91280	-0.18283	1.27963
H	1.14555	0.64785	1.60736	H	-0.65281	0.21206	1.32157
H	-0.22634	2.37263	0.35963	H	0.03680	2.29772	0.21245
H	-1.16436	1.38770	1.48322	H	0.36062	1.41717	-1.27637
H	-2.40525	1.51295	-0.65394	H	2.51156	1.75071	-0.09105
H	-0.97380	0.98151	-1.53905	H	1.84461	1.04373	1.37774
H	-2.47358	-0.94489	-1.21666	H	3.15919	-0.67361	0.21770
H	-2.51642	-0.64753	0.53054	H	2.25126	-0.39508	-1.28001
H	0.85652	-1.73938	0.89183	H	-0.65301	-1.93365	0.09367
H	-0.52291	-1.07739	1.77649	H	-0.02535	-1.10990	-1.34971
14_{ax} **Energy (hartrees) = -386.269467041** **No negative frequencies**				**14_{eq}** **Energy (hartrees) = -386.269860918** **No negative frequencies**			
O	-1.98999	0.42927	-0.31220	O	2.21130	0.26379	-0.26295
C	-1.52129	-0.88443	-0.55429	C	1.79774	-0.98281	0.25752
C	-0.58112	-1.34823	0.54988	C	0.38303	-1.32927	-0.18240
C	0.58317	-0.37827	0.69646	C	-0.58051	-0.23139	0.23026
C	0.04019	1.04262	0.85584	C	-0.06643	1.11371	-0.27400
C	-0.92962	1.36312	-0.27229	C	1.37634	1.31413	0.17283
O	1.37898	-0.52434	-0.46869	O	-1.85273	-0.56995	-0.27930
C	2.58994	0.18770	-0.44234	C	-2.89248	0.26792	0.16012
H	3.12306	0.02495	0.50103	H	-2.83014	1.26624	-0.28142
H	3.20119	-0.18329	-1.26179	H	-3.82875	-0.19115	-0.14789
H	2.44013	1.26258	-0.57816	H	-2.88611	0.36541	1.25172
H	1.19109	-0.64375	1.57049	H	-0.63583	-0.19538	1.33022
H	0.84921	1.77364	0.88255	H	-0.67488	1.93779	0.10165
H	-0.48699	1.10577	1.80979	H	-0.11743	1.11937	-1.36527
H	-1.38382	2.34236	-0.13279	H	1.78964	2.23197	-0.24035
H	-0.39898	1.36008	-1.23276	H	1.41925	1.38496	1.26906
H	-2.40264	-1.52056	-0.60884	H	2.51171	-1.72141	-0.10075
H	-1.00483	-0.91977	-1.51998	H	1.85525	-0.95697	1.35476
H	-0.19851	-2.34405	0.32491	H	0.07033	-2.28034	0.24972
H	-1.12844	-1.39250	1.49303	H	0.35228	-1.42495	-1.26948
15_{ax} **Energy (hartrees) = -422.194354330** **No negative frequencies**				**15_{eq}** **Energy (hartrees) = -422.192347961** **No negative frequencies**			
C	-0.53604	-0.43493	0.65202	C	-0.54288	0.27613	0.23445
C	0.65793	-1.35433	0.45351	C	0.45685	1.34205	-0.15986
C	1.58443	-0.75652	-0.59420	C	1.84963	0.87915	0.24642
O	1.91497	0.57662	-0.23393	O	2.11329	-0.41060	-0.27735
