ELECTRONIC SUPPORTING INFORMATION (ESI)

An examination of the relationship between molecular dipole moment and blood-gas partition for common anaesthetic gases

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Standard coordinates for the optimized geometries of the fluorinated anaesthetics. 1

Table S1. Weighted dipole moment (Db), blood-gas partition coefficient (K_{bg}), and MAC (%) for the studied fluorinated anaesthetics. 15

Table S2. Conformational Gibbs free energies (in kcal mol^{-1}) and population (%, in parenthesis), molecular dipole moments (μ, in Db), bond lengths (in Å), and dihedral angles (degrees) obtained for the main conformers of the studied fluorinated anesthetics. 16

Table S3. Important electron delocalization interactions obtained through NBO analysis (in kcal mol^{-1}) in the gas phase at the B3LYP/aug-cc-pVTZ level. 17

STANDARD COORDINATES

H

Standard orientation:

Free Gibbs Energy (Hartree) = -3408.289718

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.102819	0.360968	-0.523301
2	1	0	-0.135755	0.348512	-1.607686
3	6	0	-1.204364	-0.558340	-0.000622
4	9	0	-1.231299	-0.615950	1.327592
5	9	0	-2.395775	-0.124076	-0.427818
6	9	0	-1.029610	-1.795946	-0.476669
7	17	0	-0.382846	2.006750	0.029356
8	35	0	1.611354	-0.298722	0.012692

E*sag*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.792883

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.529131	0.199256	-0.525229
2	1	0	1.472187	0.321875	-1.603815
3	6	0	0.186844	0.577409	0.101733
4	6	0	-2.068720	-0.009704	0.039353
5	1	0	-2.171127	0.907693	0.612752
6	8	0	-0.787041	-0.185033	-0.475259
7	9	0	2.475122	1.031637	-0.018689
8	17	0	1.932380	-1.468933	-0.163139
9	9	0	0.207967	0.432362	1.439770
10	9	0	-0.037839	1.895216	-0.131574
11	9	0	-2.907932	-0.003759	-1.002672
12	9	0	-2.374954	-1.064255	0.809983

E*s'a'g*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.792795

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.500772	0.224555	-0.534985
2	1	0	1.372075	0.318041	-1.610257
3	6	0	0.171973	0.515264	0.163015
4	6	0	-2.064911	-0.142512	0.136663
5	1	0	-2.102834	0.449488	1.047081
6	8	0	-0.765894	-0.352980	-0.316831
7	9	0	2.407288	1.137851	-0.100970
8	17	0	2.052357	-1.399617	-0.167157
9	9	0	0.291927	0.420781	1.502550
10	9	0	-0.178100	1.798113	-0.094732
11	9	0	-2.770753	0.466028	-0.830726
12	9	0	-2.603603	-1.348778	0.340691

E*sag'*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.792552

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.354135	0.387545	-0.589719
2	1	0	1.249949	0.201450	-1.655604
3	6	0	0.153145	-0.205302	0.148901
4	6	0	-2.177315	-0.066060	0.152969
5	1	0	-2.067258	-0.586544	1.100474
6	8	0	-0.966859	0.401381	-0.350305
7	9	0	1.382051	1.724314	-0.358349
8	17	0	2.841156	-0.356401	-0.026037
9	9	0	0.108099	-1.541037	-0.048862
10	9	0	0.253428	-0.013900	1.479718
11	9	0	-2.974463	0.997506	0.293831
12	9	0	-2.738811	-0.885129	-0.752194

E*s'a'g'*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.792553

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.357959	0.366116	-0.612400
2	1	0	1.319671	0.149492	-1.676971
3	6	0	0.158389	-0.280363	0.082091
4	6	0	-2.172736	-0.170985	0.072421
5	1	0	-2.069364	-1.051478	0.700980
6	8	0	-0.968929	0.226112	-0.503419
7	9	0	1.294530	1.706860	-0.414982
8	17	0	2.856165	-0.272325	0.043647
9	9	0	0.212315	-1.624086	-0.073881
10	9	0	0.169348	-0.044720	1.407252
11	9	0	-2.667216	0.846481	0.793204
12	9	0	-3.021794	-0.414089	-0.932851

E*s'a'a'*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.792488

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.633563	0.419341	0.004013
2	1	0	-2.278489	0.869888	0.754889
3	6	0	-0.185984	0.503600	0.486337
4	6	0	1.995659	-0.084504	-0.073623
5	1	0	2.241589	0.622719	0.714072
6	8	0	0.650464	-0.050984	-0.429968
7	9	0	-1.740365	1.108058	-1.160500
8	17	0	-2.115808	-1.251377	-0.224158
9	9	0	0.116407	1.811809	0.691107
10	9	0	-0.077346	-0.094640	1.693907
11	9	0	2.311105	-1.328840	0.319551
12	9	0	2.695227	0.187842	-1.179497

E*saa* Standard orientation:

Free Gibbs Energy (Hartree) = -1148.792427

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.599792	0.487120	-0.070567
2	1	0	-2.226272	1.084555	0.587721
3	6	0	-0.176640	0.473714	0.485432
4	6	0	1.982069	-0.271828	0.036645
5	1	0	2.159402	0.062788	1.055377
6	8	0	0.631423	-0.285383	-0.300404
7	9	0	-1.573747	1.046846	-1.306181
8	17	0	-2.253037	-1.139251	-0.147192
9	9	0	0.266720	1.752239	0.558598
10	9	0	-0.200275	0.015960	1.760550
11	9	0	2.433503	-1.519305	-0.128895
12	9	0	2.638610	0.523033	-0.822589

E*s'g'g'* Standard orientation:

Free Gibbs Energy (Hartree) = -1148.790414

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.090682	-0.552274	-0.402712
2	1	0	-1.075599	-0.768339	-1.467771
3	6	0	-0.234305	0.688436	-0.123072
4	6	0	1.933326	-0.227435	0.201011
5	1	0	1.513551	-0.534400	1.152738
6	8	0	1.061213	0.534344	-0.565564
7	9	0	-0.542135	-1.600048	0.279657
8	17	0	-2.748731	-0.306494	0.109168
9	9	0	-0.732335	1.721131	-0.806646
10	9	0	-0.260163	0.985255	1.190931
11	9	0	2.293265	-1.306218	-0.515045
12	9	0	3.035894	0.509438	0.399141

E*g'gg* Standard orientation:

Free Gibbs Energy (Hartree) = -1148.790265

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.509275	0.082208	-0.464964
2	1	0	-1.585083	0.170655	-1.545825
3	6	0	-0.300151	-0.788561	-0.110872
4	6	0	1.779093	0.332265	0.133961
5	1	0	1.331502	0.851892	0.974614
6	8	0	0.845259	-0.288128	-0.686295
7	9	0	-2.630528	-0.495790	0.031647
8	17	0	-1.312178	1.696613	0.214547
9	9	0	-0.182846	-0.916141	1.222471
10	9	0	-0.510356	-2.009020	-0.626827
11	9	0	2.657603	-0.580959	0.585163
12	9	0	2.441743	1.189086	-0.649620

E*sga* Standard orientation:

Free Gibbs Energ (Hartree) = -1148.790018

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.318727	0.065154	0.578502
2	1	0	2.123562	0.677365	0.977331
3	6	0	0.260439	0.972065	-0.064118
4	6	0	-1.698013	-0.343579	0.101438
5	1	0	-1.661335	-0.052924	1.146412
6	8	0	-0.778906	0.336918	-0.688140
7	9	0	0.725739	-0.618766	1.600708
8	17	0	1.976631	-1.051418	-0.597469
9	9	0	-0.199213	1.795073	0.913172
10	9	0	0.850780	1.726619	-0.993756
11	9	0	-2.907525	-0.083600	-0.411361
12	9	0	-1.483184	-1.664606	-0.015049

E*g'g'g* Standard orientation:

Free Gibbs Energy (Hartree) = -1148.789663

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.150554	-0.132535	0.572762
2	1	0	-0.646158	-0.473057	1.471861
3	6	0	-0.216805	0.761695	-0.254381
4	6	0	1.987602	0.021076	0.165138
5	1	0	2.302123	0.980871	0.562761
6	8	0	0.914961	0.113594	-0.703663
7	9	0	-2.239553	0.606657	0.914469
8	17	0	-1.637055	-1.533397	-0.365729
9	9	0	-0.847282	1.215729	-1.334536
10	9	0	0.117128	1.827560	0.516340
11	9	0	1.681196	-0.798562	1.203504
12	9	0	2.969936	-0.545853	-0.531892

E*gg'a* Standard orientation:

Free Gibbs Energy (Hartree) = -1148.789659

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.624323	-0.162124	-0.018011
2	1	0	2.376428	-0.674232	0.577287
3	6	0	0.274958	-0.878234	0.118078
4	6	0	-1.673716	0.468511	0.016888
5	1	0	-1.288567	0.983823	0.890340
6	8	0	-0.718022	-0.303785	-0.631075
7	9	0	1.985698	-0.172162	-1.323365
8	17	0	1.490649	1.497898	0.556607
9	9	0	0.438836	-2.134156	-0.323591
10	9	0	-0.048265	-0.939567	1.428334
11	9	0	-2.114996	1.344982	-0.889561
12	9	0	-2.709952	-0.311598	0.376732

E*ggg'*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.789422

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.993422	-0.642604	0.035019
2	1	0	-0.564055	-1.325488	-0.691381
3	6	0	-0.159819	0.644427	0.111096
4	6	0	2.074894	0.006520	-0.333049
5	1	0	2.156381	0.666047	-1.191328
6	8	0	1.119772	0.413347	0.580784
7	9	0	-0.985869	-1.218667	1.264087
8	17	0	-2.642053	-0.272921	-0.451654
9	9	0	-0.122325	1.210728	-1.117686
10	9	0	-0.711215	1.507738	0.960301
11	9	0	3.223418	-0.036606	0.339273
12	9	0	1.799822	-1.247385	-0.775291

