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Structural Evidence of Anomeric Effects in the Anesthetic Isoflurane

SUPPLEMENTARY INFORMATION

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Table S1. Observed rotational transitions (obs.) and residuals (obs.-cal.) for the parent species of isoflurane AT (in MHz).

J'	K'_{-1}	K'_{+1}	F'	J''	K''_{-1}	K''_{+1}	F''	obs.	obs.-calc.
8	1	8	8	7	1	7	7	10977.0352	-0.0008
8	1	8	9	7	1	7	8	10977.2109	-0.0008
8	1	8	7	7	1	7	6	10977.8516	-0.0026
8	1	8	10	7	1	7	9	10977.9590	-0.0033
8	0	8	8	7	0	7	7	10987.5918	-0.0006
8	0	8	9	7	0	7	8	10987.6953	0.0003
8	0	8	7	7	0	7	6	10988.5664	-0.0017
8	0	8	10	7	0	7	9	10988.6758	-0.0003
7	4	3	7	6	4	2	7	11001.5918	-0.0044
7	3	4	6	6	3	3	5	11324.9530	-0.0012
7	3	4	9	6	3	3	8	11325.3807	0.0006
7	3	4	7	6	3	3	6	11329.2167	-0.0014
7	3	4	8	6	3	3	7	11329.6815	0.0013
7	2	5	8	6	2	4	7	11422.0604	-0.0003
7	2	5	7	6	2	4	6	11422.9178	0.0000
7	2	5	9	6	2	4	8	11422.9393	0.0012
7	2	5	6	6	2	4	5	11423.7752	-0.0012
4	4	1	4	3	3	0	3	11752.7537	0.0013
4	4	1	5	3	3	0	4	11753.2178	0.0000
4	4	1	3	3	3	0	2	11754.6250	-0.0006
4	4	1	6	3	3	0	5	11755.1172	0.0016
4	4	0	4	3	3	0	3	11753.3570	0.0034
4	4	0	5	3	3	0	4	11753.8354	-0.0008
4	4	0	6	3	3	0	5	11755.6970	0.0004
4	4	0	5	3	3	1	4	11759.7317	0.0011
4	4	0	3	3	3	1	2	11760.5122	-0.0006
4	4	0	6	3	3	1	5	11761.2200	0.0012
4	4	1	4	3	3	1	3	11758.5033	0.0021
4	4	1	5	3	3	1	4	11759.1003	-0.0117
4	4	1	3	3	3	1	2	11759.9385	-0.0007
4	4	1	6	3	3	1	5	11760.6390	0.0012
8	2	7	9	7	2	6	8	11800.1969	0.0007
8	2	7	8	7	2	6	7	11800.5563	-0.0010
8	2	7	10	7	2	6	9	11801.7165	0.0001
8	2	7	7	7	2	6	6	11801.8883	-0.0028
8	1	7	9	7	1	6	8	11981.7242	0.0046
8	1	7	8	7	1	6	7	11982.5172	-0.0006
8	1	7	10	7	1	6	9	11985.3726	0.0007
8	2	7	9	7	1	6	8	12187.7080	0.0017
8	2	7	8	7	1	6	7	12188.9313	-0.0004
8	2	7	10	7	1	6	9	12193.8263	-0.0001
8	2	7	7	7	1	6	6	12195.0953	0.0019
9	0	9	9	8	1	8	8	12293.3499	0.0002
9	0	9	10	8	1	8	9	12293.5026	0.0000
9	0	9	8	8	1	8	7	12293.9677	-0.0009
9	0	9	11	8	1	8	10	12294.0991	0.0000
9	1	9	9	8	1	8	8	12296.5509	-0.0001
9	1	9	10	8	1	8	9	12296.6938	0.0003
9	1	9	8	8	1	8	7	12297.2124	-0.0007
9	1	9	11	8	1	8	10	12297.3412	0.0011
6	3	3	7	5	2	3	6	12904.2540	0.0000
6	3	3	6	5	2	3	5	12906.6719	0.0011

Table S1. Continued.