C	0.76482	1.35703	-0.13126	C	1.14510	-1.32590	0.13745
O	-0.10725	0.89255	0.87272	O	-0.13803	-0.97571	-0.29973
O	-1.34797	-0.53689	-0.48246	O	-1.78582	0.59810	-0.26498
C	-2.54144	0.21337	-0.38975	C	-2.80711	-0.29940	0.12695
H	-2.33639	1.28435	-0.35103	H	-3.74442	0.11146	-0.23709
H	-3.13089	-0.01401	-1.27371	H	-2.64658	-1.28788	-0.30248
H	-3.10617	-0.06852	0.50434	H	-2.84814	-0.38280	1.21771
H	-1.11176	-0.69208	1.54602	H	-0.58791	0.16895	1.33389
H	0.31060	-2.34138	0.15199	H	0.20317	2.28635	0.32101
H	1.18873	-1.43669	1.40156	H	0.40161	1.46705	-1.24101
H	2.52056	-1.30549	-0.66016	H	2.62121	1.54058	-0.13914
H	1.10152	-0.76172	-1.57723	H	1.93576	0.85014	1.34088
H	1.06877	2.35745	0.16047	H	1.38787	-2.28596	-0.30682
H	0.23888	1.37205	-1.09468	H	1.15238	-1.39431	1.23713
16_{ax} **Energy (hartrees) = -422.197809147** **No negative frequencies**				**16_{eq}** **Energy (hartrees) = -422.196374757** **No negative frequencies**			
C	-0.51025	-0.41985	0.66532	C	0.50914	-0.00006	-0.63479
O	0.55218	-1.29060	0.54291	O	0.01154	1.15301	-0.01447
C	1.45249	-0.94144	-0.50630	C	-1.40245	1.22926	-0.08596
C	1.94667	0.48173	-0.30795	C	-2.02629	0.00007	0.55371
C	0.73984	1.39297	-0.15892	C	-1.40258	-1.22918	-0.08595
O	-0.11215	0.90269	0.87209	O	0.01142	-1.15308	-0.01444
O	-1.30026	-0.53805	-0.48095	O	1.86931	-0.00013	-0.58247

C	-2.48869	0.22239	-0.41849	C	2.42491	0.00008	0.72775
H	-2.27889	1.29333	-0.43403	H	3.50232	-0.00061	0.59289
H	-3.08368	-0.04745	-1.28647	H	2.12309	0.89196	1.27503
H	-3.05200	-0.01065	0.49027	H	2.12206	-0.89101	1.27575
H	-1.07214	-0.70698	1.55607	H	0.21976	-0.00007	-1.69515
H	2.26167	-1.66525	-0.45253	H	-1.68893	2.14902	0.41804
H	0.94847	-1.04683	-1.47000	H	-1.70992	1.30300	-1.13763
H	2.55889	0.79429	-1.15442	H	-3.10717	0.00013	0.40947
H	2.55251	0.53371	0.59747	H	-1.81653	0.00007	1.62363
H	1.02105	2.39967	0.14040	H	-1.68916	-2.14891	0.41807
H	0.18546	1.44900	-1.10109	H	-1.71005	-1.30290	-1.13762
17_{ax} **Energy (hartrees) = -422.177452706** **No negative frequencies**				**17_{eq}** **Energy (hartrees) = -422.179981816** **No negative frequencies**			
C	-0.61315	0.00036	0.96390	C	0.55613	-0.20686	-0.25759
C	0.23545	-1.24623	0.71506	C	-0.00560	1.12860	0.22860
