

## Chiral Recognition and Atropisomerism in the Sevoflurane Dimer

### ***Electronic Supplementary Information (ESI)***

Nathan A. Seifert,<sup>a</sup> Cristóbal Pérez,<sup>a,d</sup> Justin L. Neill,<sup>a</sup> Brooks H. Pate,<sup>\*a</sup> Montserrat Vallejo-López,<sup>b</sup> Alberto Lesarri,<sup>\*b</sup> Emilio J. Cocinero,<sup>c</sup> Fernando Castaño<sup>c</sup>

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<sup>a</sup>Department of Chemistry, University of Virginia, McCormick Rd, Charlottesville, VA 22904 (USA)

E-mail: brookspate@virginia.edu, Web: <http://faculty.virginia.edu/bpate-lab>

<sup>b</sup>Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid (Spain), E-mail: lesarri@qf.uva.es, Web: [www.uva.es/lesarri](http://www.uva.es/lesarri)

<sup>c</sup>Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV-EHU), Apartado 644, 48080 Bilbao (Spain)

<sup>d</sup>Present address: Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, D-22761 Hamburg (Germany)

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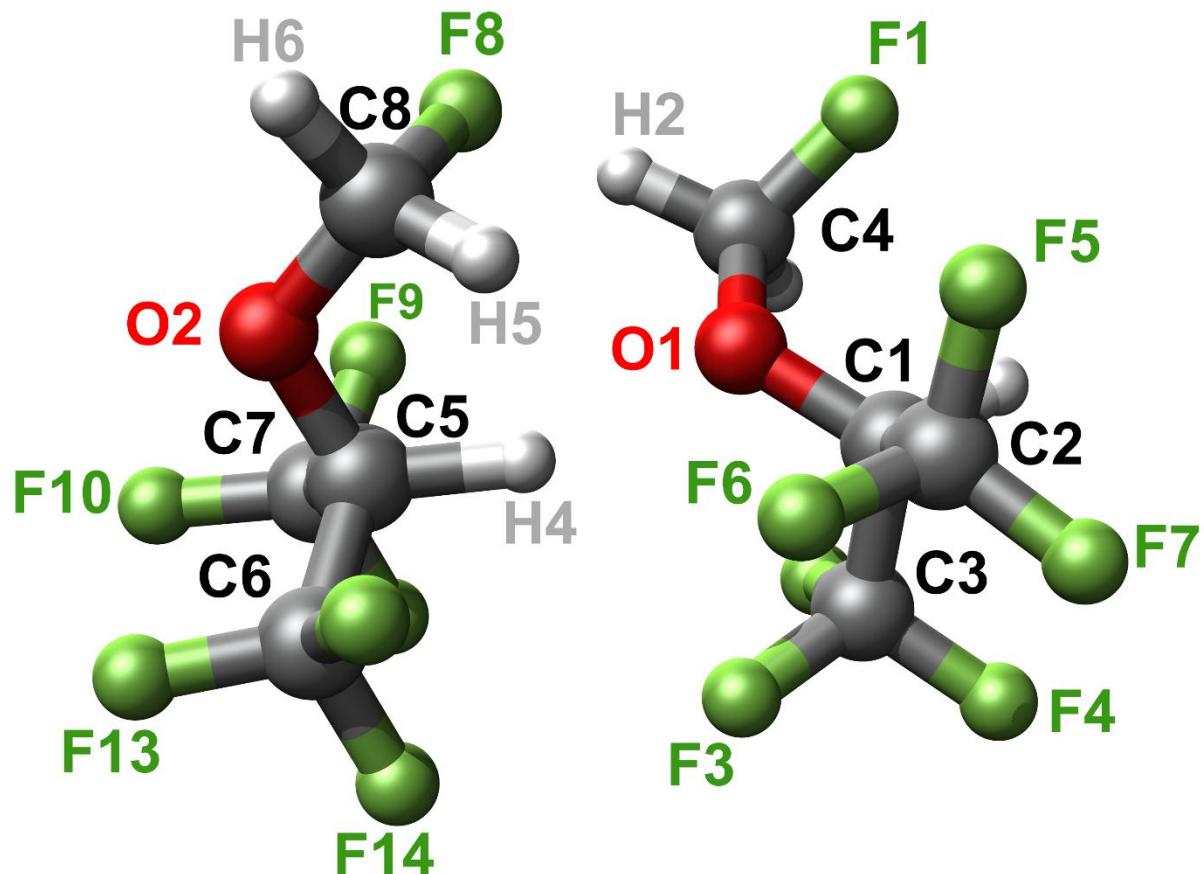
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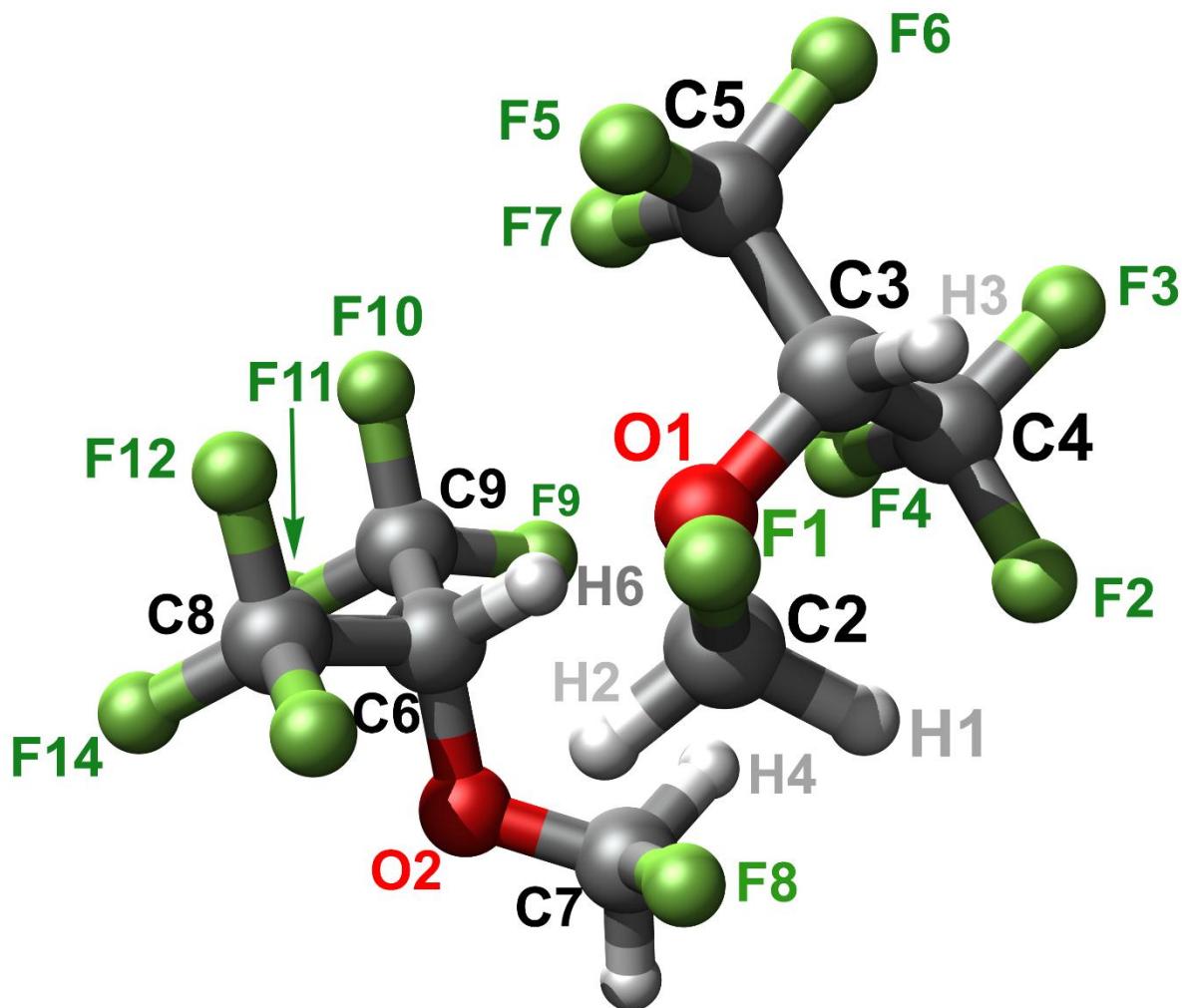




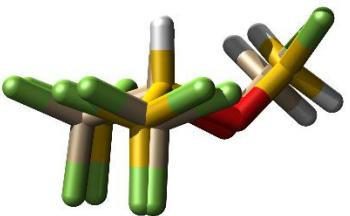
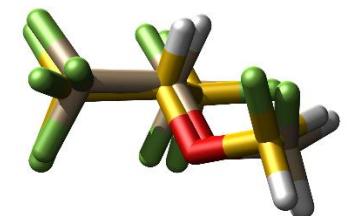
**Figure S3.** Atom labeling diagram for the heterochiral dimer, associated with parameters listed in Table S8. The monomer on the left is the *donor* (via the C-H interaction donor with H4) and the acceptor is on the right.



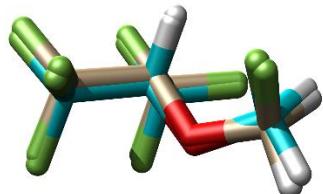
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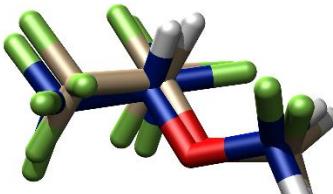
**Figure S5.** Overlaid comparison of homochiral dimer structure from experiment ( $r_0$ , beige backbone) and theory: B3LYP-D3 (top, gold backbone); MP2 (middle, teal backbone); M06-2X (bottom, dark blue backbone). The basis set used is 6-311++g(d,p) for all levels of theory.



**B3LYP-D3**

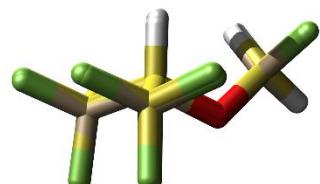
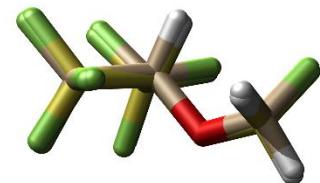


**MP2**

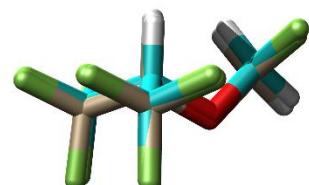
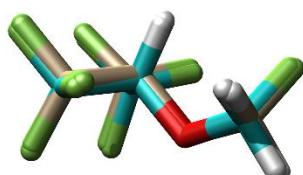


**M06-2X**

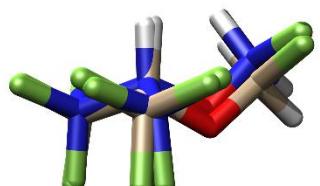
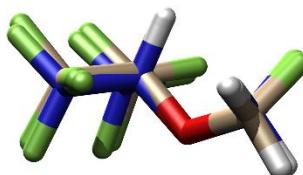
**Figure S6.** Overlaid comparison of heterochiral dimer structure from experiment ( $r_0$ , beige backbone) and theory: B3LYP-D3 (top, gold backbone); MP2 (middle, teal backbone); M06-2X (bottom, dark blue backbone). The basis set used is 6-311++g(d,p) for all levels of theory.