E*aaa*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.789353

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.493005	0.397823	0.440318
2	1	0	-1.948931	0.322606	1.424701
3	6	0	-0.061811	-0.137775	0.519562
4	6	0	1.893670	-0.105677	-0.839101
5	1	0	2.119936	-0.354185	-1.870405
6	8	0	0.512808	-0.088132	-0.724290
7	9	0	-1.446293	1.699396	0.058402
8	17	0	-2.452010	-0.536634	-0.695606
9	9	0	0.613510	0.601813	1.421176
10	9	0	-0.096550	-1.399205	0.991981
11	9	0	2.413499	1.096677	-0.537087
12	9	0	2.446674	-1.006105	-0.007733

E*aag*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.789194

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.526015	0.299965	-0.428484
2	1	0	1.652138	0.473679	-1.494080
3	6	0	0.070698	0.569636	-0.034119
4	6	0	-2.025450	-0.488236	-0.461405
5	1	0	-2.542771	-0.857497	-1.340492
6	8	0	-0.724418	-0.208202	-0.847221
7	9	0	2.316490	1.153633	0.270892
8	17	0	1.966248	-1.361627	-0.069068
9	9	0	-0.132297	0.332972	1.267120
10	9	0	-0.181467	1.878145	-0.247417
11	9	0	-2.045523	-1.423826	0.503617
12	9	0	-2.642516	0.604510	0.020292

E*a'a'g'* Standard orientation:

Free Gibbs Energy (Hartree) = -1148.789031

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.370581	0.409306	-0.549884
2	1	0	1.494261	0.300283	-1.624328
3	6	0	0.073655	-0.277548	-0.111564
4	6	0	-2.247084	0.220506	-0.378759
5	1	0	-2.890034	0.494894	-1.208328
6	8	0	-0.941102	0.319875	-0.832199
7	9	0	1.288168	1.726546	-0.230445
8	17	0	2.749023	-0.320880	0.255867
9	9	0	0.146963	-1.588988	-0.408440
10	9	0	-0.111878	-0.166960	1.209151
11	9	0	-2.529798	-1.025376	0.040049
12	9	0	-2.459200	1.053358	0.654325

E*ag'g* Standard orientation:

Free Gibbs Energy (Hartree) = -1148.788386

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.115640	-0.036098	0.605499
2	1	0	-0.650160	-0.557603	1.435000
3	6	0	-0.049688	0.664093	-0.251349
4	6	0	1.884811	-0.748064	-0.241910
5	1	0	2.253621	-1.570685	-0.844574
6	8	0	0.801106	-0.216514	-0.902681
7	9	0	-1.952798	0.921594	1.084735
8	17	0	-2.015448	-1.196265	-0.360431
9	9	0	-0.636549	1.377086	-1.212718
10	9	0	0.629600	1.507432	0.548296
11	9	0	2.856530	0.162159	-0.066804
12	9	0	1.540263	-1.199682	0.989260

Eg'ga Standard orientation:

Free Gibbs Energy (Hartree) = -1148.788315

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.312261	0.142436	0.555269
2	1	0	2.173705	0.783286	0.723426
3	6	0	0.300996	0.900453	-0.320771
4	6	0	-1.517095	-0.598117	0.029000
5	1	0	-0.925898	-1.307281	0.600051
6	8	0	-0.756224	0.192780	-0.826186
7	9	0	0.736834	-0.159911	1.754325
8	17	0	1.847900	-1.327506	-0.242991
9	9	0	-0.123425	1.959665	0.399997
10	9	0	0.962405	1.371799	-1.387043
11	9	0	-2.227164	0.171689	0.872237
12	9	0	-2.369681	-1.245385	-0.768864

E*agg'*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.787568

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.762122	-0.606644	-0.162151
2	1	0	-0.218088	-0.994763	-1.018195
3	6	0	-0.115988	0.687921	0.354707
4	6	0	2.138044	-0.086302	0.052228
5	1	0	3.102109	0.126549	0.500270
6	8	0	1.184229	0.536021	0.822493
7	9	0	-0.750490	-1.516305	0.845211
8	17	0	-2.417429	-0.287837	-0.662597
9	9	0	-0.150949	1.613692	-0.619058
10	9	0	-0.796526	1.155894	1.401312
11	9	0	1.941455	-1.424212	0.014932
12	9	0	2.109715	0.337979	-1.227571

E*gg'a'*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.786243

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.413121	-0.041834	-0.386637
2	1	0	2.396715	-0.461975	-0.194331
3	6	0	0.362971	-0.945965	0.288847
4	6	0	-1.537614	0.398887	-0.254447
5	1	0	-0.970055	1.110342	-0.846376
6	8	0	-0.928133	-0.845620	-0.154567
7	9	0	1.173661	-0.039936	-1.725945
8	17	0	1.400943	1.607455	0.230908
9	9	0	0.722987	-2.213355	0.016750
10	9	0	0.444028	-0.781180	1.621583
11	9	0	-2.718268	0.159173	-0.829933
12	9	0	-1.761131	0.911224	0.969236

E*g'gg'*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.786186

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.912187	0.629072	-0.147080
2	1	0	0.504535	1.048764	-1.063506
3	6	0	0.180232	-0.674073	0.213284
4	6	0	-1.900627	0.456224	-0.036548
5	1	0	-1.566215	1.470917	0.167630
6	8	0	-1.133713	-0.506100	0.597813
7	9	0	0.739308	1.515289	0.876999
8	17	0	2.617298	0.323398	-0.402101
9	9	0	0.250850	-1.491828	-0.855104
10	9	0	0.775585	-1.281695	1.240844
11	9	0	-1.905338	0.257724	-1.375214
12	9	0	-3.139675	0.285400	0.420380