O	1.00135	-1.15775	-0.47512	O	-1.33097	1.29073	-0.23893
C	1.78225	-0.00024	-0.48864	C	-2.14793	0.23468	0.17674
O	1.00153	1.15740	-0.47578	O	-1.71693	-0.99686	-0.32192
C	0.23567	1.24668	0.71437	C	-0.41623	-1.30745	0.13846
O	-1.84173	0.00032	0.27399	O	1.79233	-0.51565	0.33629
C	-1.78212	-0.00043	-1.14118	C	2.87204	0.24687	-0.15244
H	-1.27154	-0.88672	-1.52207	H	3.77847	-0.16125	0.28709
H	-2.81318	-0.00045	-1.48621	H	2.93869	0.17587	-1.24265
H	-1.27126	0.88530	-1.52299	H	2.78937	1.30009	0.12851
H	-0.90015	0.00069	2.01738	H	0.64547	-0.18142	-1.35053
H	-0.40459	-2.12127	0.62017	H	0.56516	1.97700	-0.14282
H	0.90990	-1.39143	1.56896	H	0.01937	1.13731	1.32689
H	2.35198	-0.00056	-1.41277	H	-3.14103	0.41771	-0.22149
H	2.45512	-0.00005	0.38451	H	-2.16466	0.19842	1.27738
H	-0.40426	2.12175	0.61902	H	-0.12776	-2.25937	-0.30036
H	0.91016	1.39223	1.56818	H	-0.40902	-1.40512	1.23188
18_{ax} **Energy (hartrees) = -458.114643421** **No negative frequencies**				**18_{eq}** **Energy (hartrees) = -458.114594065** **No negative frequencies**			
C	-0.49558	-0.39433	0.65612	C	0.49274	-0.00000	0.65232
O	0.57330	-1.26373	0.52008	O	-0.02253	-1.14726	0.02309
C	1.46721	-0.85808	-0.49214	C	-1.42515	-1.14250	0.03283
O	1.92329	0.44483	-0.25456	O	-1.92918	0.00000	-0.59916
C	0.83186	1.31830	-0.19702	C	-1.42515	1.14250	0.03283
O	-0.06472	0.93033	0.81849	O	-0.02253	1.14725	0.02309
O	-1.31075	-0.53165	-0.46365	O	1.84618	-0.00000	0.59330
C	-2.51276	0.20855	-0.37413	C	2.39962	0.00000	-0.72094
H	-2.32097	1.28229	-0.39166	H	3.47666	-0.00001	-0.58627
H	-3.11917	-0.07042	-1.23073	H	2.09454	-0.89125	-1.26641
H	-3.05170	-0.03920	0.54505	H	2.09456	0.89127	-1.26639
H	-1.03031	-0.65665	1.56984	H	0.20286	-0.00000	1.71134
H	2.32030	-1.52564	-0.44543	H	-1.76289	-2.01189	-0.52051
H	0.97115	-0.91148	-1.46694	H	-1.78536	-1.17614	1.07198
H	1.20236	2.30351	0.06441	H	-1.76289	2.01189	-0.52050
H	0.31510	1.33274	-1.16445	H	-1.78535	1.17614	1.07199

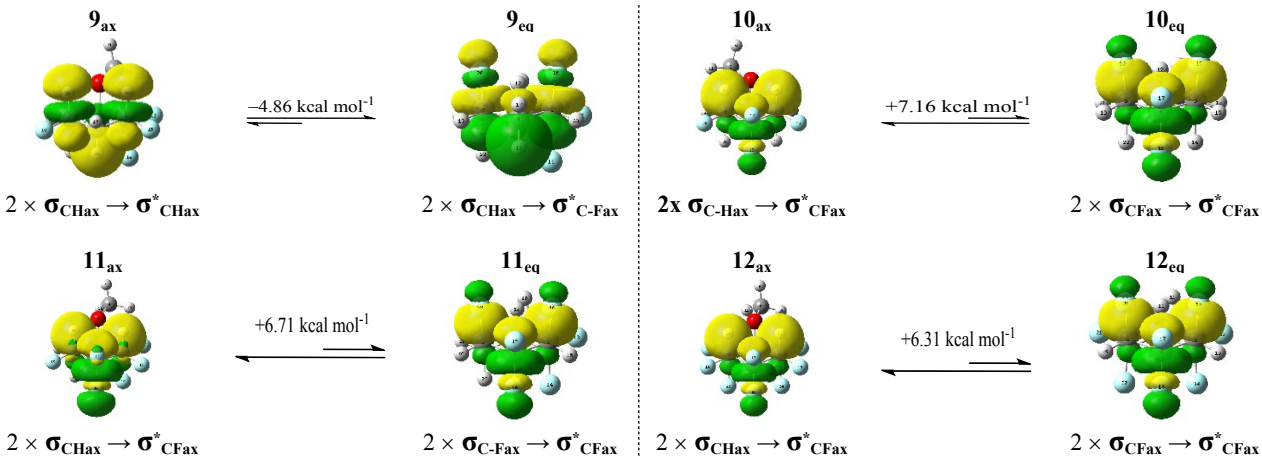

Figure S6. Calculated energies obtained at the M06-2X/aug-cc-pVTZ theory level in kcal mol^{-1} of selected hyperconjugative interactions to illustrate the trends observed in ΔE(NL) for cyclohexanes 9-12.