6	3	3	8	5	2	3	7	12910.5238	0.0030
6	3	3	5	5	2	3	4	12912.8602	-0.0006
9	2	8	10	8	2	7	9	13154.3038	-0.0003
9	2	8	9	8	2	7	8	13154.5421	0.0003
9	2	7	11	8	2	6	10	14333.6900	0.0011
10	1	10	10	9	1	9	9	13614.5490	0.0004
10	1	10	11	9	1	9	10	13614.6776	0.0039
10	1	10	9	9	1	9	8	13615.0970	0.0027
10	1	10	12	9	1	9	11	13615.2190	0.0010
10	0	10	10	9	0	9	9	13616.4556	0.0002
10	0	10	11	9	0	9	10	13616.5742	0.0008
10	0	10	9	9	0	9	8	13617.0281	0.0002
10	0	10	12	9	0	9	11	13617.1506	0.0011
9	6	4	11	8	6	3	10	14031.2831	-0.0063
9	6	3	11	8	6	2	10	14032.6848	0.0007
11	1	11	11	10	1	10	10	14931.8734	0.0000
11	1	11	12	10	1	10	11	14931.9828	-0.0037
11	1	11	10	10	1	10	9	14932.3245	-0.0047
11	1	11	13	10	1	10	12	14932.4456	0.0015
11	0	11	11	10	0	10	10	14932.6527	-0.0001
11	0	11	12	10	0	10	11	14932.7640	0.0003
11	0	11	10	10	0	10	9	14933.1195	0.0004
11	1	10	13	10	1	9	12	15846.9843	0.0024
10	6	5	12	9	6	4	11	15630.6114	0.0063
10	6	5	11	9	6	4	10	15633.3489	0.0011
10	6	4	12	9	6	3	11	15637.3595	-0.0010
10	6	4	11	9	6	3	10	15639.8408	0.0010
10	5	6	9	9	5	5	8	15695.8049	0.0009
10	5	6	12	9	5	5	11	15696.0042	0.0000
10	5	6	10	9	5	5	9	15697.8305	0.0010
10	5	6	11	9	5	5	10	15698.0202	0.0000
10	5	5	9	9	5	4	8	15788.6478	0.0000
10	5	5	12	9	5	4	11	15788.9763	0.0000
10	5	5	10	9	5	4	9	15791.6303	0.0008
10	5	5	11	9	5	4	10	15791.9427	0.0002
7	4	4	8	6	3	3	7	16098.7962	-0.0009
7	4	4	7	6	3	3	6	16100.7706	-0.0019
7	4	4	9	6	3	3	8	16106.5860	-0.0012
7	4	4	6	6	3	3	5	16108.6649	-0.0011
6	5	2	7	5	4	1	6	16438.0986	0.0006
6	5	2	6	5	4	1	5	16438.4947	0.0016
6	5	2	8	5	4	1	7	16440.3303	0.0011
6	5	2	5	5	4	1	4	16440.7222	-0.0004
11	5	6	10	10	5	5	9	17504.9900	-0.0002
11	5	6	13	10	5	5	12	17505.2811	0.0007
11	5	6	11	10	5	5	10	17508.0622	0.0011
11	5	6	12	10	5	5	11	17508.3233	0.0004
11	6	5	13	10	6	4	12	17259.9230	0.0000
11	6	5	10	10	6	4	9	17259.6500	-0.0003
11	6	5	11	10	6	4	10	17262.1063	-0.0003
11	6	5	12	10	6	4	11	17262.3617	-0.0007
11	5	7	10	10	5	6	9	17298.8079	-0.0002
11	5	7	13	10	5	6	12	17298.9058	0.0004
11	5	7	11	10	5	6	10	17300.2729	-0.0067
11	5	7	12	10	5	6	11	17300.3656	0.0068
13	5	9	12	12	5	8	11	20453.8959	-0.0031
13	5	9	15	12	5	8	14	20453.9043	0.0003
13	5	9	14	12	5	8	13	20454.3023	-0.0001
13	5	9	13	12	5	8	12	20454.3894	-0.0009

Table S2. Observed rotational transitions (obs.) and residuals (obs.-cal.) for the ^{37}Cl isotopologue of isoflurane AT (in MHz).