E*gg'g* Standard orientation:

Free Gibbs Energy (Hartree) = -1148.785920

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.095954	0.098285	-0.602338
2	1	0	-0.574046	0.247704	-1.544429
3	6	0	-0.255366	-0.762862	0.355387
4	6	0	1.703347	0.491922	-0.145671
5	1	0	1.242034	1.429929	-0.448323
6	8	0	0.939321	-0.216645	0.767040
7	9	0	-2.255951	-0.560700	-0.841555
8	17	0	-1.434292	1.669726	0.117370
9	9	0	-0.945845	-1.012387	1.469037
10	9	0	-0.039667	-1.940783	-0.266692
11	9	0	2.860629	0.733061	0.467364
12	9	0	1.946195	-0.251845	-1.248502

E*aga* Standard orientation:

Free Gibbs Energy (Hartree) = -1148.785292

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.057884	0.120169	0.714660
2	1	0	1.741937	0.780576	1.242699
3	6	0	0.119315	1.000989	-0.124449
4	6	0	-1.663212	-0.556450	-0.639396
5	1	0	-2.355638	-0.652806	-1.468858
6	8	0	-0.731755	0.392705	-1.021351
7	9	0	0.337337	-0.591412	1.617816
8	17	0	2.002409	-0.947359	-0.309867
9	9	0	-0.567138	1.782738	0.733617
10	9	0	0.887250	1.803603	-0.875639
11	9	0	-1.077674	-1.744404	-0.401453
12	9	0	-2.319455	-0.200808	0.476748

E*a'g'g'* Standard orientation:

Free Gibbs Energy (Hartree) = -1148.784915

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.808617	-0.576516	-0.342399
2	1	0	-0.641868	-0.833264	-1.385100
3	6	0	-0.183056	0.796593	-0.032129
4	6	0	2.130357	0.086160	-0.240012
5	1	0	3.054453	0.578280	-0.523661
6	8	0	1.113173	0.978662	-0.498452
7	9	0	-0.242465	-1.512845	0.459851
8	17	0	-2.541468	-0.527178	-0.044600
9	9	0	-0.883271	1.744420	-0.667137
10	9	0	-0.243873	1.036598	1.284288
11	9	0	2.173508	-0.279443	1.049579
12	9	0	1.979975	-1.038697	-0.977492

E*a'g'a'*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.783418

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.294652	0.332954	0.176751
2	1	0	-2.319363	0.166200	-0.146944
3	6	0	-0.501676	-0.944576	-0.159332
4	6	0	1.781070	-0.301710	0.371062
5	1	0	2.636673	-0.843072	0.760364
6	8	0	0.702099	-1.156570	0.477496
7	9	0	-1.272713	0.509610	1.522517
8	17	0	-0.704029	1.764290	-0.650263
9	9	0	-1.267023	-1.973248	0.252969
10	9	0	-0.376506	-1.045483	-1.492671
11	9	0	2.007637	0.071496	-0.900069
12	9	0	1.589264	0.817236	1.093942

E*agg*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.782879

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.056053	0.358690	-0.536428
2	1	0	-0.765957	0.437573	-1.580645
3	6	0	-0.416492	-0.904228	0.088410
4	6	0	1.926862	-0.346733	-0.261950
5	1	0	2.818498	-0.922605	-0.485234
6	8	0	0.864723	-1.216474	-0.346538
7	9	0	-2.406229	0.214020	-0.451681
8	17	0	-0.590194	1.829284	0.299415
9	9	0	-0.467240	-0.855399	1.425179
10	9	0	-1.145320	-1.955921	-0.310930
11	9	0	1.803515	0.652667	-1.167541
12	9	0	2.030504	0.219368	0.950299

I*ag*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.799883

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.089969	0.246587	-0.205939
2	1	0	0.296773	0.039396	-1.201098
3	6	0	-1.395659	-0.525761	-0.023955
4	9	0	-1.927166	-0.328923	1.179324
5	9	0	-2.284156	-0.161691	-0.951043
6	9	0	-1.154698	-1.833352	-0.170402
7	17	0	-0.400228	1.982172	-0.085534
8	8	0	0.781493	-0.187418	0.803218
9	6	0	2.069384	-0.414319	0.395199
10	1	0	2.653524	-0.694663	1.264564
11	9	0	2.114373	-1.399827	-0.532866
12	9	0	2.595991	0.681421	-0.194676

I*ga*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.799253

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.211771	0.223925	-0.334333
2	1	0	-0.030556	0.178297	-1.406538
3	6	0	-1.489066	-0.552510	-0.017919
4	9	0	-1.780343	-0.524619	1.278482
5	9	0	-2.515165	-0.039391	-0.700763
6	9	0	-1.335482	-1.825645	-0.392265
7	17	0	-0.435404	1.939431	0.091586
8	8	0	0.803153	-0.376018	0.401335
9	6	0	2.074309	0.048370	0.066875
10	1	0	2.215309	1.117729	0.211411
11	9	0	2.910970	-0.645516	0.837106
12	9	0	2.336804	-0.251154	-1.229255