**B3LYP-D3**



**MP2**



**M06-2X**

**Table S1.** Experimental rotational constants for all assigned species for both homochiral and heterochiral dimers.

Homochiral		A / MHz	B	C	$\Delta_J$ / kHz	$\Delta_{JK}$	$\Delta_K$	N <sub>lines</sub>	RMS
	Parent	307.789308(39)	172.119904(23)	168.437022(23)	0.011420(29)	0.029193(43)	-0.035955(67)	1051	8.19
<b><u>Donor</u></b>									
	<i>13C (perfluoro)</i>	307.40757(60)	171.58380(25)	168.20903(32)	--	--	--	57	6.56
	<i>13C (perfluoro 2)</i>	307.46892(55)	171.77412(63)	168.0777(10)	--	--	--	68	10.4
	<i>13C (fluoromethoxy)</i>	306.59142(48)	171.62923(48)	168.27076(46)	--	--	--	76	10.0
	<i>13C (isopropyl)</i>	307.79119(43)	171.89546(30)	168.26542(35)	--	--	--	94	10.8
	<i>18O</i>	306.9748(45)	171.2038(85)	167.7374(92)	--	--	--	28	9.78
<b><u>Acceptor</u></b>									
	<i>13C (perfluoro)</i>	307.44545(43)	171.72477(29)	168.10618(35)	--	--	--	105	10.8
	<i>13C (perfluoro 2)</i>	307.37722(47)	171.67171(43)	168.14898(43)	--	--	--	87	10.0
	<i>13C (fluoromethoxy)</i>	306.71699(48)	172.02105(58)	167.95566(55)	--	--	--	70	10.8
	<i>13C (isopropyl)</i>	307.79327(50)	171.78312(38)	168.13005(55)	--	--	--	102	10.7
	<i>18O</i>	307.3765(55)	171.928(15)	168.108(20)	--	--	--	26	14.3
Heterochiral		A / MHz	B	C	$\Delta_J$ / kHz	$\Delta_{JK}$	$\Delta_K$	N <sub>lines</sub>	RMS
	Parent	304.70027(32)	175.56391(12)	167.25459(13)	0.00850(24)	0.04428(62)	0.0487(13)	726	7.25
<b><u>Donor</u></b>									
	<i>13C (perfluoro)</i>	304.306(28)	175.18860(44)	166.88015(44)	--	--	--	93	10.7
	<i>13C (perfluoro 2)</i>	304.371(44)	175.15364(46)	166.96985(44)	--	--	--	103	9.57
	<i>13C (fluoromethoxy)</i>	303.506(33)	175.25105(54)	166.87794(57)	--	--	--	101	10.0
	<i>13C (isopropyl)</i>	304.695(22)	175.35294(38)	167.06513(38)	--	--	--	137	8.82
<b><u>Acceptor</u></b>									
	<i>13C (perfluoro)</i>	304.236(22)	175.20023(36)	166.92694(32)	--	--	--	155	10.7
	<i>13C (perfluoro 2)</i>	304.393(24)	175.11316(39)	166.93244(39)	--	--	--	131	9.59
	<i>13C (fluoromethoxy)</i>	303.626(28)	175.34532(36)	166.87283(37)	--	--	--	132	10.0
	<i>13C (isopropyl)</i>	304.700(29)	175.22266(42)	166.94644(39)	--	--	--	143	10.3

**Table S2.** Optimized geometries for the homochiral and heterochiral sevoflurane dimers, optimized at the MP2/6-311++g(d,p) level of theory.

Homochiral				Heterochiral		
C	-2.261555	-0.762348	1.139877	C	2.338197	-0.245413
F	-2.379053	-0.030533	2.260896	F	2.652513	0.862577
C	-2.286325	0.175562	-0.068084	C	2.288719	0.064577
O	-1.197464	1.061836	0.031086	O	1.224562	0.969245
C	-1.527880	2.350007	0.470934	C	1.533092	2.091927
F	-2.338220	2.961483	-0.462619	F	2.494151	2.846399
C	-2.141648	-0.535456	-1.414747	C	2.044320	-1.159005
F	-3.117593	-1.435001	-1.591371	F	3.060764	-2.023900
F	-3.262412	-1.643321	1.113212	F	3.249571	-1.182413
F	-1.103935	-1.436072	1.220221	F	1.145601	-0.671174
F	-2.212241	0.359075	-2.401036	F	1.926332	-0.751329
F	-0.964774	-1.165519	-1.503711	F	0.918512	-1.793531
F	0.590629	1.446764	2.409762	F	-1.886622	-1.156281
C	1.535962	0.434992	2.521609	C	-2.292951	-1.157800
O	2.393349	0.455625	1.429959	O	-3.622669	-1.268503
C	1.815119	0.004032	0.223696	C	-1.811070	0.134727
C	2.148879	1.032942	-0.853927	C	-2.385636	1.216873
F	1.625149	0.676549	-2.032292	F	-1.483141	1.973381
C	2.329675	-1.405606	-0.064334	C	-0.758071	2.806383
F	1.944311	-2.212056	0.944540	F	-2.179406	0.275935
F	1.819473	-1.896052	-1.197206	F	-1.679886	-0.738500
F	3.660609	-1.455825	-0.140067	F	-1.772150	-2.236555
F	1.620773	2.218346	-0.510577	F	-1.648481	1.413363
F	3.464457	1.198769	-1.007022	F	-3.497809	0.323441
H	-3.251271	0.693141	-0.076553	H	3.257485	0.495319
H	-2.076711	2.322326	1.414234	H	0.613709	2.665712
H	-0.589052	2.891067	0.543194	H	1.937720	1.800625
H	0.726196	-0.038265	0.275997	H	-0.720821	0.144342
H	0.986123	-0.505016	2.595796	H	-0.764245	1.344817
H	2.148674	0.639229	3.397479	H	-2.075676	2.596356

**Table S3.** Optimized geometries for the homochiral and heterochiral sevoflurane dimers, optimized at the M06-2X/6-311++g(d,p) level of theory.

Homochiral				Heterochiral		
C	-2.274125	-0.552743	1.185625	C	2.294638	-0.425902
F	-2.509742	0.381361	2.112828	F	2.605586	0.589390
C	-2.255240	0.100783	-0.199364	C	2.268292	0.064708
O	-1.218832	1.037638	-0.254339	O	1.233594	1.005100
C	-1.575408	2.358849	0.030380	C	1.535896	2.186999
F	-2.459352	2.794270	-0.925453	F	2.559361	2.826294
C	-1.981050	-0.897160	-1.325751	C	1.992675	-1.045978
F	-2.881002	-1.880576	-1.326779	F	2.948597	-1.970217
F	-3.215616	-1.483791	1.289224	F	3.186534	-1.396494
F	-1.094060	-1.114764	1.477403	F	1.093752	-0.887123
F	-2.036961	-0.276733	-2.498287	F	1.941614	-0.507243
F	-0.768236	-1.441201	-1.198742	F	0.823812	-1.640403
F	0.285240	1.621433	2.139359	F	-1.850153	-1.492039
C	1.349887	0.797774	2.455422	C	-2.293623	-1.254565
O	2.235260	0.753560	1.392631	O	-3.623090	-1.290130
C	1.766224	0.075725	0.257686	C	-1.750748	0.097424
C	2.039276	0.955852	-0.959320	C	-2.195244	1.074639
F	1.532274	0.407368	-2.062076	F	-1.208866	1.759222
C	2.446312	-1.290505	0.190760	C	-0.652501	2.723828
F	2.083329	-1.998232	1.271955	F	-2.191646	0.493875
F	2.075031	-1.972206	-0.890278	F	-1.848176	-0.436380
F	3.772360	-1.199421	0.196111	F	-1.861969	-2.241822
F	1.457592	2.147324	-0.786261	F	-1.579803	1.633633
F	3.339516	1.163281	-1.153576	F	-3.501698	0.694371
H	-3.238357	0.546297	-0.384928	H	3.250636	0.496749
H	-2.066475	2.443487	1.000393	H	0.638506	2.796465
H	-0.658948	2.937719	-0.029608	H	1.871068	1.978090
H	0.686646	-0.085213	0.283085	H	-0.661965	0.016419
H	0.934394	-0.185079	2.685278	H	-0.399011	1.097558
H	1.885967	1.237188	3.293179	H	-1.695688	2.259367

**Table S4.** Optimized geometries for the homochiral and heterochiral sevoflurane dimers, optimized at the B3LYP-D3/6-311++g(d,p) level of theory.

Homochiral				Heterochiral			
C	-2.328682	0.482247	-1.229821	O	1.230390	1.005816	0.287978
F	-2.510558	-0.485692	-2.153306	C	2.313789	0.114281	0.165413
C	-2.314521	-0.156760	0.171984	C	2.339846	-0.328994	-1.308189
O	-1.220750	-1.036711	0.272057	C	2.142792	-1.048152	1.162229
C	-1.480127	-2.393868	0.027849	C	1.449452	2.161789	1.053190
F	-2.353466	-2.877861	0.992709	F	2.440758	2.929610	0.459809
C	-2.157657	0.860760	1.316813	F	2.026704	-0.537838	2.407515
F	-3.144855	1.772315	1.293747	F	1.043835	-1.772833	0.912318
F	-3.315576	1.375225	-1.371201	F	3.206747	-1.865548	1.151095
F	-1.160500	1.092759	-1.514824	F	2.653232	0.717668	-2.086518
F	-2.206492	0.222652	2.492974	F	1.136500	-0.788755	-1.707121
F	-0.982952	1.510332	1.241180	F	3.247439	-1.294251	-1.516335
H	-3.274045	-0.659132	0.321564	H	3.275273	0.592112	0.370512
H	-1.946880	-2.549836	-0.945658	H	0.511211	2.708668	1.034208
H	-0.523131	-2.899251	0.119812	H	1.787763	1.918003	2.062559
F	0.477985	-1.904949	-2.085258	C	-1.839464	0.112159	-0.202032
C	1.406737	-0.904524	-2.399609	O	-2.425053	1.184592	-0.907453
O	2.306081	-0.741843	-1.356062	C	-2.337126	-1.205773	-0.820405
C	1.831831	-0.046278	-0.221577	C	-2.176395	0.277619	1.288433
C	2.245952	-0.849566	1.021210	C	-1.576229	1.926161	-1.719300
F	1.823694	-0.245168	2.143970	F	-0.833838	2.823494	-0.949787
C	2.378772	1.391531	-0.255169	F	-1.629056	1.425485	1.742975
F	1.948814	1.983613	-1.394281	F	-3.493337	0.332336	1.520457
F	1.925733	2.116694	0.778006	F	-1.660131	-0.730986	2.012775
F	3.717124	1.439844	-0.252431	F	-1.989386	-1.221548	-2.126386
F	1.675443	-2.071074	0.971975	F	-3.667766	-1.344096	-0.749670
F	3.571510	-1.021356	1.107884	F	-1.768863	-2.270442	-0.232307
H	0.743693	0.019300	-0.190775	H	-0.751108	0.110961	-0.271925
H	0.833674	0.001383	-2.605475	H	-0.860384	1.298887	-2.256529
H	1.983268	-1.244446	-3.257912	H	-2.210727	2.506061	-2.387353

**Table S5.** Kraitchman coordinates for atoms with assigned isotopologues, homochiral dimer. Values with entry [0] are imaginary and set to zero. Labeling scheme can be found in Figure S4.

	Acceptor		
	$ a $ (Å)	$ b $ (Å)	$ c $ (Å)
C2 (fluoromethoxy)	1.5039(26)	2.5278(15)	[0]
C3 (isopropyl)	/2.3715(14)	[0]	0.3589(94)
C4 ( <i>anti</i> -perfluoro)	2.341(11)	0.6956(37)	1.1655(22)
C5 ( <i>syn</i> -perfluoro)	2.3000(14)	[0]	1.5379(20)
O1	2.44246(90)	0.5252(40)	1.3885(16)

	Donor		
	$ a $ (Å)	$ b $ (Å)	$ c $ (Å)
C7 (fluoromethoxy)	1.5681(21)	0.6691(46)	2.442(14)
C6 (isopropyl)	1.8574(14)	[0]	0.6167(42)
C8 ( <i>syn</i> -perfluoro)	2.3014(25)	1.0490(54)	0.7849(74)
C9 ( <i>anti</i> -perfluoro)	2.3641(58)	[0]	1.8706(72)
O2	1.2274(18)	1.2067(18)	[0]

**Table S6.** Kraitchman coordinates for atoms with assigned isotopologues, heterochiral dimer. Values with entry [0] are imaginary and set to zero. Labeling scheme can be found in Figure S3.

	Acceptor		
	$ a $ (Å)	$ b $ (Å)	$ c $ (Å)
C1 (isopropyl)	2.363(21)	[0]	0.12(39)
C2 ( <i>syn</i> -perfluoro)	2.402(18)	0.22(20)	1.278(34)
C3 ( <i>anti</i> -perfluoro)	2.162(17)	1.111(33)	1.141(33)
C4 (fluoromethoxy)	1.517(26)	2.136(18)	1.147(35)

	Donor		
	$ a $ (Å)	$ b $ (Å)	$ c $ (Å)
C5 (isopropyl)	1.851(20)	[0]	0.18(20)
C6 ( <i>anti</i> -perfluoro)	2.320(20)	1.174(39)	0.882(53)
C7 ( <i>syn</i> -perfluoro)	2.244(33)	0.32(23)	1.303(57)
C8 (fluoromethoxy)	1.643(34)	2.01(28)	1.580(37)

**Table S7.** Least-squares fit effective ground-state experimental geometries ( $r_0$ ) for the homochiral and heterochiral sevoflurane dimers. The homochiral fit has a  $\chi^2$  of 1.79 and a deviation of fit of 0.253 amu Å<sup>2</sup>. The heterochiral fit has a  $\chi^2$  of 0.962 and a deviation of 0.209 amu Å<sup>2</sup>.