J'	K'_{-1}	K'_{+1}	F'	J''	K''_{-1}	K''_{+1}	F''	obs.	obs.-calc.
8	1	8	8	7	1	7	7	10867.9292	-0.0008
8	1	8	9	7	1	7	8	10868.0670	0.0000
8	1	8	7	7	1	7	6	10868.5551	-0.0006
8	1	8	10	7	1	7	9	10868.6568	0.0003
8	0	8	8	7	0	7	7	10876.1333	-0.0003
8	0	8	9	7	0	7	8	10876.2277	0.0004
8	0	8	7	7	0	7	6	10876.8621	0.0001
8	0	8	10	7	0	7	9	10876.9596	0.0007
7	4	3	6	6	4	2	5	10980.9721	-0.0013
7	4	3	9	6	4	2	8	10981.6533	0.0010
7	4	3	7	6	4	2	6	10984.6432	0.0018
7	4	3	8	6	4	2	7	10985.2781	-0.0015
7	3	4	6	6	3	3	5	11330.2432	0.0002
7	3	4	9	6	3	3	8	11330.5606	-0.0003
7	3	4	7	6	3	3	6	11333.5389	-0.0002
7	3	4	8	6	3	3	7	11333.8465	0.0000
8	2	7	9	7	2	6	8	11701.0364	0.0004
8	2	7	8	7	2	6	7	11701.2778	0.0007
8	2	7	10	7	2	6	9	11702.2332	0.0010
8	2	7	7	7	2	6	6	11702.4350	0.0000
8	1	7	9	7	1	6	8	11856.3782	-0.0016
8	1	7	8	7	1	6	7	11856.9705	0.0010
8	1	7	10	7	1	6	9	11859.1541	0.0017
8	1	7	7	7	1	6	6	11859.7391	-0.0020
9	2	8	10	8	2	7	9	13036.6971	-0.0003
9	2	8	9	8	2	7	8	13036.8777	-0.0004
9	2	8	11	8	2	7	10	13037.8784	0.0002
9	2	8	8	8	2	7	7	13038.0477	-0.0008
9	2	7	10	8	2	6	9	14206.1040	-0.0004
9	2	7	9	8	2	6	8	14206.8131	0.0012
9	2	7	11	8	2	6	10	14208.9726	0.0000
9	2	7	8	8	2	6	7	14209.6803	-0.0005
11	1	11	11	10	1	10	10	14780.8757	-0.0003
11	1	11	12	10	1	10	11	14780.9684	0.0002
11	1	11	10	10	1	10	9	14781.2248	0.0007
11	1	11	13	10	1	10	12	14781.3168	-0.0005
11	0	11	11	10	0	10	10	14781.4072	-0.0009
11	0	11	12	10	0	10	11	14781.4997	0.0006
11	0	11	10	10	0	10	9	14781.7628	0.0010
11	0	11	13	10	0	10	12	14781.8540	-0.0006

Table S3. Observed rotational transitions (obs.) and residuals (obs.-cal.) for the $^{13}C(1)$ isotopologue of isoflurane AT (in MHz).