I*g'a*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.797772

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.240217	0.209529	-0.389237
2	1	0	-0.127651	0.155691	-1.473084
3	6	0	-1.533831	-0.512235	-0.008890
4	9	0	-1.750485	-0.489677	1.300903
5	9	0	-2.573614	0.049443	-0.629152
6	9	0	-1.455591	-1.787970	-0.405529
7	17	0	-0.365922	1.924922	0.043329
8	8	0	0.787593	-0.445278	0.277991
9	6	0	2.028851	-0.341521	-0.314921
10	1	0	1.975383	-0.376594	-1.404266
11	9	0	2.638413	0.802936	0.052656
12	9	0	2.757207	-1.360863	0.147246

I*s'g'*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.795881

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.416341	0.491188	-0.702818
2	1	0	-0.838338	0.657281	-1.689205
3	6	0	-1.236396	-0.616760	-0.028275
4	9	0	-0.871968	-0.818285	1.240629
5	9	0	-2.532239	-0.296230	-0.048882
6	9	0	-1.075988	-1.758146	-0.698777
7	17	0	-0.618875	1.998838	0.222258
8	8	0	0.914937	0.151922	-0.909464
9	6	0	1.711584	-0.071271	0.201423
10	1	0	1.349648	0.430436	1.094936
11	9	0	1.803825	-1.396100	0.431308
12	9	0	2.936034	0.368507	-0.116542

I*a'g'*

Standard orientation:

Free Gibbs Energy (Hartree) = -1148.790664

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.419849	0.424075	0.766278
2	1	0	0.977343	0.452852	1.697672
3	6	0	1.021570	-0.722856	-0.059763
4	9	0	0.556498	-0.788131	-1.302210
5	9	0	2.348142	-0.554363	-0.116371
6	9	0	0.783080	-1.886725	0.552418
7	17	0	0.731986	1.963467	-0.059365
8	8	0	-0.911966	0.259924	1.160899
9	6	0	-1.923191	-0.022378	0.266342
10	1	0	-2.857082	0.148974	0.791876
11	9	0	-1.861842	0.743972	-0.836649
12	9	0	-1.867842	-1.307331	-0.142152

D*ag*

Standard orientation:

Free Gibbs Energy (Hartree) = -788.819857

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.102359	-0.420753	-0.248139
2	1	0	-0.267280	-0.151653	-1.236684
3	6	0	1.478986	0.203166	-0.024264
4	9	0	1.955575	-0.083075	1.183865
5	9	0	2.334977	-0.254839	-0.941165
6	9	0	1.395713	1.530251	-0.151218
7	8	0	-0.727160	0.035430	0.771809
8	6	0	-2.027015	0.272171	0.402961
9	1	0	-2.589881	0.533164	1.291860
10	9	0	-2.090915	1.279748	-0.499128
11	9	0	-2.566612	-0.809341	-0.198462
12	9	0	0.232202	-1.773016	-0.173113

D*ga*

Standard orientation:

Free Gibbs Energy (Hartree) = -788.818501

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.236492	0.499303	0.241313
2	1	0	0.053323	0.651926	1.304826
3	6	0	1.554991	-0.246714	0.042731
4	9	0	1.812499	-0.450570	-1.244788
5	9	0	2.550739	0.470692	0.570164
6	9	0	1.506905	-1.424752	0.667091
7	8	0	-0.749422	-0.253158	-0.367002
8	6	0	-2.036009	0.176188	-0.096139
9	1	0	-2.210081	1.209805	-0.387380
10	9	0	-2.847954	-0.640769	-0.764591
11	9	0	-2.296013	0.049348	1.227743
12	9	0	0.342634	1.728371	-0.356605

D*g'a*

Standard orientation:

Free Gibbs Energy (Hartree) = -788.817401

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.253162	0.433741	-0.366110
2	1	0	-0.140207	0.453485	-1.452993
3	6	0	-1.588856	-0.218112	-0.006336
4	9	0	-1.767198	-0.279032	1.307809
5	9	0	-2.587097	0.487153	-0.544010
6	9	0	-1.631911	-1.456375	-0.507566
7	8	0	0.738576	-0.300441	0.251628
8	6	0	1.990622	-0.182559	-0.318707
9	1	0	1.953667	-0.192967	-1.408984
10	9	0	2.588864	0.955354	0.083646
11	9	0	2.711711	-1.211452	0.130664
12	9	0	-0.271447	1.720417	0.084553

D*s'g'*

Standard orientation:

Free Gibbs Energy (Hartree) = -788.815255

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.409973	0.859343	0.533083
2	1	0	0.819250	1.254582	1.459507
3	6	0	1.338264	-0.250984	0.020559
4	9	0	0.963397	-0.697532	-1.181373
5	9	0	2.581321	0.227366	-0.079786
6	9	0	1.343954	-1.271959	0.874998
7	8	0	-0.874056	0.442108	0.823129
8	6	0	-1.645039	-0.045352	-0.221223
9	1	0	-1.321519	0.308072	-1.195843
10	9	0	-1.629736	-1.392308	-0.198976
11	9	0	-2.901717	0.348337	0.021183
12	9	0	0.406729	1.844144	-0.418624