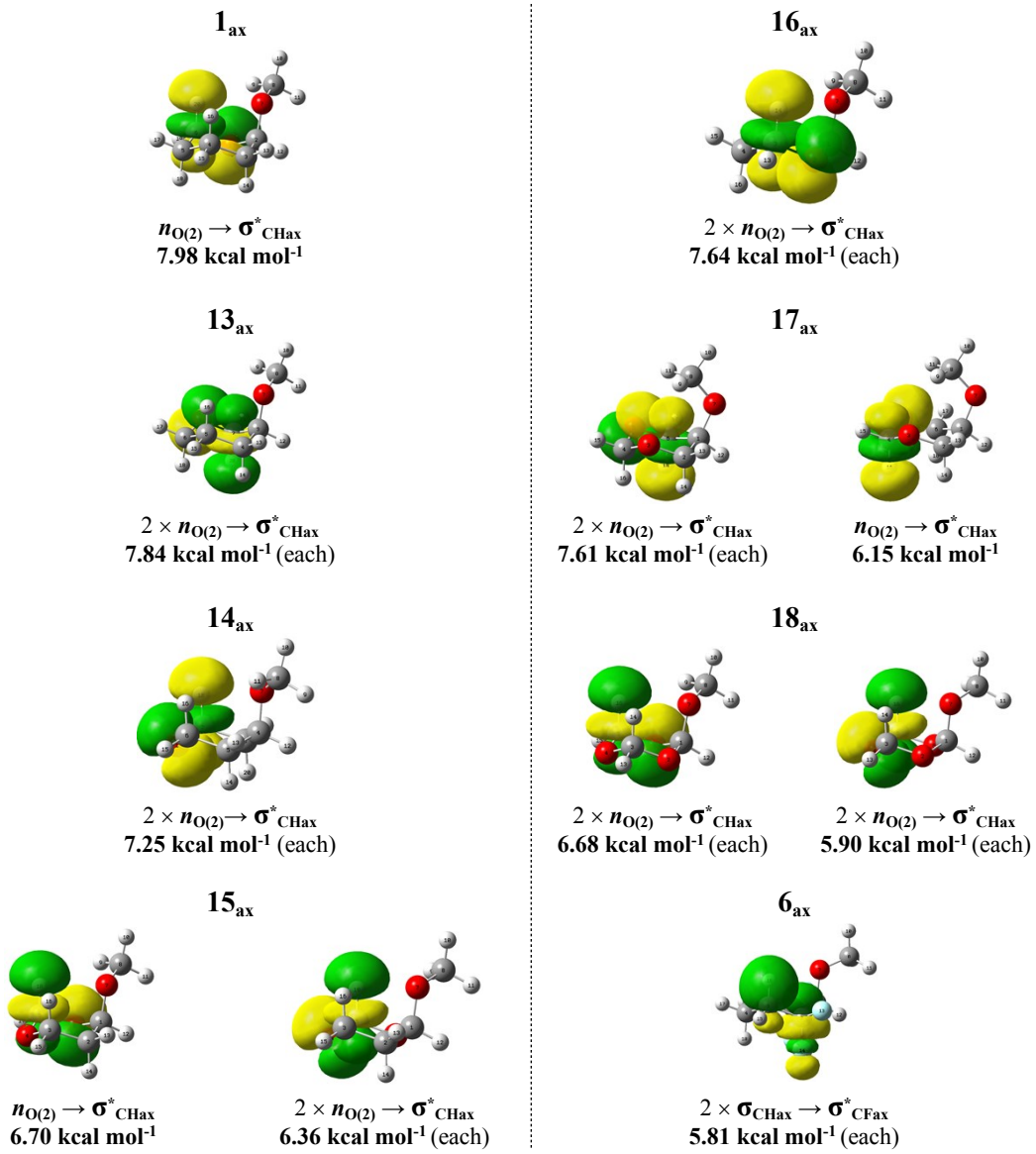

Figure S7. Hyperconjugative interactions in compounds 1 and 13-18 between ring O atoms and σ^*_{CHax} donate charge to H_{ax} and thus are responsible for lowering the energy of NCHBs in oxygenated compounds, while in 6 the $\sigma_{CHax} \rightarrow \sigma^*_{CFax}$ hyperconjugation withdraws charge from H_{ax} and thus strengthen the NCHBs. Interaction energies were calculated at the M06-2X/aug-cc-pVTZ theoretical level.