J'	K'_{-1}	K'_{+1}	F'	J''	K''_{-1}	K''_{+1}	F''	obs.	obs.-calc.
8	0	8	8	7	0	7	7	10957.2944	0.0017
8	0	8	9	7	0	7	8	10957.3944	0.0007
8	0	8	7	7	0	7	6	10958.2759	0.0028
8	0	8	10	7	0	7	9	10958.3802	0.0006
7	3	4	9	6	3	3	8	11286.0791	-0.0008
7	2	5	8	6	2	4	7	11386.9464	0.0000
7	2	5	9	6	2	4	8	11387.7912	0.0000
7	2	5	7	6	2	4	6	11387.7994	0.0020
7	2	5	6	6	2	4	5	11388.6220	0.0000
8	2	7	9	7	2	6	8	11766.8900	-0.0010
8	2	7	8	7	2	6	7	11767.2759	0.0007
8	2	7	10	7	2	6	9	11768.4314	0.0006
8	2	7	7	7	2	6	6	11768.5684	-0.0023
8	1	7	9	7	1	6	8	11950.4217	-0.0004
8	1	7	8	7	1	6	7	11951.2230	-0.0013
8	1	7	10	7	1	6	9	11954.0845	0.0004
8	1	7	7	7	1	6	6	11954.8882	0.0030
9	1	9	9	8	1	8	8	12262.3986	-0.0004
9	1	9	10	8	1	8	9	12262.5411	0.0001
9	1	9	8	8	1	8	7	12263.0637	0.0013
9	1	9	11	8	1	8	10	12263.1902	0.0013
9	0	9	9	8	0	8	8	12267.0649	0.0010
9	0	9	10	8	0	8	9	12267.1828	0.0008
9	0	9	8	8	0	8	7	12267.7972	0.0017
9	0	9	11	8	0	8	10	12267.9191	0.0009
9	1	8	10	8	1	7	9	13223.1567	-0.0032
9	1	8	9	8	1	7	8	13223.6474	-0.0007
9	1	8	11	8	1	7	10	13225.9345	-0.0002
9	1	8	8	8	1	7	7	13226.4194	0.0000
10	2	9	11	9	2	8	10	14451.8248	-0.0001
10	2	9	10	9	2	8	9	14452.0018	-0.0005
10	2	9	12	9	2	8	11	14453.2149	0.0005
10	2	9	9	9	2	8	8	14453.3808	-0.0003
10	1	9	11	9	1	8	10	14506.9255	-0.0001
10	1	9	10	9	1	8	9	14507.2163	0.0002
10	1	9	12	9	1	8	11	14508.9823	0.0007
10	1	9	9	9	1	8	8	14509.2672	0.0000
11	1	11	11	10	1	10	10	14890.3796	0.0008
11	1	11	12	10	1	10	11	14890.4863	-0.0052
11	1	11	10	10	1	10	9	14890.8318	-0.0041
11	1	11	13	10	1	10	12	14890.9512	0.0008

Table S4. Observed rotational transitions (obs.) and residuals (obs.-cal.) for the $^{13}C(2)$ isotopologue of isoflurane AT (in MHz).

J'	K'_{-1}	K'_{+1}	F'	J''	K''_{-1}	K''_{+1}	F''	obs.	obs.-calc.
8	0	8	8	7	0	7	7	10923.6625	0.0001
8	0	8	9	7	0	7	8	10923.7620	0.0014
8	0	8	7	7	0	7	6	10924.6521	0.0006
8	0	8	10	7	0	7	9	10924.7551	-0.0001
7	3	4	9	6	3	3	8	11233.5980	0.0034
7	3	4	8	6	3	3	7	11237.9037	-0.0040
7	2	5	8	6	2	4	7	11341.9521	0.0007
7	2	5	9	6	2	4	8	11342.7386	0.0018
7	2	5	7	6	2	4	6	11342.7904	-0.0006
7	2	5	6	6	2	4	5	11343.5531	-0.0009
8	2	7	9	7	2	6	8	11727.8094	0.0001
8	2	7	8	7	2	6	7	11728.2551	0.0007
8	2	7	10	7	2	6	9	11729.4055	0.0004
8	2	7	7	7	2	6	6	11729.4473	-0.0040
8	1	7	9	7	1	6	8	11915.0511	0.0040
8	1	7	10	7	1	6	9	11918.7237	-0.0021
8	1	7	7	7	1	6	6	11919.5323	-0.0016
9	1	9	9	8	1	8	8	12224.4327	0.0000
9	1	9	10	8	1	8	9	12224.5749	0.0010
9	1	9	8	8	1	8	7	12225.0980	-0.0006
9	1	9	11	8	1	8	10	12225.2235	-0.0001
9	0	9	9	8	0	8	8	12229.3007	0.0005
9	0	9	10	8	0	8	9	12229.4176	0.0008
9	0	9	8	8	0	8	7	12230.0377	0.0002
9	0	9	11	8	0	8	10	12230.1582	-0.0003
9	1	8	10	8	1	7	9	13183.7948	0.0019
9	1	8	9	8	1	7	8	13184.2900	0.0018
9	1	8	11	8	1	7	10	13186.5925	-0.0012
9	1	8	8	8	1	7	7	13187.0816	-0.0039
10	2	9	11	9	2	8	10	14405.9012	0.0004
10	2	9	10	9	2	8	9	14406.0811	0.0016
10	2	9	12	9	2	8	11	14407.2910	0.0014
10	1	9	11	9	1	8	10	14463.0674	0.0017
10	1	9	10	9	1	8	9	14463.3595	-0.0015
10	1	9	12	9	1	8	11	14465.1445	0.0010
10	1	9	9	9	1	8	8	14465.4319	-0.0024
11	1	11	11	10	1	10	10	14844.4202	0.0019
11	1	11	12	10	1	10	11	14844.5280	-0.0024
11	1	11	10	10	1	10	9	14844.8739	-0.0037
11	1	11	13	10	1	10	12	14844.9933	0.0018