Dgg'

Standard orientation:

Free Gibbs Energy (Hartree) = -788.813402

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.416271	0.546315	-0.805838
2	1	0	-0.838916	0.581751	-1.807296
3	6	0	-1.344187	-0.299384	0.080428
4	9	0	-1.034598	-0.199771	1.376524
5	9	0	-2.602262	0.110308	-0.081163
6	9	0	-1.268428	-1.587133	-0.271995
7	8	0	0.862385	0.043999	-0.955581
8	6	0	1.592277	-0.310892	0.170605
9	1	0	1.080047	-1.019842	0.815357
10	9	0	2.717795	-0.856238	-0.300971
11	9	0	1.919825	0.779809	0.887350
12	9	0	-0.413568	1.805232	-0.280254

D*a'g'*

Standard orientation:

Free Gibbs Energy (Hartree) = -788.811079

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.359030	0.793841	0.682728
2	1	0	0.901782	1.050415	1.589858
3	6	0	1.180013	-0.274571	-0.057472
4	9	0	0.720261	-0.542214	-1.273747
5	9	0	2.433248	0.183764	-0.176685
6	9	0	1.217156	-1.400661	0.657503
7	8	0	-0.905921	0.416100	1.118639
8	6	0	-1.842050	-0.126938	0.261788
9	1	0	-2.797065	-0.084507	0.774925
10	9	0	-1.909441	0.539873	-0.903203
11	9	0	-1.545916	-1.410556	-0.029297
12	9	0	0.302547	1.891049	-0.123032

S*gg*

Standard orientation:

Free Gibbs Energy (Hartree) = -927.165191

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.138325	0.066696	-0.212311
2	1	0	0.521900	0.150787	-1.231005
3	6	0	-0.245030	-1.398367	-0.006157
4	9	0	-0.639684	-1.640512	1.242436
5	9	0	-1.232524	-1.752566	-0.837083
6	9	0	0.812346	-2.170512	-0.266331
7	8	0	1.110128	0.378833	0.754759
8	6	0	2.208851	1.070400	0.253962
9	1	0	2.821078	1.329627	1.111169
10	9	0	2.939831	0.254113	-0.583006
11	6	0	-1.036331	1.036857	-0.079454
12	9	0	-0.572861	2.294045	-0.187497
13	9	0	-1.656740	0.931034	1.092915
14	9	0	-1.931324	0.850408	-1.053266
15	1	0	1.909712	1.941301	-0.327974

S*sg*

Standard orientation:

Free Gibbs Energy (Hartree) = -927.158997

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.187479	-0.004332	-0.701369
2	1	0	0.471437	-0.361067	-1.691419
3	6	0	1.508731	0.317814	0.010601
4	9	0	1.346156	0.640598	1.301716
5	9	0	2.346371	-0.720124	-0.050667
6	9	0	2.091162	1.356352	-0.594502
7	8	0	-0.575072	1.152479	-0.925848
8	6	0	-1.247852	1.753001	0.143547
9	1	0	-1.357387	2.798307	-0.127166
10	9	0	-2.506553	1.215706	0.269894
11	6	0	-0.592407	-1.157412	-0.058143
12	9	0	0.150779	-2.271232	-0.065742
13	9	0	-0.942113	-0.907283	1.207387
14	9	0	-1.698709	-1.395103	-0.760639
15	1	0	-0.733020	1.618271	1.090525

M*gaa* Standard orientation:

Free Gibbs Energy (Hartree) = -1310.466432

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.845395	-0.000000	0.472341
2	1	0	-1.120270	0.000001	1.522287
3	6	0	0.681512	0.000001	0.382291
4	8	0	1.094003	-0.000000	-0.891801
5	6	0	2.522663	-0.000001	-1.062281
6	1	0	2.956013	-0.893505	-0.619784
7	1	0	2.679107	-0.000000	-2.134358
8	1	0	2.956015	0.893500	-0.619782
9	17	0	-1.500971	-1.458371	-0.267193
10	17	0	-1.500974	1.458369	-0.267195
11	9	0	1.147637	1.081245	1.073139
12	9	0	1.147639	-1.081239	1.073143

M*gag* Standard orientation:

Free Gibbs Energy (Hartree) = -1310.466116

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.736649	0.107999	-0.516555
2	1	0	-0.708058	0.115244	-1.601124
3	6	0	0.644222	-0.306917	-0.001786
4	8	0	1.556590	0.556765	-0.489185
5	6	0	2.908404	0.299593	-0.067066
6	1	0	3.219194	-0.695951	-0.374715
7	1	0	3.508832	1.050158	-0.567206
8	1	0	2.992984	0.408627	1.011039
9	17	0	-1.128616	1.734532	0.036717
10	17	0	-1.954959	-1.056747	-0.001984
11	9	0	0.663698	-0.360376	1.352093
12	9	0	0.898439	-1.579468	-0.422375

M*gg'g* Standard orientation:

Free Gibbs Energy (Hartree) = -1310.461402

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.498458	0.202629	-0.451891
2	1	0	-0.218974	0.312053	-1.494563
3	6	0	0.617033	-0.547061	0.298400
4	8	0	1.788909	0.126956	0.396134
5	6	0	2.368793	0.535049	-0.848338
6	1	0	1.826450	1.383687	-1.265178
7	1	0	3.381331	0.839789	-0.609398
8	1	0	2.394168	-0.292812	-1.554831
9	17	0	-0.700558	1.815918	0.232121
10	17	0	-1.999517	-0.718047	-0.404620
11	9	0	0.235398	-0.830902	1.547279
12	9	0	0.796027	-1.731972	-0.358573

M*gga* Standard orientation:

Free Gibbs Energy (Hartree) = -1310.460963

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.633429	-0.145761	-0.582698
2	1	0	0.833704	-0.400568	-1.618280
3	6	0	-0.894532	-0.243180	-0.369480
4	8	0	-1.361918	-0.322401	0.891400
5	6	0	-1.093570	0.791174	1.757176
6	1	0	-1.317518	1.731255	1.258260
7	1	0	-1.756329	0.653273	2.604230
8	1	0	-0.058047	0.775535	2.089052
9	17	0	1.448642	-1.327156	0.438336
10	17	0	1.261422	1.485994	-0.319595
11	9	0	-1.463408	0.790516	-1.051290
12	9	0	-1.286539	-1.378730	-0.983492

Table S1. Weighted dipole moment (Db), blood-gas partition coefficient (K_{bg}), and MAC(%) for the studied fluorinated anaesthetics.

Molecule	Dipole moment	K_{bg}	MAC (%)
Halothane	1.49	2.40	0.74
Enflurane	1.51	1.90	1.58
Isoflurane	1.93	1.40	1.15
Sevoflurane	2.56	0.65	2.00
Desflurane	1.97	0.45	5.80
Methoxyflurane	2.04	12.00	0.20

Table S2. Conformational Gibbs free energies (in kcal mol^{-1}) and population (%, in parenthesis), molecular dipole moments (μ, in Db), bond lengths (in Å), and dihedral angles (degrees) obtained for the main conformers of the studied fluorinated anesthetics.[a]

C$\phi_1\phi_2\phi_3$	G^0_{rel} (%)	μ	O–C_1	C_2–O	C_1–Faxial	C_2–R^2	Φ_1	ϕ_2	Φ_3
H	-- (100)	1.49	-	-	-	-	-	-	58.29
E*sag*	0.0(21)	1.26	1.39	1.36	1.34	1.36	17.26	176.77	56.14
E*s'a'g*	0.1(19)	0.45	1.39	1.37	1.34	1.35	340.46	185.33	57.62
E*sag'*	0.2(14)	1.06	1.39	1.37	1.34	1.35	20.12	176.57	300.55
E*s'a'g'*	0.2(14)	1.81	1.39	1.37	1.34	1.35	342.37	184.84	301.67
E*s'a'a'*	0.3(13)	2.37	1.39	1.36	1.34	1.36	340.40	182.66	180.03
E*saa*	0.3(13)	2.51	1.39	1.36	1.34	1.36	19.33	174.25	178.90
E*s'g'g'*	1.6(2)	1.48	1.39	1.38	1.34	1.35	353.25	282.10	302.91
E*g'gg*	1.6(1)	1.78	1.39	1.38	1.35	1.35	327.29	107.34	55.14
E*sga*	1.8(1)	2.52	1.39	1.37	1.34	1.36	17.39	69.43	175.99
E*g'g'g*	2.0(1)	2.06	1.38	1.38	1.36	1.36	306.15	276.46	62.44
E*gg'a*	2.0(1)	2.97	1.39	1.37	1.35	1.35	31.72	255.70	180.00
E*ggg'*	2.2(0)	2.39	1.38	1.39	1.36	1.35	53.48	84.38	295.59
E*aaa*	2.2(0)	1.11	1.39	1.37	1.34	1.35	163.58	159.42	178.13
E*aag*	2.3(0)	3.25	1.39	1.38	1.34	1.35	164.43	160.17	54.65
E*a'a'g'*	2.4(0)	2.95	1.39	1.38	1.34	1.35	195.91	199.90	302.19
E*ag'g*	2.8(0)	2.78	1.38	1.39	1.36	1.35	166.53	277.08	66.14
E*g'ga*	2.9(0)	2.74	1.39	1.37	1.34	1.35	306.06	49.93	169.72
E*agg'*	3.3(0)	2.28	1.37	1.39	1.35	1.34	166.27	51.31	297.27
E*gg'a'*	4.2(0)	2.69	1.39	1.37	1.35	1.35	53.86	309.42	199.45
E*g'gg'*	4.2(0)	2.45	1.38	1.38	1.35	1.35	293.20	37.14	291.53
E*gg'g*	4.4(0)	2.77	1.39	1.38	1.35	1.35	68.27	320.62	64.09
E*aga*	4.8(0)	0.80	1.38	1.38	1.35	1.35	164.80	58.03	171.75
E*a'g'g'*	5.0(0)	2.46	1.38	1.39	1.35	1.34	192.38	308.32	313.10
E*a'g'a'*	5.9(0)	0.57	1.38	1.38	1.35	1.35	193.94	299.14	198.47
E*agg*	6.3(0)	2.84	1.38	1.39	1.35	1.34	168.88	56.53	36.67
I*ag*	0.0(61)	1.72	1.37	1.40	1.35	1.77	177.22	136.85	58.40
I*ga*	0.4(31)	2.11	1.38	1.39	1.36	1.78	60.05	169.45	59.41
I*g'a*	1.3(7)	2.91	1.38	1.39	1.35	1.77	322.35	154.39	59.46
I*s'g'*	2.5(1)	1.84	1.39	1.39	1.35	1.78	335.79	295.71	68.55
I*a'g'*	5.8(0)	2.48	1.38	1.40	1.35	1.77	193.80	306.44	72.24
D*ag*	0.0(76)	1.89	1.37	1.39	1.35	1.36	174.93	143.71	56.48
D*ga*	0.9(18)	2.02	1.38	1.38	1.36	1.37	57.98	170.26	57.35
D*g'a*	1.5(5)	3.13	1.38	1.38	1.35	1.36	318.43	157.60	57.24
D*s'g'*	2.9(1)	1.59	1.39	1.38	1.35	1.37	336.92	296.68	67.23
D*gg'*	4.1(0)	1.86	1.39	1.38	1.35	1.36	54.79	309.10	73.28
D*a'g'*	5.5(0)	2.61	1.38	1.39	1.35	1.36	194.64	306.13	71.52
S*gg*	0.0(100)	2.56	1.39	1.41	1.38	1.53	51.09	133.73	54.89
S*gg'*	3.9(0)	1.71	1.40	1.40	1.37	1.54	30.89	285.23	72.63
M*gaa*	0.00(58)	1.62	1.44	1.34	-	1.37	61.22	180.00	180.00
M*gag*	0.20(42)	2.62	1.44	1.35	-	1.36	59.25	179.07	57.60
M*gg'g*	3.16(0)	3.60	1.43	1.36	-	1.37	74.78	303.19	66.44
M*gga*	3.43(0)	1.73	1.44	1.35	-	1.36	46.81	62.13	162.67