	Homochiral			Heterochiral			
O	1.312201	1.081806	0.053448	C	-2.375928	0.089056	0.200647
C	1.417271	2.326059	0.489586	C	-2.436388	-0.288819	-1.279864
C	2.414714	0.212611	-0.046049	C	-2.135477	-1.094533	1.139090
C	2.384567	-0.749209	1.142837	O	-1.268240	1.008571	0.377056
C	2.300585	-0.473597	-1.408426	C	-1.520097	2.171266	1.117426
F	2.185151	3.059149	-0.390762	F	-2.493680	2.916879	0.488870
F	2.474683	-0.038127	2.279623	F	-2.007074	-0.629769	2.393228
F	3.397912	-1.615736	1.114556	F	-1.016366	-1.752345	0.827872
F	1.235370	-1.440129	1.191985	F	-3.158671	-1.953713	1.118528
F	2.373760	0.441107	-2.375843	F	-2.746397	0.789407	-2.004105
F	3.291575	-1.356071	-1.587369	F	-1.249596	-0.743753	-1.713235
F	1.134117	-1.117791	-1.527980	F	-3.356270	-1.230467	-1.507652
H	1.905582	2.368333	1.465066	H	-3.339870	0.539296	0.459275
H	0.406857	2.723812	0.504462	H	-0.587539	2.727891	1.122105
H	3.372359	0.743383	-0.029392	H	-1.886783	1.932350	2.118371
C	-1.898249	-0.036952	0.209488	C	1.890253	0.110494	-0.219883
O	-2.471012	0.381840	1.430106	C	2.372873	-1.212801	-0.811450
C	-1.649378	0.376963	2.503641	C	2.221629	0.306521	1.257241
C	-2.257367	1.008421	-0.843865	O	2.496425	1.157082	-0.944670
C	-2.395285	-1.447873	-0.102069	C	1.623121	1.893695	-1.736023
F	-0.732558	1.416639	2.412200	F	0.886955	2.767855	-0.953663
F	-1.988448	-2.268720	0.886559	F	1.692684	1.468288	1.676264
F	-1.889258	-1.907972	-1.249451	F	3.534994	0.346608	1.484405
F	-3.72604	-1.51596	-0.166085	F	1.690786	-0.672457	2.001782
F	-1.743013	2.194262	-0.481668	F	2.000295	-1.258089	-2.103675
F	-1.740190	0.683444	-2.034146	F	3.700391	-1.338324	-0.762125
F	-3.576637	1.158091	-0.981000	F	1.823203	-2.260787	-0.189141
H	-1.073391	-0.547296	2.577293	H	0.629411	0.113482	-0.333327
H	-2.278812	0.555912	3.373161	H	0.910518	1.252652	-2.260265
H	-0.842404	-0.052668	0.248281	H	2.240693	2.482524	-2.411711

**Table S8.** Full parameter listing for  $r_0$  experimental geometry of heterochiral dimer, associated with the geometry listing in Table S5. Labeling scheme can be found in Figure S3.

<b>Bond Lengths</b>				<b>Bond Angles</b>			
<b>Acceptor</b>				<b>Acceptor</b>			
O1 C4 = 1.40123 +- 0.01257	C1 O1 C4 F1 = 116.93951 +- 2.80477	C4 F1 = 1.37800 +- 0.04353	O1 C4 F1 = 109.56968 +- 1.75500	C1 H1 = 1.09489 +- 0.01513	F1 C4 H3 = 107.40522 +- 3.75864	C1 O1 = 1.45038 +- 0.02974	F1 C4 H2 = 109.34868 +- 1.71858
C1 H1 = 1.09489 +- 0.01513	O1 C1 H1 = 112.51645 +- 1.25936	C1 C2 = 1.52917 +- 0.00421	C3 C2 C1 = 32.93224 +- 0.38966	C1 C2 = 1.52917 +- 0.00421	C1 C2 F6 = 111.17612 +- 1.18952	C3 F4 = 1.33624 +- 0.02441	F6 C2 F5 = 107.67872 +- 1.21774
C1 C2 = 1.52917 +- 0.00421	F5 C2 F7 = 108.46937 +- 1.40167	C3 F4 = 1.33624 +- 0.02441	F5 C2 F7 = 108.46937 +- 1.40167	<b>Donor</b>			
C5 H4 = 1.26594 +- 0.03541	C5 O2 C8 = 114.57969 +- 0.91424	C5 O2 = 1.41001 +- 0.01093	O2 C8 F8 = 110.29707 +- 0.52198	O2 C8 = 1.38979 +- 0.01563	F8 C8 H5 = 107.14028 +- 1.78487	C8 F8 = 1.38498 +- 0.01402	F8 C8 H6 = 108.10903 +- 1.07751
O2 C8 = 1.38979 +- 0.01563	O2 C5 H4 = 112.35609 +- 1.13222	C8 H5 = 1.09251 +- 0.02219	C7 C5 C6 = 114.66776 +- 0.53932	C8 F8 = 1.38498 +- 0.01402	C5 C7 F10 = 112.49000 +- 1.02733	C8 H5 = 1.09251 +- 0.02219	F14 C6 F13 = 108.54613 +- 0.92413
C8 F8 = 1.38498 +- 0.01402	F14 C6 F13 = 108.54613 +- 0.92413	C8 H5 = 1.09251 +- 0.02219	C7 C5 C6 = 114.66776 +- 0.53932	C8 H5 = 1.09251 +- 0.02219	C5 C7 F10 = 112.49000 +- 1.02733	C8 H5 = 1.09251 +- 0.02219	F14 C6 F13 = 108.54613 +- 0.92413
C8 H5 = 1.09251 +- 0.02219	F14 C6 F13 = 108.54613 +- 0.92413	C5 C7 = 1.52647 +- 0.00544	O2 C5 C7 F10 = -57.18185 +- 0.95648	C5 C7 = 1.52647 +- 0.00544	O2 C5 C7 F10 = -57.18185 +- 0.95648	C5 C6 = 1.52773 +- 0.01095	O2 C5 C6 F13 = 58.73625 +- 0.83505
C5 C6 = 1.52773 +- 0.01095	O2 C5 C6 F13 = 58.73625 +- 0.83505	C7 F10 = 1.33346 +- 0.02423	O2 C5 C6 F13 = 58.73625 +- 0.83505	<b>Bond Dihedrals</b>			
<b>Acceptor</b>				<b>Donor</b>			
C1 O1 C4 F1 = -61.26898 +- 2.13365	C5 O2 C8 F8 = 76.80511 +- 1.15311	C4 O1 C1 H1 = 14.36991 +- 1.22874	C8 O2 C5 H4 = -6.05479 +- 1.69061	C4 O1 C1 C2 = 132.30224 +- 0.92940	C8 O2 C5 C7 = -124.57999 +- 0.80208	C4 O1 C1 C3 = -104.42389 +- 1.22484	C8 O2 C5 C6 = 110.92401 +- 0.71120
C4 O1 C1 C2 = 132.30224 +- 0.92940	C8 O2 C5 C7 = -124.57999 +- 0.80208	O1 C1 C3 F7 = -144.86886 +- 1.11022	O2 C5 C7 F10 = -57.18185 +- 0.95648	O1 C1 C3 F7 = -144.86886 +- 1.11022	O2 C5 C7 F10 = -57.18185 +- 0.95648	O1 C1 C2 F6 = 53.28472 +- 1.28418	O2 C5 C6 F13 = 58.73625 +- 0.83505
O1 C1 C3 F7 = -144.86886 +- 1.11022	O2 C5 C6 F13 = 58.73625 +- 0.83505	O1 C1 C2 F6 = 53.28472 +- 1.28418	<b>Intermolecular Parameters</b>				
<b>Lengths</b>				<b>Angles / Dihedrals</b>			
O1 H4 = 2.21516 +- 0.04515	C5 H4 O1 = 145.63228 +- 1.88795	F6 H4 = 2.48388 +- 0.03830	C5 H4 C1 = 164.77194 +- 2.34596	F3 H4 = 2.74560 +- 0.02989	C7 C5 C1 C2 = -173.05380 +- 0.58406	H2 F9 = 2.66328 +- 0.04197	C6 C5 C1 C3 = 61.16463 +- 0.40131
F6 H4 = 2.48388 +- 0.03830	C6 C5 C1 C3 = 61.16463 +- 0.40131	F3 H4 = 2.74560 +- 0.02989	C8 C5 C1 C4 = -66.32546 +- 0.25408	H2 F8 = 2.54648 +- 0.02904			
F3 H4 = 2.74560 +- 0.02989				F6 H5 = 2.99182 +- 0.02495			

**Table S9.** Full parameter listing for  $r_0$  experimental geometry of homochiral dimer, associated with the geometry listing in Table S5. Labeling scheme can be found in Figure S4.

<b>Bond Lengths</b>				<b>Bond Angles</b>			
<b>Acceptor</b>				<b>Donor</b>			
C1 C2 = 1.32265 +- 0.02191		C3 O1 C2 = 122.82284 +- 1.56728		C6 O2 C7 = 116.03441 +- 2.05580		O2 C7 F8 = 110.25120 +- 3.69275	
C2 F1 = 1.37916 +- 0.05648		O1 C2 F1 = 109.49863 +- 3.21481		F8 C7 H5 = 108.13424 +- 5.91697		F8 C7 H4 = 106.85198 +- 4.67763	
C2 H1 = 1.09169 +- 0.05933		F1 C2 H1 = 107.50258 +- 3.60473		O2 C6 H6 = 112.21200 +- 0.93940		O2 C6 H6 = 112.21200 +- 0.93940	
O1 C3 = 1.40746 +- 0.00699		F1 C2 H2 = 109.39542 +- 3.09691		C8 C6 C9 = 114.52023 +- 1.72254		C8 C6 C9 = 114.52023 +- 1.72254	
C3 C4 = 1.52953 +- 0.02646		O1 C3 H3 = 112.62164 +- 0.76815		C6 C8 F14 = 112.34078 +- 1.96397		C6 C8 F14 = 112.34078 +- 1.96397	
C3 H3 = 1.09503 +- 0.00801		C5 C3 C4 = 114.12381 +- 1.83323		F10 C9 F9 = 107.81386 +- 2.86927		F10 C9 F9 = 107.81386 +- 2.86927	
C3 C5 = 1.52970 +- 0.02545		C3 C5 F7 = 111.13902 +- 1.69125					
C4 F3 = 1.33362 +- 0.03759		F7 C5 F5 = 108.26013 +- 2.35301					
		F5 C5 F6 = 108.33324 +- 2.26464					
<b>Bond Dihedrals</b>				<b>Intermolecular Parameters</b>			
<b>Acceptor</b>				<b>Lengths</b>			
C3 O1 C2 F1 = 65.06818 +- 4.33624		C6 O2 C7 F8 = 72.42318 +- 5.30478		O1 H6 = 2.44281 +- 0.02241		C6 H6 O1 = 150.63216 +- 1.15230	
C2 O1 C3 H3 = -17.70456 +- 4.52712		C7 O2 C6 H6 = -15.28614 +- 4.87835		F7 H6 = 2.86290 +- 0.03595		C6 H6 C3 = 170.89740 +- 0.96807	
C2 O1 C3 C5 = -134.88059 +- 3.22398		C7 O2 C6 C8 = -130.97971 +- 3.95710		H4 H6 = 2.67072 +- 0.03369		O2 C6 C3 O1 = -66.88152 +- 3.02104	
C2 O1 C3 C4 = 101.91283 +- 3.05166		C7 O2 C6 C9 = 104.73194 +- 4.06179		H2 F12 = 2.42380 +- 0.04970		C8 C6 C3 C5 = -71.23418 +- 1.82303	
O1 C3 C4 F4 = 57.54450 +- 2.57867		O2 C6 C8 F14 = -58.70455 +- 2.52641		H2 F8 = 2.57807 +- 0.05036		C9 C6 C3 C4 = -64.99871 +- 2.10622	
O1 C3 C5 F7 = -57.50304 +- 3.41121		O2 C6 C9 F11 = 57.61184 +- 3.61983		F4 H4 = 2.83665 +- 0.06037			
<b>Donor</b>				<b>Angles / Dihedrals</b>			

Table S10. Linelist for sevoflurane dimer (homochiral), parent species. RMS error for the fit is 8.19 kHz.