Table S5. Observed rotational transitions (obs.) and residuals (obs.-cal.) for the parent species of isoflurane AG (in MHz).

J'	K'_{-1}	K'_{+1}	F'	J''	K''_{-1}	K''_{+1}	F''	obs.	obs.-calc.
4	4	1	6	3	3	1	5	12110.4020	-0.0018
4	4	0	6	3	3	1	5	12110.4347	-0.0016
8	2	7	9	7	1	6	8	12286.8739	-0.0084
8	2	7	8	7	1	6	7	12289.0991	0.0028
8	2	7	7	7	1	6	6	12299.3814	-0.0100
7	2	5	9	6	1	5	8	12396.3692	0.0050
7	2	5	6	6	1	5	5	12396.3801	0.0006
7	2	5	8	6	1	5	7	12398.5303	-0.0009
7	2	5	7	6	1	5	6	12398.6336	0.0050
9	1	8	10	8	1	7	9	12528.8704	0.0051
9	1	8	9	8	1	7	8	12529.5090	0.0085
9	1	8	11	8	1	7	10	12531.4667	0.0062
9	1	8	8	8	1	7	7	12532.0967	0.0035
9	3	6	8	8	3	5	7	12757.0751	-0.0037
9	3	6	11	8	3	5	10	12757.2443	-0.0018
9	3	6	9	8	3	5	8	12759.4895	-0.0007
9	3	6	10	8	3	5	9	12759.6303	-0.0049
6	3	4	7	5	2	3	6	12763.1087	-0.0111
6	3	4	5	5	2	3	4	12774.4470	-0.0069
6	3	3	7	5	2	3	6	12819.1681	-0.0070
6	3	3	6	5	2	3	5	12821.2272	0.0036
6	3	3	8	5	2	3	7	12826.0215	0.0047
6	3	3	5	5	2	3	4	12828.4876	-0.0063
9	2	7	10	8	2	6	9	12934.3040	-0.0061
9	2	7	11	8	2	6	10	12934.3135	-0.0033
10	0	10	10	9	1	9	9	12942.1314	0.0008
10	0	10	11	9	1	9	10	12942.2319	0.0000
10	0	10	9	9	1	9	8	12942.3275	-0.0009
10	0	10	12	9	1	9	11	12942.4543	0.0017
10	1	10	10	9	1	9	9	12971.2854	0.0005
10	1	10	11	9	1	9	10	12971.3415	0.0003
10	1	10	9	9	1	9	8	12971.8424	-0.0002
10	1	10	12	9	1	9	11	12971.9109	0.0025
10	0	10	9	9	0	9	8	12993.5656	-0.0028
10	0	10	12	9	0	9	11	12993.5779	0.0010
10	1	9	9	9	2	8	8	13015.9653	-0.0077
10	1	9	12	9	2	8	11	13016.5024	0.0010
10	1	9	10	9	2	8	9	13019.5803	0.0013
10	1	9	11	9	2	8	10	13020.0025	-0.0048
10	1	10	11	9	0	9	10	13021.8205	-0.0004
10	1	10	10	9	0	9	9	13021.8595	-0.0010
10	1	10	12	9	0	9	11	13023.0313	-0.0013
10	1	10	9	9	0	9	8	13023.0818	-0.0007
6	3	4	5	5	2	4	4	13133.1727	-0.0023
6	3	4	7	5	2	4	6	13133.9984	0.0040
6	3	3	5	5	2	4	4	13187.2225	0.0074
6	3	3	8	5	2	4	7	13187.4392	0.0101
6	3	3	6	5	2	4	5	13189.4434	0.0048
6	3	3	7	5	2	4	6	13190.0572	0.0075
9	2	8	10	8	1	7	9	13302.8319	0.0082
9	2	8	9	8	1	7	8	13304.4035	0.0049
9	2	8	11	8	1	7	10	13311.5244	0.0041