Table S3. Important electron delocalization interactions obtained through NBO analysis (in kcal mol^{-1}) in the gas phaseat the B3LYP/aug-cc-pVTZ level.

$C\phi_1\phi_2\phi_3$	$\sigma_{C3H}\rightarrow\sigma^*_{C4F}$	$\sigma_{C3F/Cl}\rightarrow\sigma^*_{C4F}$	$\sigma_{C3F/Cl}\rightarrow\sigma^*_{C4X}$	$\sigma_{C3O}\rightarrow\sigma^*_{C4F}$	$\sigma_{C4H}\rightarrow\sigma^*_{C3F}$	$\sigma_{C4H}\rightarrow\sigma^*_{C3O}$	$\sigma_{C4F}\rightarrow\sigma^*_{C3F/Cl}$	$\sigma_{C4F}\rightarrow\sigma^*_{C3O}$	$\sigma_{C4X}\rightarrow\sigma^*_{C3F}$	$\sigma_{C4X}\rightarrow\sigma^*_{C3O}$
H	-	1.57	1.75	-	3.80	-	2.39	-	3.01	-
E*sag*	-	-	1.26	0.93	3.79	-	-	1.25	2.59	-
E*s'a'g*	-	-	1.26	0.93	3.79	-	-	1.26	2.59	-
E*sag'*	-	0.91	-	-	3.79	-	1.30	-	-	2.37
E*s'a'g'*	-	0.91	-	-	3.79	-	1.31	-	-	2.38
E*s'a'a'*	-	0.93	1.28	-	-	3.34	1.30	-	2.59	-
E*saa*	-	0.94	1.27	-	-	3.35	1.29	-	2.60	-
E*s'g'g'*	-	0.99	-	-	3.46	-	1.16	-	-	2.29
E*g'gg*	-	-	1.29	0.99	3.55	-	-	1.09	2.41	
E*sga*	-	1.00	1.35	-	-	3.43	1.14	-	2.33	-
E*g'g'g*	-	-	1.30	0.86	3.34	-	-	1.23	2.46	-
E*gg'a*	-	0.96	1.29	-	-	3.23	1.17	-	2.35	-
I*ag*	3.29	2.28	-	1.24	-	-	1.42	0.97	-	-
I*ga*	3.23	2.29	-	1.18	-	-	1.47	0.93	-	-
I*g'a*	3.24	2.29	-	1.16	-	-	1.43	0.93	-	-
I*s'g'*	3.67	2.42	-	0.89	-	-	1.37	1.14	-	-
D*ag*	2.99	1.03	-	1.12	-	-	0.76	0.71	-	-
D*ga*	2.94	1.02	-	1.08	-	-	0.79	0.70	-	-
D*g'a*	2.95	1.02	-	1.06	-	-	0.77	0.69	-	-
D*s'g'*	3.33	1.11	-	0.83	-	-	0.73	0.85	-	-
Sgg	7.66	-	-	2.44	-	-	-	1.74	-	-
Mgaa	-	-	3.40	-	-	3.46	-	-	5.22	-
Mgag	-	-	1.66	-	4.09	-	-	-	2.62	2.26