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}$ (MHz)	OMC (MHz)
7	1	6	6	2	4	2016.1547	-0.0001
6	1	6	5	1	5	2031.7140	-0.0025
6	0	6	5	0	5	2040.7739	-0.0013
6	2	5	5	2	4	2042.9958	-0.0017
6	4	3	5	4	2	2043.5757	-0.0017
6	3	4	5	3	3	2043.7251	0.0152
6	3	3	5	3	2	2043.7655	0.0037
6	2	4	5	2	3	2045.5523	-0.0014
8	2	6	7	3	4	2048.4345	-0.0006
4	3	2	3	2	1	2049.6083	0.0095
4	3	2	3	2	2	2049.9604	-0.0080
28	8	21	28	7	21	2052.0446	0.0061
27	8	20	27	7	20	2053.4372	0.0025
6	1	5	5	1	4	2053.7610	-0.0009
26	8	19	26	7	19	2054.6886	0.0046
25	8	18	25	7	18	2055.7988	0.0008
24	8	17	24	7	17	2056.7877	0.0000
23	8	16	23	7	16	2057.6624	-0.0007
22	8	15	22	7	15	2058.4355	0.0016
21	8	14	21	7	14	2059.1098	0.0008
20	8	13	20	7	13	2059.6962	-0.0009
19	8	12	19	7	12	2060.2070	0.0008
18	8	11	18	7	11	2060.6430	-0.0008
17	8	10	17	7	10	2061.0165	-0.0009
16	8	9	16	7	9	2061.3337	0.0002
15	8	8	15	7	8	2061.5994	0.0009
14	8	7	14	7	7	2061.8172	-0.0010
13	8	6	13	7	6	2061.9995	0.0009
12	8	5	12	7	5	2062.1429	-0.0014
11	8	4	11	7	4	2062.2597	-0.0009
10	8	3	10	7	3	2062.3470	-0.0047
9	8	2	9	7	2	2062.4246	0.0030
5	2	3	4	1	3	2099.4480	0.0000
5	2	3	4	1	4	2136.2670	-0.0033
6	1	6	5	0	5	2143.6714	-0.0064
11	4	8	11	1	11	2199.6665	0.0040
6	1	5	5	0	5	2220.9399	-0.0005
8	1	8	7	2	6	2243.3899	-0.0006
7	0	7	6	1	6	2276.9324	0.0000
12	6	6	11	7	5	2300.2396	-0.0016
4	4	1	3	3	0	2324.8098	-0.0018
32	9	24	32	8	24	2325.3815	0.0006
31	9	23	31	8	23	2326.8019	-0.0002
30	9	22	30	8	22	2328.0918	-0.0011
29	9	21	29	8	21	2329.2721	0.0098
28	9	20	28	8	20	2330.3168	-0.0014
27	9	19	27	8	19	2331.2670	-0.0020
26	9	18	26	8	18	2332.1223	0.0001
25	9	17	25	8	17	2332.8841	-0.0006
24	9	16	24	8	16	2333.5631	-0.0006
23	9	15	23	8	15	2334.1657	0.0000
22	9	14	22	8	14	2334.6969	-0.0001
21	9	13	21	8	13	2335.1634	0.0000
20	9	12	20	8	12	2335.5706	0.0000
19	9	11	19	8	11	2335.9244	0.0003
18	9	10	18	8	10	2336.2285	-0.0003
17	9	9	17	8	9	2336.4896	0.0000
16	9	8	16	8	8	2336.7115	0.0004
15	9	7	15	8	7	2336.8990	0.0014
14	9	6	14	8	6	2337.0513	-0.0015

13	9	5	13	8	5	2337.1793	-0.0017
12	9	4	12	8	4	2337.2928	0.0075
11	9	3	11	8	3	2337.3656	-0.0034
10	9	2	10	8	2	2337.4326	-0.0027
8	1	7	7	2	5	2366.3664	-0.0003
7	1	7	6	1	6	2370.0770	-0.0016
9	2	8	8	3	5	2371.4524	-0.0422
9	2	8	8	3	6	2371.9212	-0.0006
7	0	7	6	0	6	2379.8338	-0.0014
7	2	6	6	2	5	2383.3035	-0.0028
7	6	1	6	6	0	2384.0640	-0.0112
7	5	2	6	5	1	2384.1358	0.0006
7	4	4	6	4	3	2384.2409	-0.0030
7	3	5	6	3	4	2384.4333	-0.0033
7	3	4	6	3	3	2384.5510	-0.0023
7	2	5	6	2	4	2387.3515	-0.0013
5	3	2	4	2	2	2389.7391	-0.0024
5	3	3	4	2	3	2390.8230	0.0000
9	2	7	8	3	5	2394.9951	-0.0017
7	1	6	6	1	5	2395.7398	-0.0025
6	2	5	5	1	4	2428.2108	-0.0046
14	8	6	13	9	4	2431.1495	0.0013
6	2	4	5	1	4	2433.3489	-0.0004
10	3	8	9	4	6	2445.3805	0.0024
10	3	7	9	4	5	2446.9426	0.0000
7	1	7	6	0	6	2472.9795	-0.0018
6	2	5	5	1	5	2483.4324	-0.0002
6	2	4	5	1	5	2488.5634	-0.0032
15	9	6	14	10	4	2496.6204	-0.0023
8	0	8	7	1	6	2522.3794	-0.0028
9	1	9	8	2	7	2566.3377	-0.0017
12	5	8	11	6	5	2575.8359	0.0088
7	1	6	6	0	6	2575.9074	-0.0001
34	10	25	34	9	25	2601.4386	-0.0021
33	10	24	33	9	24	2602.6584	-0.0002
32	10	23	32	9	23	2603.7736	0.0013
31	10	22	31	9	22	2604.7885	0.0001
30	10	21	30	9	21	2605.7096	-0.0032
29	10	20	29	9	20	2606.5383	-0.0135
28	10	19	28	9	19	2607.3097	-0.0012
27	10	18	27	9	18	2607.9931	-0.0024
26	10	17	26	9	17	2608.6102	-0.0008
25	10	16	25	9	16	2609.1626	0.0002
24	10	15	24	9	15	2609.6532	-0.0010
23	10	14	23	9	14	2610.0901	-0.0009
22	10	13	22	9	13	2610.4756	-0.0018
21	10	12	21	9	12	2610.8168	-0.0008
20	10	11	20	9	11	2611.1145	-0.0009
19	10	10	19	9	10	2611.3733	-0.0013
18	10	9	18	9	9	2611.5968	-0.0020
17	10	8	17	9	8	2611.7897	-0.0017
16	10	7	16	9	7	2611.9534	-0.0023
15	10	6	15	9	6	2612.0931	-0.0017
14	10	5	14	9	5	2612.2098	-0.0015
13	10	4	13	9	4	2612.3074	-0.0006
8	0	8	7	1	7	2625.3088	0.0003
13	6	8	12	7	6	2641.1242	-0.0024
5	4	1	4	3	1	2665.3719	-0.0049
18	5	14	18	2	16	2706.5043	0.0044
8	1	8	7	1	7	2708.3325	-0.0017
10	2	9	9	3	7	2709.5791	0.0010
9	1	8	8	2	6	2716.0607	-0.0015
8	0	8	7	0	7	2718.4521	-0.0025

8	2	7	7	2	6	2723.5257	-0.0015
8	5	4	7	5	3	2724.7837	0.0016
8	4	5	7	4	4	2724.9416	-0.0010
8	3	6	7	3	5	2725.2025	0.0008
8	3	5	7	3	4	2725.4327	-0.0016
6	3	3	5	2	3	2729.4212	0.0016
8	2	6	7	2	5	2729.4966	-0.0049
6	3	4	5	2	4	2731.9169	-0.0025
8	1	7	7	1	6	2737.5629	-0.0017
10	2	8	9	3	6	2743.3733	-0.0009
10	2	8	9	3	7	2744.2293	0.0028
7	2	6	6	1	5	2757.7573	-0.0025
7	2	5	6	1	5	2766.9387	-0.0016
11	3	9	10	4	7	2786.6036	-0.0059
11	3	8	10	4	6	2789.3275	0.0005
8	1	8	7	0	7	2801.4821	0.0016
7	2	6	6	1	6	2835.0219	-0.0005
9	0	9	8	1	7	2841.4381	-0.0034
12	4	9	11	5	7	2851.9577	-0.0004
12	4	8	11	5	6	2852.0765	-0.0045
36	11	26	36	10	26	2877.1501	-0.0048
35	11	25	35	10	25	2878.2233	-0.0051
34	11	24	34	10	24	2879.2143	-0.0017
33	11	23	33	10	23	2880.1241	0.0014
32	11	22	32	10	22	2880.9540	0.0009
31	11	21	31	10	21	2881.7100	-0.0018
30	11	20	30	10	20	2882.4038	0.0004
29	11	19	29	10	19	2883.0303	-0.0017
28	11	18	28	10	18	2883.6020	0.0001
27	11	17	27	10	17	2884.1164	-0.0001
26	11	16	26	10	16	2884.5803	0.0000
25	11	15	25	10	15	2884.9968	0.0003
24	11	14	24	10	14	2885.3696	0.0010
23	11	13	23	10	13	2885.7007	0.0007
22	11	12	22	10	12	2885.9945	0.0006
21	11	11	21	10	11	2886.2535	0.0001
20	11	10	20	10	10	2886.4822	0.0010
19	11	9	19	10	9	2886.6800	-0.0002
18	11	8	18	10	8	2886.8527	-0.0004
17	11	7	17	10	7	2887.0013	-0.0011
16	11	6	16	10	6	2887.1311	0.0007
12	11	2	12	10	2	2887.4736	0.0014
13	5	8	12	6	6	2916.9077	0.0023
8	1	7	7	0	7	2933.6361	-0.0009
5	5	1	4	4	1	2940.3894	0.0003
9	0	9	8	1	8	2973.5955	-0.0025
14	6	9	13	7	7	2982.0794	-0.0022
6	4	2	5	3	2	3005.9167	0.0023
11	2	10	10	3	8	3046.2894	-0.0014
9	1	9	8	1	8	3046.4747	-0.0014
15	7	9	14	8	7	3047.3953	0.0043
9	0	9	8	0	8	3056.6222	-0.0016
9	2	8	8	2	7	3063.6460	-0.0025
10	1	9	9	2	7	3064.6679	-0.0022
9	7	2	8	7	1	3065.2488	-0.0027
9	6	3	8	6	2	3065.3358	0.0078
9	5	4	8	5	3	3065.4517	0.0001
9	4	6	8	4	5	3065.6834	0.0058
9	3	7	8	3	6	3066.0012	-0.0008
9	3	6	8	3	5	3066.4250	-0.0020
7	3	5	6	2	4	3068.2226	-0.0020
7	3	4	6	2	4	3068.4178	-0.0013
9	2	7	8	2	6	3071.9935	-0.0024

7	3	5	6	2	5	3073.3566	-0.0020
7	3	4	6	2	5	3073.5505	-0.0026
9	1	8	8	1	7	3079.1953	-0.0018
8	2	7	7	1	6	3085.5425	-0.0023
11	2	9	10	3	7	3093.6860	0.0012
8	2	6	7	1	6	3100.6981	-0.0014
16	8	8	15	9	6	3112.7648	-0.0009
12	3	10	11	4	8	3127.8853	0.0000
9	1	9	8	0	8	3129.5002	-0.0018
12	3	9	11	4	7	3132.3716	-0.0002
39	12	28	39	11	28	3151.5915	-0.0021
38	12	27	38	11	27	3152.6340	-0.0036
37	12	26	37	11	26	3153.6036	-0.0014
36	12	25	36	11	25	3154.4980	-0.0016
35	12	24	35	11	24	3155.3233	-0.0020
34	12	23	34	11	23	3156.0851	-0.0010
10	0	10	9	1	8	3156.6033	-0.0020
33	12	22	33	11	22	3156.8098	0.0241
32	12	21	32	11	21	3157.4262	-0.0011
31	12	20	31	11	20	3158.0134	-0.0011
30	12	19	30	11	19	3158.5496	-0.0010
29	12	18	29	11	18	3159.0391	0.0001
28	12	17	28	11	17	3159.4829	0.0006
27	12	16	27	11	16	3159.8835	-0.0002
26	12	15	26	11	15	3160.2457	-0.0003
25	12	14	25	11	14	3160.5730	0.0009
24	12	13	24	11	13	3160.8643	0.0000
23	12	12	23	11	12	3161.1258	0.0004
22	12	11	22	11	11	3161.3587	0.0010
21	12	10	21	11	10	3161.5631	-0.0002
19	12	8	19	11	8	3161.9045	0.0005
18	12	7	18	11	7	3162.0449	0.0020
17	12	6	17	11	6	3162.1638	0.0003
16	12	5	16	11	5	3162.2686	0.0011
15	12	4	15	11	4	3162.3551	-0.0015
13	12	2	13	11	2	3162.5116	0.0147
8	2	7	7	1	7	3188.4704	-0.0005
13	4	10	12	5	8	3193.3760	-0.0068
13	4	9	12	5	7	3193.6127	-0.0013
8	2	6	7	1	7	3203.6199	-0.0057
11	1	11	10	2	9	3205.9355	-0.0014
18	10	8	17	11	6	3243.5999	0.0005
14	5	9	13	6	7	3258.0929	-0.0039
6	5	2	5	4	2	3280.9560	-0.0023
9	1	8	8	0	8	3294.3790	-0.0005
10	0	10	9	1	9	3321.4835	0.0007
15	6	10	14	7	8	3323.1168	0.0011
7	4	3	6	3	3	3346.3867	-0.0110
7	4	4	6	3	4	3346.4638	-0.0102
10	1	10	9	1	9	3384.4982	-0.0017
10	0	10	9	0	9	3394.3592	-0.0016
10	2	9	9	2	8	3403.6554	-0.0028
10	8	2	9	8	1	3405.8051	-0.0001
10	7	3	9	7	2	3405.8737	-0.0014
27	6	21	27	3	24	3405.9756	0.0315
10	5	6	9	5	5	3406.1460	-0.0001
8	3	5	7	2	5	3406.4921	-0.0086
10	3	8	9	3	7	3406.8301	-0.0020
10	3	7	9	3	6	3407.5545	-0.0023
11	1	10	10	2	8	3411.6093	-0.0024
10	2	8	9	2	7	3414.8035	-0.0008
8	3	6	7	2	6	3415.2521	-0.0019
8	3	5	7	2	6	3415.6845	0.0033