Table S5. Continued.

9	2	8	8	8	1	7	7	13313.2015	0.0107
5	4	2	6	4	3	1	5	13490.5804	0.0016
5	4	1	6	4	3	1	5	13490.8929	0.0025
5	4	2	4	4	3	1	3	13493.7314	-0.0001
5	4	1	4	4	3	1	3	13494.0209	-0.0002
5	4	2	6	4	3	2	5	13495.5080	-0.0014
5	4	1	6	4	3	2	5	13495.8209	-0.0001
5	4	2	5	4	3	2	4	13496.1733	0.0006
5	4	1	5	4	3	2	4	13496.4789	0.0007
5	4	2	7	4	3	2	6	13497.8426	0.0016
5	4	1	7	4	3	2	6	13498.1366	0.0022
5	4	2	4	4	3	2	3	13498.2393	0.0005
5	4	1	4	4	3	2	3	13498.5291	0.0006
7	3	5	8	6	2	4	7	13936.1642	-0.0084
7	3	5	7	6	2	4	6	13938.6987	-0.0054
7	3	5	9	6	2	4	8	13946.0303	-0.0055
7	3	5	6	6	2	4	5	13948.5825	-0.0082

Table S6. Observed rotational transitions (obs.) and residuals (obs.-cal.) for the ^{37}Cl isotopologue of isoflurane AG (in MHz).

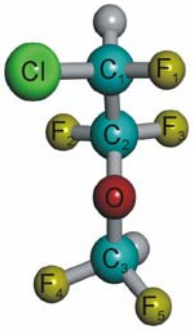
J'	K'_{-1}	K'_{+1}	F'	J''	K''_{-1}	K''_{+1}	F''	obs.	obs.-calc.
6	3	4	7	5	2	3	6	12517.3297	-0.0085
6	3	4	8	5	2	3	7	12524.4779	-0.0087
10	0	10	10	9	1	9	9	12829.1987	-0.0015
10	0	10	11	9	1	9	10	12829.2736	-0.0017
10	0	10	9	9	1	9	8	12829.4240	-0.0018
10	0	10	12	9	1	9	11	12829.5134	-0.0012
10	1	10	11	9	0	9	10	12889.4955	-0.0036
10	1	10	10	9	0	9	9	12889.5061	-0.0034
10	1	10	12	9	0	9	11	12890.3389	-0.0020
10	1	10	9	9	0	9	8	12890.3544	-0.0035
6	3	3	5	5	2	4	4	12999.6890	0.0030
6	3	3	8	5	2	4	7	13000.0513	-0.0039
6	3	3	6	5	2	4	5	13001.9510	-0.0059
6	3	3	7	5	2	4	6	13002.4185	0.0024
10	1	9	9	9	2	8	8	13022.0837	0.0001
10	1	9	12	9	2	8	11	13022.4034	0.0043
10	1	9	10	9	2	8	9	13024.3315	0.0032
10	1	9	11	9	2	8	10	13024.6059	0.0014
9	2	8	10	8	1	7	9	13074.3060	0.0058
9	2	8	9	8	1	7	8	13075.4794	0.0042
9	2	8	11	8	1	7	10	13080.7489	0.0044
9	2	8	8	8	1	7	7	13081.9639	0.0075
5	4	2	6	4	3	1	5	13208.4631	-0.0003
5	4	2	5	4	3	1	4	13208.9768	0.0077
5	4	2	7	4	3	1	6	13210.5182	0.0065
5	4	2	6	4	3	2	5	13214.5208	0.0010
5	4	1	6	4	3	2	5	13214.9387	0.0000
5	4	1	5	4	3	2	4	13215.3799	0.0005
5	4	2	7	4	3	2	6	13216.3101	0.0000
5	4	1	7	4	3	2	6	13216.7118	0.0012
5	4	1	4	4	3	2	3	13217.0757	-0.0017
7	3	5	9	6	2	4	8	13670.5722	-0.0065