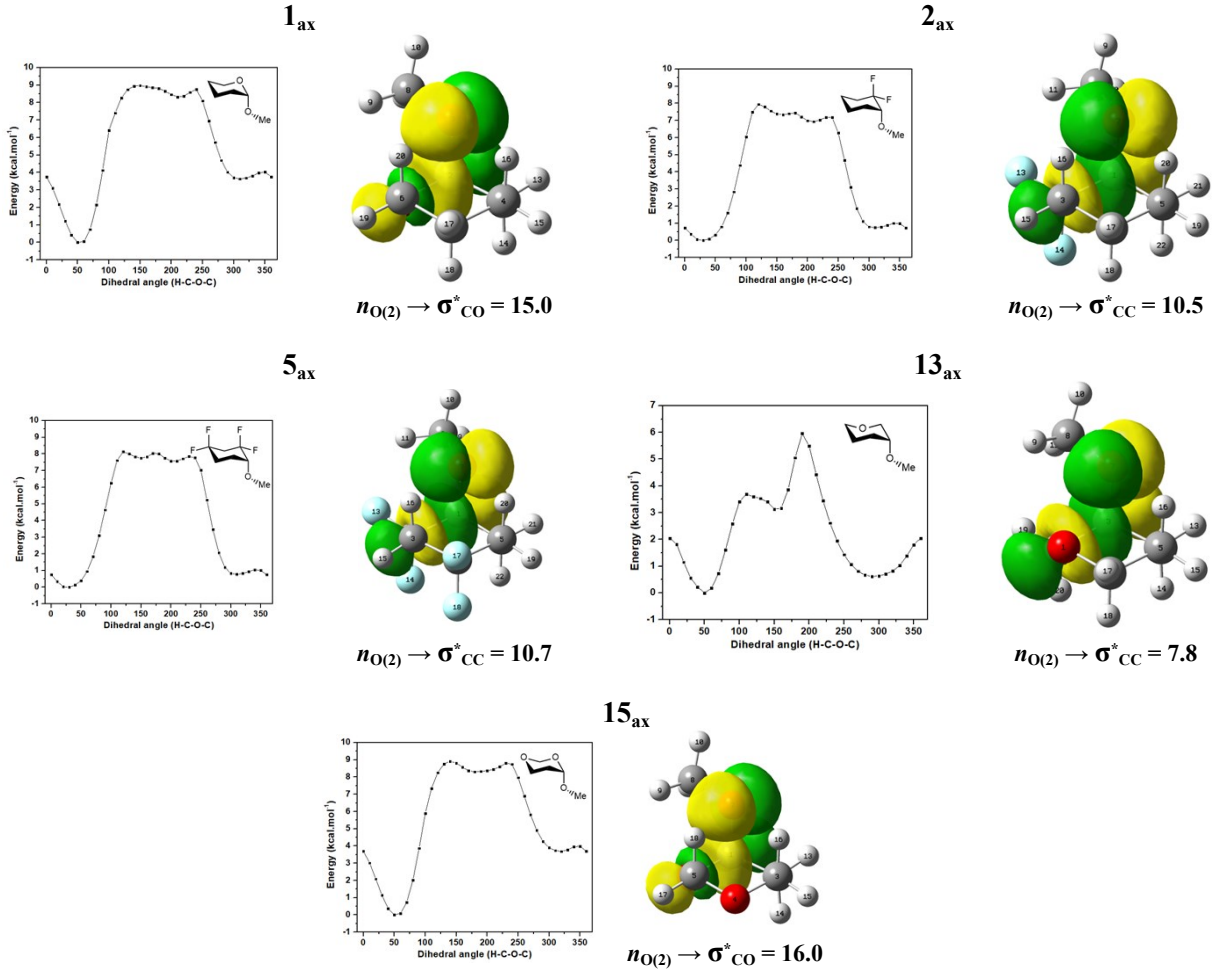

Figure S8. Calculated potential energy curves (left) obtained by scanning the H-C-O-Me dihedral angles in 10° increments at the M06-2X/aug-cc-pVTZ theoretical level for 1_{ax}, 2_{ax}, 5_{ax}, 13_{ax} and 15_{ax}. $n_O \rightarrow \sigma^*_{CO}$ and $n_O \rightarrow \sigma^*_{CC}$ hyperconjugative interactions (right) are also shown together with their energy stabilization in kcal mol^{-1}.