10	1	9	9	1	8	3420.6033	-0.0005
36	13	24	36	12	25	3431.1391	-0.0013
35	13	23	35	12	23	3431.7922	-0.0029
34	13	22	34	12	22	3432.3918	-0.0074
32	13	20	32	12	20	3433.4495	-0.0171
31	13	19	31	12	19	3433.9334	-0.0018
30	13	18	30	12	18	3434.3628	-0.0012
29	13	17	29	12	17	3434.7539	-0.0013
28	13	16	28	12	16	3435.1301	0.0188
27	13	15	27	12	15	3435.4338	-0.0005
26	13	14	26	12	14	3435.7263	-0.0004
25	13	13	25	12	13	3435.9899	-0.0006
24	13	12	24	12	12	3436.2287	0.0008
23	13	11	23	12	11	3436.4410	0.0006
22	13	10	22	12	10	3436.6310	0.0006
21	13	9	21	12	9	3436.7998	0.0006
20	13	8	20	12	8	3436.9498	0.0011
19	13	7	19	12	7	3437.0823	0.0017
18	13	6	18	12	6	3437.1973	0.0008
17	13	5	17	12	5	3437.2993	0.0017
16	13	4	16	12	4	3437.3854	0.0000
15	13	3	15	12	3	3437.4578	-0.0034
14	13	2	14	12	2	3437.5290	0.0024
13	13	1	13	12	1	3437.5802	-0.0019
12	2	10	11	3	8	3445.9359	0.0004
11	1	10	10	2	9	3446.2632	0.0031
17	8	10	16	9	8	3453.6407	0.0003
10	1	10	9	0	9	3457.3768	-0.0013
11	0	11	10	1	9	3467.7093	-0.0020
13	3	11	12	4	9	3469.1578	0.0003
13	3	10	12	4	8	3476.2512	-0.0009
12	1	12	11	2	10	3522.5797	-0.0018
14	4	11	13	5	8	3534.9800	0.0025
14	4	10	13	5	8	3535.3910	-0.0042
9	2	8	8	1	8	3543.7840	-0.0013
6	6	0	5	5	0	3555.9640	-0.0008
9	2	7	8	1	8	3567.2858	-0.0016
19	10	10	18	11	8	3584.3948	0.0017
15	5	10	14	6	8	3599.4122	-0.0079
7	5	2	6	4	2	3621.5102	-0.0054
10	1	9	9	0	9	3658.3580	-0.0014
16	6	10	15	7	8	3664.2386	-0.0006
11	0	11	10	1	10	3668.6909	-0.0018
8	4	5	7	3	4	3686.7912	0.0056
8	4	5	7	3	5	3686.9707	-0.0093
40	14	26	40	13	27	3704.7685	0.0203
38	14	25	38	13	25	3706.1347	0.0009
37	14	24	37	13	24	3706.7507	-0.0036
36	14	23	36	13	23	3707.3274	-0.0024
35	14	22	35	13	22	3707.8576	-0.0051
34	14	21	34	13	21	3708.3516	-0.0037
33	14	20	33	13	20	3708.8077	-0.0019
32	14	19	32	13	19	3709.2264	-0.0015
31	14	18	31	13	18	3709.6117	-0.0005
30	14	17	30	13	17	3709.9634	-0.0012
29	14	16	29	13	16	3710.2850	-0.0018
27	14	14	27	13	14	3710.8493	0.0009
26	14	13	26	13	13	3711.0891	-0.0021
25	14	12	25	13	12	3711.3110	0.0000
24	14	11	24	13	11	3711.5093	0.0000
23	14	10	23	13	10	3711.6867	-0.0011
22	14	9	22	13	9	3711.8487	0.0008
21	14	8	21	13	8	3711.9906	-0.0002

20	14	7	20	13	7	3712.1175	-0.0005
19	14	6	19	13	6	3712.2306	-0.0003
18	14	5	18	13	5	3712.3304	-0.0002
17	14	4	17	13	4	3712.4201	0.0017
16	14	3	16	13	3	3712.4902	-0.0049
15	14	2	15	13	2	3712.5656	0.0036
13	2	12	12	3	10	3716.2647	-0.0015
11	1	11	10	1	10	3722.4012	-0.0029
17	7	11	16	8	9	3729.3345	0.0003
11	0	11	10	0	10	3731.7081	-0.0018
10	2	9	9	1	8	3736.0912	0.0014
9	3	7	8	2	6	3742.5704	-0.0036
9	3	6	8	2	6	3743.4244	-0.0017
11	2	10	10	2	9	3743.5423	-0.0026
11	9	2	10	9	1	3746.3527	-0.0014
11	8	3	10	8	2	3746.4226	0.0021
11	7	4	10	7	3	3746.5106	-0.0009
11	6	5	10	6	4	3746.6474	0.0004
11	5	7	10	5	6	3746.8689	0.0000
11	4	8	10	4	7	3747.2648	-0.0059
11	3	9	10	3	8	3747.6829	-0.0010
11	3	8	10	3	7	3748.8514	-0.0019
12	1	11	11	2	9	3756.3232	-0.0021
9	3	7	8	2	7	3757.7267	-0.0020
11	2	9	10	2	8	3757.8654	-0.0020
9	3	6	8	2	7	3758.5802	-0.0006
11	1	10	10	1	9	3761.7445	-0.0014
10	2	8	9	1	8	3770.7367	-0.0014
12	0	12	11	1	10	3774.6988	-0.0031
11	1	11	10	0	10	3785.4194	-0.0020
18	8	11	17	9	9	3794.5651	-0.0004
13	2	11	12	3	9	3800.0080	0.0002
12	1	11	11	2	10	3805.2981	0.0019
14	3	12	13	4	10	3810.3594	-0.0011
14	3	11	13	4	9	3821.1668	-0.0015
13	1	13	12	2	11	3837.1405	-0.0023
19	9	10	18	10	8	3859.8471	-0.0245
15	4	12	14	5	10	3876.7691	0.0035
15	4	11	14	5	9	3877.4722	-0.0037
7	6	2	6	5	2	3896.5300	-0.0022
10	2	9	9	1	9	3900.9651	-0.0021
20	10	11	19	11	9	3925.2227	0.0031
10	2	8	9	1	9	3935.5873	-0.0283
16	5	12	15	6	9	3940.8555	-0.0062
16	5	11	15	6	9	3940.8941	0.0004
8	5	3	7	4	3	3962.0500	-0.0024
39	15	25	39	14	25	3981.6783	0.0060
38	15	24	38	14	24	3982.2207	-0.0053
37	15	23	37	14	23	3982.7391	-0.0023
36	15	22	36	14	22	3983.2195	-0.0007
35	15	21	35	14	21	3983.6621	-0.0022
34	15	20	34	14	20	3984.0716	-0.0040
33	15	19	33	14	19	3984.4549	-0.0009
32	15	18	32	14	18	3984.8028	-0.0037
31	15	17	31	14	17	3985.1275	-0.0020
30	15	16	30	14	16	3985.4250	-0.0013
29	15	15	29	14	15	3985.6983	-0.0001
28	15	14	28	14	14	3985.9472	-0.0002
27	15	13	27	14	13	3986.1748	0.0000
26	15	12	26	14	12	3986.3795	-0.0023
25	15	11	25	14	11	3986.5700	0.0001
24	15	10	24	14	10	3986.7400	-0.0002
23	15	9	23	14	9	3986.8957	0.0016

22	15	8	22	14	8	3987.0343	0.0015
21	15	7	21	14	7	3987.1578	0.0006
20	15	6	20	14	6	3987.2698	0.0012
19	15	5	19	14	5	3987.3699	0.0019
18	15	4	18	14	4	3987.4563	0.0000
17	15	3	17	14	3	3987.5327	-0.0018
16	15	2	16	14	2	3987.6023	-0.0012
15	15	0	15	14	1	3987.6722	0.0079
21	11	11	20	12	9	3990.5934	0.0031
12	0	12	11	1	11	4015.0228	-0.0023
11	1	10	10	0	10	4025.7458	0.0012
9	4	5	8	3	5	4027.0429	0.0016
9	4	6	8	3	6	4027.4491	-0.0068
14	2	13	13	3	11	4049.2224	-0.0020
12	1	12	11	1	11	4060.1884	-0.0011
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10	3	8	9	2	7	4077.4093	-0.0008
13	0	13	12	1	11	4077.6346	-0.0034
10	3	7	9	2	7	4078.9853	-0.0017
12	2	11	11	2	10	4083.2967	-0.0013
12	10	2	11	10	1	4086.8933	-0.0040
12	8	4	11	8	3	4087.0428	-0.0028
12	7	5	11	7	4	4087.1611	-0.0007
12	6	6	11	6	5	4087.3352	-0.0007
12	5	8	11	5	7	4087.6221	-0.0006
12	4	9	11	4	8	4088.1329	-0.0023
12	4	8	11	4	7	4088.1918	-0.0050
12	3	10	11	3	9	4088.5454	-0.0012
12	3	9	11	3	8	4090.3474	-0.0013
13	1	12	12	2	10	4098.2856	-0.0005
10	3	8	9	2	8	4100.9111	-0.0011
12	2	10	11	2	9	4101.1031	-0.0009
12	1	11	11	1	10	4102.5798	-0.0012
11	2	9	10	1	9	4108.0007	-0.0010
14	1	14	13	2	12	4149.6525	-0.0016
15	3	13	14	4	11	4151.4116	-0.0007
14	2	12	13	3	10	4155.6543	0.0003
15	3	12	14	4	10	4167.3432	0.0010
7	7	0	6	6	0	4171.5377	-0.0020
16	4	13	15	5	11	4218.7392	-0.0038
16	4	12	15	5	10	4219.9095	-0.0085
8	6	2	7	5	2	4237.0879	-0.0034
39	16	24	39	15	24	4257.5960	0.0010
37	16	22	37	15	22	4258.4989	-0.0020
36	16	21	36	15	21	4258.9084	0.0005
35	16	20	35	15	20	4259.2854	-0.0006
34	16	19	34	15	19	4259.6364	-0.0004
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32	16	17	32	15	17	4260.2627	0.0000
31	16	16	31	15	16	4260.5384	-0.0018
30	16	15	30	15	15	4260.7969	0.0009
29	16	14	29	15	14	4261.0297	-0.0015
28	16	13	28	15	13	4261.2444	-0.0026
27	16	12	27	15	12	4261.4421	-0.0026
26	16	11	26	15	11	4261.6265	0.0010
25	16	10	25	15	10	4261.7894	-0.0008
24	16	9	24	15	9	4261.9397	-0.0003
23	16	8	23	15	8	4262.0759	-0.0002
22	16	7	22	15	7	4262.1993	0.0000
21	16	6	21	15	6	4262.3104	0.0000
20	16	5	20	15	5	4262.4102	-0.0001
19	16	4	19	15	4	4262.4987	-0.0013
18	16	3	18	15	3	4262.5737	-0.0066

17	16	2	17	15	2	4262.6505	-0.0014
16	16	1	16	15	1	4262.7195	0.0038
9	5	4	8	4	4	4302.5555	-0.0026
13	0	13	12	1	12	4360.3411	-0.0117
10	4	6	9	3	6	4367.0814	-0.0019
10	4	7	9	3	7	4367.9033	-0.0031
14	0	14	13	1	12	4376.6998	-0.0022
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13	1	13	12	1	12	4397.8921	0.0325
19	7	13	18	8	11	4411.5704	0.0014
11	3	8	10	2	8	4413.0335	-0.0024
13	2	12	12	2	11	4422.9052	-0.0027
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13	8	5	12	8	4	4427.6788	-0.0027
13	7	6	12	7	5	4427.8248	-0.0025
13	6	7	12	6	6	4428.0451	-0.0020
13	5	9	12	5	8	4428.4096	-0.0006
13	4	10	12	4	9	4429.0457	-0.0018
13	4	9	12	4	8	4429.1545	-0.0023
13	3	11	12	3	10	4429.4051	-0.0021
13	3	10	12	3	9	4432.0752	-0.0020
14	1	13	13	2	11	4437.0148	-0.0030
13	1	12	12	1	11	4443.0595	-0.0053
13	2	11	12	2	10	4444.4209	-0.0002
11	3	9	10	2	9	4444.9366	-0.0014
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15	1	15	14	2	13	4460.1641	-0.0003
20	8	13	19	9	11	4476.5905	0.0021
16	3	14	15	4	12	4492.2140	0.0011
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15	2	13	14	3	11	4512.5032	0.0000
33	17	17	33	16	17	4535.3763	0.0031
32	17	16	32	16	16	4535.6367	0.0005
31	17	15	31	16	15	4535.8771	-0.0025
30	17	14	30	16	14	4536.0991	-0.0054
29	17	13	29	16	13	4536.3118	-0.0003
28	17	12	28	16	12	4536.5006	-0.0026
27	17	11	27	16	11	4536.6781	-0.0008
26	17	10	26	16	10	4536.8418	0.0017
25	17	9	25	16	9	4536.9870	-0.0006
24	17	8	24	16	8	4537.1234	0.0009
23	17	7	23	16	7	4537.2463	0.0009
22	17	6	22	16	6	4537.3450	-0.0121
19	17	3	19	16	3	4537.6301	-0.0031
18	17	2	18	16	2	4537.7021	-0.0057
17	17	1	17	16	1	4537.7731	-0.0017
17	4	14	16	5	12	4560.9183	0.0033
17	4	13	16	5	11	4562.7985	0.0016
9	6	4	8	5	4	4577.6328	-0.0043
12	2	11	11	1	11	4620.9030	-0.0032
18	5	14	17	6	12	4624.2846	0.0094
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10	5	5	9	4	5	4643.0212	0.0019
15	0	15	14	1	13	4672.1868	-0.0018
14	0	14	13	1	13	4704.6218	-0.0003
11	4	7	10	3	7	4706.8285	-0.0018
11	4	8	10	3	8	4708.3400	-0.0052
16	2	15	15	3	13	4710.3674	-0.0032
14	1	14	13	1	13	4735.4193	0.0000
12	3	10	11	2	9	4740.9655	-0.0034