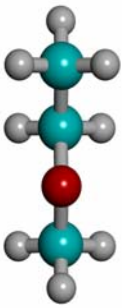
Table S7. Substitution coordinates of isoflurane.

	Substitution coordinates[a]			***Ab initio***[b]		
	Conformer 1			Conformer AT		
	$\|a\|$ / Å	$\|b\|$ / Å	$\|c\|$ / Å	a / Å	b / Å	c / Å
Cl	0.344(4)[c]	1.9868(8)	0.085(18)	-0.340	1.982	-0.105
C_1	1.3855(11)	0.491(3)	0.000[d]	-1.386	-0.502	-0.028
C_3	2.0837(7)	0.438(3)	0.420(4)	2.078	-0.443	0.422
	Conformer 2			Conformer AG		
	$\|a\|$	$\|b\|$	$\|c\|$	a	b	c
Cl	0.454(3)	1.9589(7)	0.000[d]	-0.465	1.957	0.065

[a] Principal inertial axis denoted as *a*, *b*, *c*. [b] MP2/6-311++G(2df,p). [c] Errors in parenthesis in units of the last digit, calculated as the sum of the standard errors and the Costain's estimates: $\delta z = K/|z|$ (K=0.15 Å). [d] Values in square brackets constrained to zero.

Table S8. *Ab initio* structures of the most stable conformations of enflurane and ethyl methyl ether (MP2/6-311++G(2df,p)).





	Enflurane	***Ethyl methyl ether***
	Ab initio[a] r_e	*Ab initio* r_e
r(C_1-F_1) / Å [7 b]	1.354	
r(C_1-Cl) / Å	1.753	
r(C_1-C_2) / Å	1.526	1.509
r(C_2-F_2) / Å	1.348	
r(C_2-F_3) / Å	1.354	
r(C_2-O) / Å	1.357	1.413
r(C_3-O) / Å	1.389	1.409
r(C_3-F_4) / Å	1.340	
r(C_3-F_5) / Å	1.333	
∠(C_2-C_1-F_1) / deg	108.4	
∠(Cl-C_1-C_2) / deg	110.8	
∠(C_1-C_2-O) / deg	110.2	108.4
∠(C_2-O-C_3) / deg	115.9	111.5
∠(C_1-C_2-F_2) / deg	109.5	
∠(C_1-C_2-F_3) / deg	108.1	
∠(O-C_3-F_4) / deg	109.1	
∠(O-C_3-F_5) / deg	106.7	
τ(F_1-C_1-C_2-O) / deg	60.9	
τ(Cl-C_1-C_2-O) / deg	-60.7	
τ(C_1-C_2-O-C_3) / deg	176.8	180.0
τ(F_2-C_2-O-C_3) / deg	54.7	
τ(F_3-C_2-O-C_3) / deg	-63.5	
τ(F_4-C_3-O-C_2) / deg	-99.8	
τ(F_5-C_3-O-C_2) / deg	143.6	

[a] A. Lesarri, A. Vega-Toribio, R. D. Suenram, D. J. Brugh, J.-U. Grabow, unpublished. [b] Valence angles and dihedrals denoted ∠ and τ, respectively.