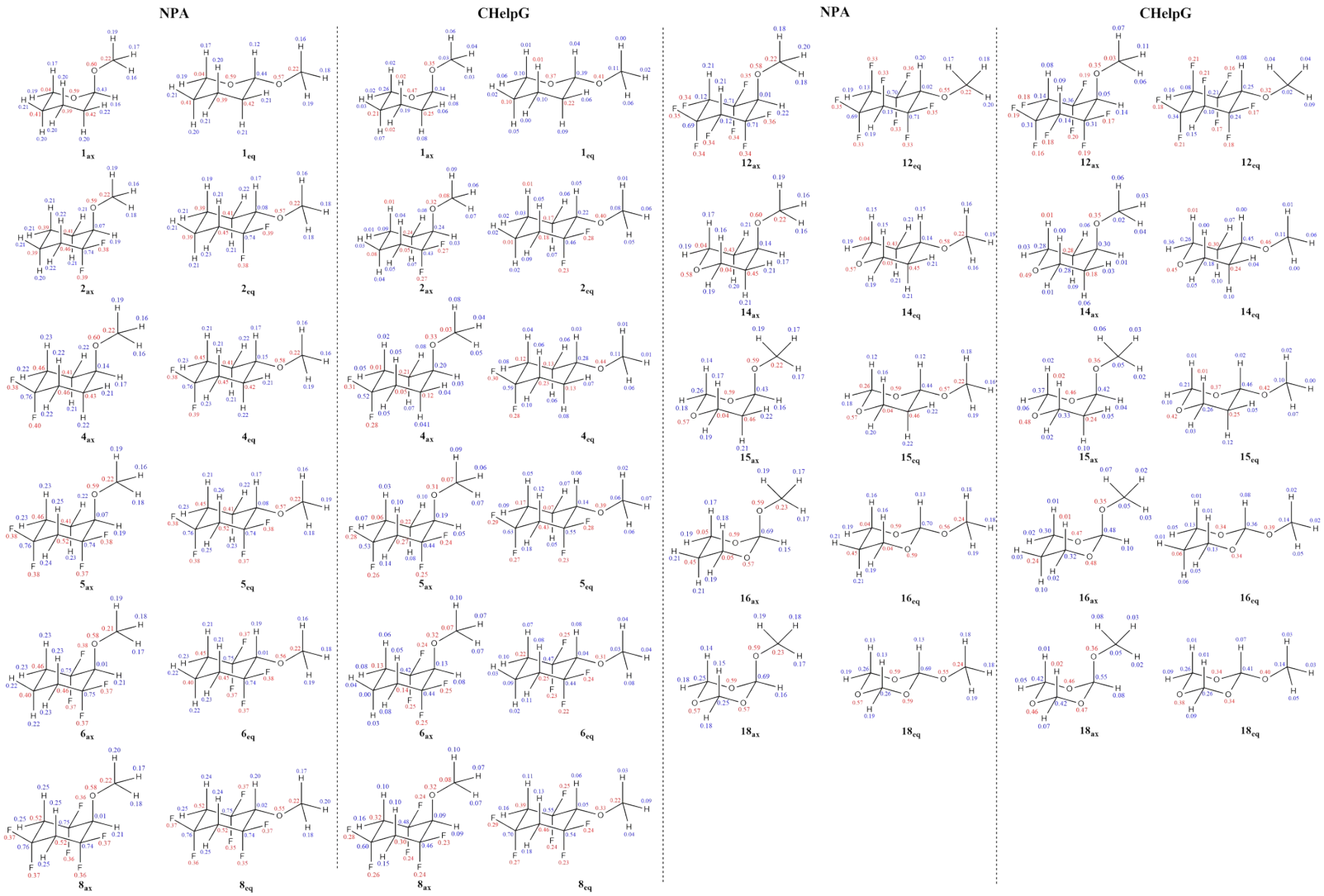

Figure S9. Comparison between NPA and CHelpG atomic charges for compounds 1, 2, 4, 5, 6, 8, 12, 14, 15, 16 and 18 calculated at the M06-2X/aug-cc-pVTZ theoretical level.

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