14	0	14	13	0	13	4742.1279	-0.0008
12	3	9	11	2	9	4745.5151	-0.0022
20	7	14	19	8	12	4752.8190	0.0038
14	2	13	13	2	12	4762.3637	-0.0017
14	12	2	13	12	1	4767.9584	-0.0047
14	11	3	13	11	2	4768.0187	-0.0086
14	10	4	13	10	3	4768.1024	-0.0019
14	9	5	13	9	4	4768.2000	-0.0010
14	8	6	13	8	5	4768.3278	-0.0012
14	7	7	13	7	6	4768.5082	-0.0011
14	6	8	13	6	7	4768.7795	-0.0028
14	5	9	13	5	8	4769.2347	-0.0038
14	4	11	13	4	10	4770.0075	-0.0012
14	3	12	13	3	11	4770.2464	-0.0043
13	1	12	12	0	12	4770.9443	0.0003
15	1	14	14	2	12	4772.0941	-0.0038
14	1	14	13	0	13	4772.9260	0.0001
14	3	11	13	3	10	4774.0694	-0.0036
14	1	13	13	1	12	4783.1504	-0.0024
8	8	0	7	7	0	4787.1103	-0.0031
14	2	12	13	2	11	4787.7226	-0.0006
13	2	11	12	1	11	4789.1994	-0.0004
12	3	10	11	2	10	4789.9378	-0.0019
12	3	9	11	2	10	4794.4926	0.0044
33	18	16	33	17	16	4810.7191	-0.0006
32	18	15	32	17	15	4810.9538	-0.0002
32	18	15	32	17	15	4810.9538	-0.0002
31	18	14	31	17	14	4811.1710	-0.0006
30	18	13	30	17	13	4811.3655	-0.0078
29	18	12	29	17	12	4811.5615	0.0014
28	18	11	28	17	11	4811.7346	0.0020
27	18	10	27	17	10	4811.8921	0.0004
26	18	9	26	17	9	4812.0381	-0.0001
25	18	8	25	17	8	4812.1680	-0.0049
24	18	7	24	17	7	4812.2961	-0.0004
23	18	6	23	17	6	4812.4074	-0.0024
22	18	5	22	17	5	4812.5122	-0.0010
21	18	4	21	17	4	4812.6066	-0.0010
20	18	3	20	17	3	4812.6923	-0.0012
19	18	2	19	17	2	4812.7651	-0.0064
18	18	1	18	17	1	4812.8372	-0.0050
9	7	2	8	6	2	4852.6566	-0.0044
17	3	14	16	4	12	4864.4005	0.0039
16	2	14	15	3	12	4870.0806	0.0036
18	4	15	17	5	13	4903.2764	0.0009
18	4	14	17	5	12	4906.2019	-0.0006
10	6	4	9	5	4	4918.1582	-0.0057
6	5	2	5	2	4	4931.5425	0.0120
16	0	16	15	1	14	4964.4866	-0.0020
19	5	15	18	6	13	4966.2668	0.0045
19	5	14	18	6	12	4966.4376	0.0023
11	5	7	10	4	7	4983.4393	-0.0086
13	2	12	12	1	12	4983.6231	-0.0014
14	2	13	13	1	12	5020.2029	-0.0075
20	6	14	19	7	12	5029.8518	-0.0004
17	2	16	16	3	14	5038.3064	-0.0008
12	4	9	11	3	8	5046.0461	-0.0040
12	4	8	11	3	8	5046.1700	-0.0037
15	0	15	14	1	14	5047.8379	-0.0044
12	4	9	11	3	9	5048.7935	-0.0029
12	4	8	11	3	9	5048.9164	-0.0036
13	3	11	12	2	10	5069.2697	-0.0024
15	1	15	14	1	14	5072.8758	0.0000

17	1	17	16	2	15	5075.4597	0.0046
13	3	10	12	2	10	5076.4879	-0.0025
15	0	15	14	0	14	5078.6387	-0.0007
37	19	19	37	18	19	5085.0124	0.0016
36	19	18	36	18	18	5085.2998	0.0100
35	19	17	35	18	17	5085.5534	0.0025
34	19	16	34	18	16	5085.7954	0.0005
33	19	15	33	18	15	5085.9981	-0.0246
32	19	14	32	18	14	5086.2364	0.0012
31	19	13	31	18	13	5086.4349	0.0019
30	19	12	30	18	12	5086.6090	-0.0079
29	19	11	29	18	11	5086.7873	-0.0005
28	19	10	28	18	10	5086.9470	0.0008
27	19	9	27	18	9	5087.0732	-0.0197
26	19	8	26	18	8	5087.2303	0.0018
25	19	7	25	18	7	5087.3513	-0.0023
24	19	6	24	18	6	5087.4670	-0.0020
23	19	5	23	18	5	5087.5757	0.0005
22	19	4	22	18	4	5087.6739	0.0013
21	19	3	21	18	3	5087.8198	0.0578
21	7	14	20	8	12	5094.1622	0.0033
15	2	14	14	2	13	5101.6608	-0.0022
16	1	15	15	2	13	5103.1540	-0.0036
15	1	15	14	0	14	5103.6688	-0.0040
15	13	2	14	13	1	5108.4754	-0.0090
15	12	3	14	12	2	5108.5502	0.0005
15	11	4	14	11	3	5108.6252	-0.0003
15	10	5	14	10	4	5108.7151	-0.0024
15	9	6	14	9	5	5108.8345	0.0005
15	8	7	14	8	6	5108.9890	-0.0004
15	7	8	14	7	7	5109.2093	0.0000
15	6	10	14	6	9	5109.5449	0.0014
15	5	11	14	5	10	5110.1030	0.0057
15	3	13	14	3	12	5111.0398	-0.0206
15	4	11	14	4	10	5111.3205	0.0012
15	3	12	14	3	11	5116.3677	0.0001
15	1	14	14	1	13	5122.8014	-0.0020
9	8	1	8	7	1	5127.6692	-0.0039
15	2	13	14	2	12	5130.9223	0.0000
14	2	12	13	1	12	5133.8594	0.0011
13	3	11	12	2	11	5136.0489	0.0000
14	1	13	13	0	13	5148.5799	0.0003
10	7	3	9	6	3	5193.2029	-0.0053
18	3	15	17	4	13	5215.7249	0.0062
17	2	15	16	3	13	5227.8115	0.0027
19	4	16	18	5	14	5245.8100	0.0013
11	6	5	10	5	5	5258.6590	-0.0054
12	5	7	11	4	7	5323.7467	0.0069
15	2	14	14	1	13	5338.7183	-0.0023
14	2	13	13	1	13	5348.1286	-0.0018
36	20	17	36	19	17	5360.6179	-0.0087
35	20	16	35	19	16	5360.8662	0.0011
34	20	15	34	19	15	5361.0479	-0.0405
33	20	14	33	19	14	5361.2972	-0.0004
32	20	13	32	19	13	5361.4898	-0.0033
31	20	12	31	19	12	5361.6798	0.0039
30	20	11	30	19	11	5361.8489	0.0026
29	20	10	29	19	10	5362.0071	0.0020
28	20	9	28	19	9	5362.1531	0.0003
27	20	8	27	19	8	5362.2926	0.0025
26	20	7	26	19	7	5362.4211	0.0035
25	20	6	25	19	6	5362.5301	-0.0055
24	20	5	24	19	5	5362.6452	0.0003

23	20	4	23	19	4	5362.7449	-0.0008
22	20	3	22	19	3	5362.8403	0.0013
21	20	2	21	19	2	5362.9236	-0.0011
20	20	1	20	19	1	5363.0019	-0.0017
18	2	17	17	3	15	5364.3398	-0.0021
18	1	18	17	2	16	5380.4128	0.0047
13	4	10	12	3	9	5384.7464	-0.0025
13	4	9	12	3	9	5384.9797	-0.0021
12	3	9	11	0	11	5385.8068	-0.0009
13	4	10	12	3	10	5389.2964	-0.0010
13	4	9	12	3	10	5389.5270	-0.0033
16	0	16	15	1	15	5390.0708	0.0007
14	3	12	13	2	11	5395.0997	-0.0021
9	9	0	8	8	0	5402.6826	-0.0033
14	3	11	13	2	11	5406.1391	-0.0033
16	1	16	15	1	15	5410.2373	0.0004
16	0	16	15	0	15	5415.1033	-0.0001
19	0	19	18	2	16	5419.9109	-0.0308
17	1	16	16	2	14	5429.8793	-0.0021
16	2	15	15	2	14	5440.7944	-0.0001
16	14	2	15	14	1	5449.0139	0.0170
16	13	3	15	13	2	5449.0636	-0.0001
16	12	4	15	12	3	5449.1468	0.0071
16	11	5	15	11	4	5449.2228	-0.0060
16	10	6	15	10	5	5449.3370	-0.0008
16	9	7	15	9	6	5449.4769	0.0000
16	8	8	15	8	7	5449.6634	0.0001
16	7	9	15	7	8	5449.9282	0.0000
16	6	11	15	6	10	5450.3342	0.0018
16	5	11	15	5	10	5451.0109	-0.0061
16	3	14	15	3	13	5451.8179	-0.0010
16	4	13	15	4	12	5452.0787	0.0040
16	4	12	15	4	11	5452.5486	0.0008
16	3	13	15	3	12	5458.9863	0.0015
16	1	15	15	1	14	5461.9817	-0.0001
10	8	2	9	7	2	5468.2223	-0.0045
16	2	14	15	2	13	5473.9412	-0.0001
15	2	13	14	1	13	5481.6289	0.0011
14	3	12	13	2	12	5483.3907	-0.0010
14	3	11	13	2	12	5494.4380	0.0056
19	3	17	18	4	15	5511.8752	0.0001
15	1	14	14	0	14	5529.2541	-0.0001
11	7	4	10	6	4	5533.7394	-0.0022
19	3	16	18	4	14	5569.1447	0.0070
18	2	16	17	3	14	5585.0759	0.0086
20	4	17	19	5	14	5588.2745	-0.0381
20	4	17	19	5	15	5588.4878	0.0000
20	4	16	19	5	14	5595.0545	0.0050
12	6	6	11	5	6	5599.1267	-0.0042
38	21	18	38	20	18	5635.4596	0.0107
37	21	17	37	20	17	5635.7141	0.0160
36	21	16	36	20	16	5635.9256	-0.0070
35	21	15	35	20	15	5636.1514	-0.0019
34	21	14	34	20	14	5636.3361	-0.0246
33	21	13	33	20	13	5636.5577	0.0022
32	21	12	32	20	12	5636.7380	0.0000
31	21	11	31	20	11	5636.9119	0.0028
30	21	10	30	20	10	5637.0707	0.0016
29	21	9	29	20	9	5637.2206	0.0018
28	21	8	28	20	8	5637.3610	0.0025
27	21	7	27	20	7	5637.4915	0.0027
26	21	6	26	20	6	5637.6105	0.0004
25	21	5	25	20	5	5637.7225	-0.0004

24	21	4	24	20	4	5637.8285	0.0006
21	5	17	20	6	15	5650.8834	0.0071
21	5	16	20	6	14	5651.3404	0.0018
16	2	15	15	1	14	5656.7075	-0.0041
13	5	8	12	4	8	5663.9573	0.0020
13	5	9	12	4	9	5664.0713	-0.0036
19	1	19	18	2	17	5683.7112	0.0094
22	6	16	21	7	15	5713.5162	0.0034
15	2	14	14	1	14	5714.3730	-0.0012
14	4	10	13	3	10	5723.0980	-0.0003
14	4	11	13	3	11	5729.8982	-0.0006
17	0	17	16	1	16	5731.3961	0.0031
15	3	12	14	2	12	5734.7849	-0.0018
10	9	1	9	8	1	5743.2366	-0.0040
17	1	17	16	1	16	5747.5125	0.0011
12	4	9	11	2	10	5750.1894	-0.0001
17	0	17	16	0	16	5751.5614	0.0016
18	1	17	17	2	15	5752.0079	-0.0040
17	1	17	16	0	16	5767.6771	-0.0010
23	7	16	22	8	14	5777.1803	0.0062
17	2	16	16	2	15	5779.7555	0.0002
17	15	2	16	15	1	5789.4979	-0.0021
17	14	3	16	14	2	5789.5693	0.0002
17	13	4	16	13	3	5789.6486	0.0027
17	12	5	16	12	4	5789.7344	0.0007
17	11	6	16	11	5	5789.8383	0.0005
17	10	7	16	10	6	5789.9663	0.0004
17	9	8	16	9	7	5790.1309	0.0008
17	8	9	16	8	8	5790.3524	0.0008
17	7	10	16	7	9	5790.6695	0.0019
17	6	12	16	6	11	5791.1533	0.0022
17	5	13	16	5	12	5791.9330	-0.0177
17	3	15	16	3	14	5792.5084	0.0005
17	4	14	16	4	13	5793.1756	0.0016
23	3	20	22	5	17	5793.8981	-0.0347
17	1	16	16	1	15	5800.6643	-0.0008
17	3	14	16	3	13	5801.9376	0.0010
11	8	3	10	7	3	5808.7688	-0.0033
17	2	15	16	2	14	5816.7141	-0.0025
19	0	19	18	1	17	5827.1303	0.0053
15	3	13	14	2	13	5832.0868	0.0000
16	2	14	15	1	14	5832.7650	-0.0006
15	3	12	14	2	13	5848.4499	0.0153
20	3	18	19	4	16	5850.3761	0.0011
12	7	5	11	6	5	5874.2499	-0.0065
37	22	16	37	21	16	5910.9990	-0.0008
35	22	14	35	21	14	5911.4245	-0.0016
34	22	13	34	21	13	5911.6205	-0.0005
33	22	12	33	21	12	5911.8058	0.0012
32	22	11	32	21	11	5911.9804	0.0031
31	22	10	31	21	10	5912.1408	0.0014
30	22	9	30	21	9	5912.2940	0.0023
29	22	8	29	21	8	5912.4330	-0.0013
16	1	15	15	0	15	5912.6004	0.0036
21	4	18	20	5	16	5931.2769	0.0032
13	6	7	12	5	7	5939.5513	-0.0029
21	4	17	20	5	15	5940.7750	0.0042
19	2	17	18	3	15	5941.1847	0.0031
18	1	17	17	2	16	5965.0356	0.0084
20	1	20	19	2	18	5985.4650	0.0146
22	5	17	21	6	15	5994.1738	-0.0846
14	5	9	13	4	9	6004.0383	0.0012
14	5	10	13	4	10	6004.2569	-0.0046

10	10	0	9	9	0	6018.2541	-0.0031
16	3	14	15	2	13	6039.3354	-0.0001
15	4	12	14	3	11	6059.6252	-0.0006
15	4	11	14	3	11	6060.3448	0.0001
16	3	13	15	2	13	6062.8489	-0.0002
19	1	18	18	2	16	6069.3556	-0.0030
15	4	12	14	3	12	6070.6668	0.0002
15	4	11	14	3	12	6071.3864	0.0011
18	0	18	17	1	17	6071.9170	0.0021
16	2	15	15	1	15	6082.2908	-0.0022
11	9	2	10	8	2	6083.7866	-0.0029
18	1	18	17	1	17	6084.7117	0.0035
18	0	18	17	0	17	6088.0362	0.0029
18	2	17	17	2	16	6118.5427	0.0000
18	16	2	17	16	1	6129.9890	-0.0042
18	15	3	17	15	2	6130.0643	-0.0004
18	14	4	17	14	3	6130.1453	0.0022
18	13	5	17	13	4	6130.2327	0.0019
18	12	6	17	12	5	6130.3328	0.0009
18	11	7	17	11	6	6130.4530	0.0005
18	10	8	17	10	7	6130.6017	0.0000
18	9	9	17	9	8	6130.7964	0.0020
18	8	10	17	8	9	6131.0574	0.0022
18	7	11	17	7	10	6131.4309	0.0022
18	6	13	17	6	12	6132.0048	0.0032
18	5	13	17	5	12	6132.9710	-0.0191
18	3	16	17	3	15	6133.1100	0.0007
18	4	15	17	4	14	6134.3133	0.0021
18	4	14	17	4	13	6135.3860	0.0031
18	1	17	17	1	16	6138.8493	0.0022
18	3	15	17	3	14	6145.2230	0.0051
12	8	4	11	7	4	6149.3022	-0.0039
18	2	16	17	2	15	6159.1971	0.0020
16	3	14	15	2	14	6182.2447	0.0020
25	8	17	24	9	15	6182.9352	0.0081
17	2	15	16	1	15	6187.5057	0.0053
21	3	19	20	4	17	6187.9252	0.0038
13	7	6	12	6	6	6214.7448	-0.0029
24	1	23	23	4	19	6218.3853	-0.0152
26	9	17	25	10	15	6247.4378	0.0108
22	4	19	21	5	17	6274.1206	0.0079
14	6	8	13	5	8	6279.9243	0.0002
21	3	18	20	4	16	6282.5444	0.0105
16	2	14	15	0	15	6283.3648	-0.0156
22	4	18	21	5	16	6287.5821	0.0010
18	2	17	17	1	16	6292.3609	-0.0016
20	2	18	19	3	16	6295.4695	0.0017
17	1	16	16	0	16	6298.1591	0.0005
19	1	18	18	2	17	6323.0341	0.0077
21	2	20	20	3	18	6330.2661	-0.0003
23	5	18	22	6	16	6337.5598	0.0075
15	5	10	14	4	10	6343.9489	-0.0001
15	5	11	14	4	11	6344.3460	-0.0041
11	10	1	10	9	1	6358.8022	-0.0038
20	1	19	19	2	17	6381.8092	-0.0040
17	3	14	16	2	14	6390.8446	0.0002
21	0	21	20	1	19	6395.5409	0.0110
16	4	12	15	3	12	6396.5247	-0.0001
24	6	19	23	7	17	6397.8512	0.0127
24	6	18	23	7	16	6397.9097	0.0043
16	4	13	15	3	13	6411.6821	0.0013
19	1	19	18	1	18	6421.8402	0.0037
12	9	3	11	8	3	6424.3275	-0.0033

19	0	19	18	0	18	6424.5426	0.0050
19	1	19	18	0	18	6434.6335	0.0037
17	2	16	16	1	16	6451.8099	-0.0016
19	2	18	18	2	17	6457.1581	0.0023
19	18	2	18	18	1	6470.4016	-0.0033
19	17	2	18	17	1	6470.4742	-0.0014
19	16	3	18	16	2	6470.5491	-0.0012
19	15	4	18	15	3	6470.6342	0.0036
19	14	5	18	14	4	6470.7211	0.0021
19	13	6	18	13	5	6470.8225	0.0039
19	12	7	18	12	6	6470.9377	0.0032
19	11	8	18	11	7	6471.0757	0.0023
19	10	9	18	10	8	6471.2490	0.0027
19	9	10	18	9	9	6471.4725	0.0020
19	8	11	18	8	10	6471.7774	0.0021
19	7	13	18	7	12	6472.2159	0.0030
19	6	14	18	6	13	6472.8898	0.0042
19	3	17	18	3	16	6473.6068	0.0016
19	5	15	18	5	14	6473.9871	-0.0015
19	5	14	18	5	13	6474.0656	0.0042
19	4	16	18	4	15	6475.4823	0.0033
19	1	18	18	1	17	6476.5459	0.0040
19	4	15	18	4	14	6477.0340	0.0025
19	3	16	18	3	15	6488.8048	0.0029
13	8	5	12	7	5	6489.8221	-0.0037
19	2	17	18	2	16	6501.3342	0.0021
17	3	15	16	2	15	6533.9585	0.0025
18	2	16	17	1	16	6546.0366	0.0064
14	7	7	13	6	7	6555.2078	-0.0022
23	4	20	22	5	18	6616.9443	0.0076
15	6	9	14	5	9	6620.2263	-0.0027
11	11	0	10	10	0	6633.8238	-0.0033
23	4	19	22	5	17	6635.5951	-0.0804
22	3	19	21	4	17	6642.3951	0.0127
21	2	19	20	3	17	6647.2572	0.0018
22	2	21	21	3	19	6648.0258	0.0023
13	4	10	12	1	12	6656.6720	0.0163
22	0	22	21	1	20	6679.1770	0.0200
24	5	20	23	6	18	6679.5791	-0.0024
24	5	19	23	6	17	6681.2837	0.0070
16	5	11	15	4	11	6683.6414	-0.0053
16	5	12	15	4	12	6684.3313	-0.0023
18	1	17	17	0	17	6685.4453	-0.0004
21	1	20	20	2	18	6689.3597	-0.0045
12	10	2	11	9	2	6699.3458	-0.0034
18	3	15	17	2	15	6719.3471	0.0014
17	4	13	16	3	13	6731.4341	-0.0017
25	6	20	24	7	18	6740.3194	0.0049
25	6	19	24	7	17	6740.4266	0.0036
17	4	14	16	3	14	6753.0374	0.0014
20	1	20	19	1	19	6758.9103	0.0059
20	0	20	19	0	19	6761.0841	0.0060
13	9	4	12	8	4	6764.8586	-0.0038
20	1	20	19	0	19	6769.0027	0.0059
20	2	19	19	2	18	6795.5992	0.0033
20	19	1	19	19	0	6810.8630	-0.0091
20	18	2	19	18	1	6810.9453	-0.0014
20	17	3	19	17	2	6811.0255	0.0007
20	16	4	19	16	3	6811.1117	0.0040
20	15	5	19	15	4	6811.1983	0.0009
20	14	6	19	14	5	6811.2983	0.0015
20	13	7	19	13	6	6811.4118	0.0021
20	12	8	19	12	7	6811.5448	0.0032

20	11	9	19	11	8	6811.7027	0.0019
20	10	10	19	10	9	6811.9027	0.0028
20	9	11	19	9	10	6812.1619	0.0029
20	8	12	19	8	11	6812.5152	0.0027
20	7	14	19	7	13	6813.0251	0.0036
20	6	14	19	6	13	6813.8174	0.0086
20	3	18	19	3	17	6813.9809	0.0021
20	5	16	19	5	15	6815.0836	0.0025
20	5	15	19	5	14	6815.1997	0.0031
20	4	17	19	4	16	6816.6708	0.0029
20	4	16	19	4	15	6818.8714	0.0043
18	2	17	17	1	17	6822.8392	-0.0037
14	8	6	13	7	6	6830.3241	-0.0035
20	3	17	19	3	16	6832.6420	0.0034
20	2	18	19	2	17	6843.0903	0.0022
27	8	19	26	9	17	6866.1278	0.0128
18	3	16	17	2	16	6887.3125	0.0027
15	7	8	14	6	8	6895.6342	-0.0027
19	2	17	18	1	17	6908.5234	0.0081
16	6	10	15	5	10	6960.4643	0.0082
23	2	22	22	3	20	6963.6485	0.0035
12	11	1	11	10	1	6974.3665	-0.0029
22	1	21	21	2	19	6992.1069	-0.0037
22	2	20	21	3	18	6995.9110	0.0017
23	3	20	22	4	18	7004.0543	0.0140
17	5	12	16	4	12	7023.0748	-0.0012
17	5	13	16	4	13	7024.2078	-0.0019
25	5	20	24	6	18	7025.5107	0.0113
15	4	11	14	1	13	7029.4717	0.0024
13	10	3	12	9	3	7039.8821	-0.0031
19	3	16	18	2	16	7048.9538	0.0013
18	4	14	17	3	14	7064.8822	0.0000
19	1	18	18	0	18	7073.9535	-0.0009
21	0	21	20	1	20	7089.7406	0.0037
18	4	15	17	3	15	7094.8410	0.0017
21	1	21	20	1	20	7095.9269	0.0069
21	0	21	20	0	20	7097.6615	0.0061
14	9	5	13	8	5	7105.3776	-0.0044
21	2	20	20	2	19	7133.8696	0.0036
27	7	20	26	8	18	7144.8122	0.0100
21	20	2	20	20	1	7151.3227	-0.0043
21	19	2	20	19	1	7151.4032	-0.0027
21	18	3	20	18	2	7151.4855	-0.0021
21	17	4	20	17	3	7151.5799	0.0063
21	16	5	20	16	4	7151.6682	0.0028
21	15	6	20	15	5	7151.7670	0.0016
21	14	7	20	14	6	7151.8793	0.0024
21	13	9	20	13	8	7152.0072	0.0031
21	12	10	20	12	9	7152.1584	0.0048
21	11	11	20	11	10	7152.3384	0.0033
21	10	12	20	10	11	7152.5664	0.0035
21	9	12	20	9	11	7152.8651	0.0044
21	8	13	20	8	12	7153.2732	0.0053
21	7	15	20	7	14	7153.8600	0.0041
21	3	19	20	3	18	7154.2168	0.0026
21	6	15	20	6	14	7154.7709	0.0025
21	5	17	20	5	16	7156.2280	0.0044
21	5	16	20	5	15	7156.4082	0.0053
21	4	18	20	4	17	7157.8710	0.0041
21	4	17	20	4	16	7160.9218	0.0040
15	8	7	14	7	7	7170.8038	-0.0038
21	3	18	20	3	17	7176.6613	0.0051
21	2	19	20	2	18	7184.4283	0.0023

24	3	22	23	4	20	7193.2192	0.0007
19	2	18	18	1	18	7195.2865	-0.0039
16	7	9	15	6	9	7236.0203	-0.0012
19	3	17	18	2	17	7242.3760	0.0036
12	12	0	11	11	0	7249.3914	-0.0041
10	8	3	9	6	4	7255.5549	-0.0050
17	3	14	16	0	16	7259.1270	0.0056
20	2	18	19	1	18	7275.0714	0.0097
24	2	23	23	3	21	7277.1507	0.0043
23	1	22	22	2	20	7290.2660	-0.0018
17	6	12	16	5	12	7300.6222	0.0008
20	3	18	19	2	17	7301.3474	-0.0039
13	11	3	12	10	3	7314.9026	-0.0034
34	15	20	33	16	18	7319.1863	-0.1301
25	4	21	24	5	19	7336.5922	0.0160
23	2	21	22	3	19	7340.8509	0.0016
18	5	13	17	4	13	7362.1701	-0.0003
18	5	14	17	4	14	7363.9808	-0.0006
26	5	22	25	6	20	7366.6485	0.0085
24	3	21	23	4	19	7367.1429	0.0137
20	3	17	19	2	17	7380.2618	0.0029
14	10	4	13	9	4	7380.4086	-0.0037
19	4	15	18	3	15	7396.6932	-0.0023
22	1	22	21	1	21	7432.8962	0.0055
22	0	22	21	0	21	7434.2741	0.0078
19	4	16	18	3	16	7437.2130	0.0039
15	9	6	14	8	6	7445.8837	-0.0032
20	1	19	19	0	19	7463.2007	-0.0029
22	2	21	21	2	20	7471.9744	0.0032
22	1	21	21	1	20	7487.1736	0.0011
22	21	1	21	21	0	7491.7707	0.0015
22	20	2	21	20	1	7491.8547	0.0022
22	19	3	21	19	2	7491.9415	0.0032
22	18	4	21	18	3	7492.0336	0.0060
22	17	5	21	17	4	7492.1264	0.0044
22	16	6	21	16	5	7492.2242	0.0007
22	15	7	21	15	6	7492.2892	-0.0453
22	14	8	21	14	7	7492.4651	0.0060
22	13	9	21	13	8	7492.6050	0.0030
22	12	10	21	12	9	7492.7758	0.0050
22	11	12	21	11	11	7492.9825	0.0060
22	10	12	21	10	11	7493.2410	0.0050
22	9	14	21	9	13	7493.5818	0.0057
22	8	15	21	8	14	7494.0491	0.0066
22	3	20	21	3	19	7494.2981	0.0011
22	7	16	21	7	15	7494.7221	0.0047
22	6	17	21	6	16	7495.7710	0.0121
22	5	18	21	5	17	7497.4218	0.0055
22	5	17	21	5	16	7497.6952	0.0067
22	4	19	21	4	18	7499.0640	0.0013
22	4	18	21	4	17	7503.2175	0.0043
16	8	8	15	7	8	7511.2578	-0.0038
22	3	19	21	3	18	7520.7723	0.0060
20	2	19	19	1	19	7569.0455	-0.0044
17	7	10	16	6	10	7576.3535	-0.0029
24	1	23	23	2	21	7584.1635	-0.0014
25	2	24	24	3	22	7588.5678	0.0037
13	12	1	12	11	1	7589.9268	-0.0038
20	3	18	19	2	18	7599.1997	0.0044
18	6	13	17	5	13	7640.6523	-0.0198
21	2	19	20	1	19	7645.7109	0.0099
14	11	3	13	10	3	7655.4302	-0.0054
24	2	22	23	3	20	7681.5621	0.0009

26	4	22	25	5	20	7689.8476	0.0242
19	5	14	18	4	14	7700.8483	-0.0006
19	5	15	18	4	15	7703.6593	0.0003
21	3	18	20	2	18	7713.8326	0.0057
27	5	22	26	6	20	7715.7945	0.0181
15	10	5	14	9	5	7720.9251	-0.0037
20	4	16	19	3	16	7726.7587	-0.0021
25	3	22	24	4	20	7731.1673	0.0157
23	0	23	22	0	22	7770.9141	0.0078
20	4	17	19	3	17	7780.2761	0.0043
16	9	7	15	8	7	7786.3702	-0.0041
23	2	22	22	2	21	7809.9250	0.0065
23	1	22	22	1	21	7823.4691	0.0018
23	21	2	22	21	1	7832.2911	0.0052
23	20	3	22	20	2	7832.3794	0.0034
23	19	5	22	19	4	7832.4770	0.0078
23	18	6	22	18	5	7832.5718	0.0052
23	17	7	22	17	6	7832.6755	0.0054
23	16	8	22	16	7	7832.7886	0.0067
23	15	9	22	15	8	7832.9118	0.0068
23	14	10	22	14	9	7833.0492	0.0056
20	11	9	20	8	13	7833.2099	0.0426
23	12	11	22	12	10	7833.4014	0.0080
23	11	12	22	11	11	7833.6307	0.0050
23	10	13	22	10	12	7833.9267	0.0072
23	9	15	22	9	14	7834.3135	0.0075
23	8	16	22	8	15	7834.8446	0.0074
23	7	17	22	7	16	7835.6155	0.0080
23	6	17	22	6	16	7836.8148	0.0011
23	5	19	22	5	18	7838.6633	0.0047
23	5	18	22	5	17	7839.0683	0.0053
23	4	20	22	4	19	7840.2428	0.0024
23	4	19	22	4	18	7845.7897	0.0067
17	8	9	16	7	9	7851.6812	-0.0038
21	1	20	20	0	20	7852.7589	-0.0057
26	3	24	25	4	22	7855.7478	0.0006
23	3	20	22	3	19	7864.8734	0.0023
13	13	0	12	12	0	7864.9594	-0.0029
23	2	21	22	2	20	7865.7115	0.0052
25	1	24	24	2	22	7874.2339	-0.0005
18	7	11	17	6	11	7916.6312	-0.0023
14	12	2	13	11	2	7930.4546	-0.0053
21	2	20	20	1	20	7944.0030	-0.0084
21	3	19	20	2	19	7957.8172	0.0034
19	6	13	18	5	13	7980.5098	-0.0037
19	6	14	18	5	14	7980.6047	-0.0073
15	11	5	14	10	5	7995.9520	-0.0048

Table S11. Linelist for sevoflurane dimer (homochiral),  $^{13}\text{C}$  (acceptor, perfluoro) species. RMS error for the fit is 10.8 kHz.

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
5	5	1	4	4	1	2936.9375	0.0065
6	4	2	5	3	2	3001.6989	0.0068
8	2	7	7	1	6	3080.7048	0.0173
8	2	6	7	1	6	3095.3049	-0.0229
10	0	10	9	1	8	3151.7278	0.0295
13	12	2	13	11	2	3162.9513	0.0021
6	5	1	5	4	1	3276.7742	0.0008
8	3	6	7	2	6	3409.4156	-0.0156
8	3	5	7	2	6	3409.8409	0.0044
6	6	0	5	5	0	3551.8220	0.0030
7	5	2	6	4	2	3616.5918	-0.0125
8	4	4	7	3	4	3681.1297	0.0046
8	4	5	7	3	5	3681.2924	-0.0125
9	3	7	8	2	6	3736.4943	0.0183
9	3	6	8	2	6	3737.2831	-0.0010
9	3	7	8	2	7	3751.1056	-0.0106
10	2	8	9	1	8	3763.8306	0.0321
12	0	12	11	1	10	3769.6831	-0.0238
15	4	12	14	5	10	3865.5007	0.0016
7	6	1	6	5	1	3891.6576	-0.0019
8	5	3	7	4	3	3956.4121	-0.0033
11	1	10	10	0	10	4015.0215	0.0001
14	2	13	13	3	11	4039.9760	-0.0025
10	3	8	9	2	8	4093.4585	-0.0291
11	2	9	10	1	9	4100.1887	0.0095
15	3	13	14	4	10	4139.9146	0.0063
7	7	0	6	6	0	4166.7040	-0.0020
8	6	2	7	5	2	4231.4912	-0.0008
9	5	4	8	4	4	4296.1964	0.0000
10	4	6	9	3	6	4359.9996	0.0010
12	2	10	11	1	10	4438.5665	-0.0121
16	3	14	15	4	12	4480.3880	-0.0172
8	7	1	7	6	1	4506.5398	-0.0034
9	6	3	8	5	3	4571.3089	-0.0027
10	5	5	9	4	5	4635.9361	0.0018
11	4	7	10	3	7	4699.0624	0.0099
11	4	8	10	3	8	4700.4924	0.0016
12	3	9	11	2	9	4737.7625	0.0201
8	8	0	7	7	0	4781.5973	0.0052
9	7	2	8	6	2	4846.3688	-0.0050
10	6	4	9	5	4	4911.1081	-0.0045
11	5	6	10	4	6	4975.6197	0.0061
12	4	8	11	3	8	5037.7294	0.0091
12	4	9	11	3	9	5040.2128	0.0020
13	3	10	12	2	10	5068.2068	-0.0054
16	1	15	15	2	13	5092.9099	0.0044
9	8	1	8	7	1	5121.4180	-0.0069
10	7	3	9	6	3	5186.1943	-0.0003
11	6	5	10	5	5	5250.8815	-0.0067
13	4	10	12	3	10	5379.9701	-0.0045
9	9	0	8	8	0	5396.4739	-0.0028
10	8	2	9	7	2	5461.2491	-0.0027
14	3	12	13	2	12	5472.4528	0.0261
11	7	4	10	6	4	5526.0017	0.0000
12	6	6	11	5	6	5590.6282	-0.0025
13	5	8	12	4	8	5654.7235	0.0067
13	5	9	12	4	9	5654.8255	-0.0028
14	4	11	13	3	11	5719.8295	-0.0013
10	9	1	9	8	1	5736.3024	-0.0021
12	7	5	11	6	5	5865.7901	-0.0008

13	6	7	12	5	7	5930.3316	0.0000
10	10	0	9	9	0	6011.3904	0.0301
15	4	11	14	3	11	6050.0641	0.0377
15	4	12	14	3	12	6059.8360	-0.0051
16	2	15	15	1	15	6066.9658	-0.0067
11	9	2	10	8	2	6076.1215	-0.0051
12	8	4	11	7	4	6140.8727	-0.0054
13	7	6	12	6	6	6205.5539	-0.0033
14	6	8	13	5	8	6269.9815	0.0009
19	1	18	18	2	17	6306.3863	-0.0064
15	5	10	14	4	10	6333.3023	0.0026
11	10	1	10	9	1	6351.1817	-0.0006
16	4	13	15	3	13	6400.0817	-0.0007
12	9	3	11	8	3	6415.9396	-0.0016
13	8	5	12	7	5	6480.6682	-0.0035
14	7	7	13	6	7	6545.2936	-0.0018
11	11	0	10	10	0	6626.2410	-0.0014
12	10	2	11	9	2	6690.9944	-0.0041
17	4	14	16	3	14	6740.6356	-0.0090
13	9	4	12	8	4	6755.7433	-0.0030
14	8	6	13	7	6	6820.4284	-0.0194
15	7	8	14	6	8	6884.9989	-0.0002
16	6	11	15	5	11	6949.0912	-0.0015
12	11	1	11	10	1	6966.0571	-0.0007
22	2	20	21	3	18	6978.2412	-0.0293
19	3	17	18	2	16	6979.3208	0.0010
13	10	3	12	9	3	7030.8057	-0.0019
14	9	5	13	8	5	7095.5378	-0.0016
15	8	7	14	7	7	7160.2007	-0.0021
19	2	18	18	1	18	7176.3849	0.0092
16	7	9	15	6	9	7224.6632	0.0013
12	12	0	11	11	0	7241.1229	-0.0001
20	2	18	19	1	18	7255.5542	0.0004
13	11	2	12	10	2	7305.8645	-0.0029
18	5	14	17	4	14	7351.1867	0.0137
14	10	4	13	9	4	7370.6054	-0.0028
15	9	6	14	8	6	7435.3175	-0.0008
20	1	19	19	0	19	7440.3077	0.0088
17	7	10	16	6	10	7564.2772	0.0007
13	12	1	12	11	1	7580.9293	-0.0019
15	10	5	14	9	5	7710.3969	-0.0012
16	9	7	15	8	7	7775.0783	-0.0019
17	8	9	16	7	9	7839.6509	0.0186
13	13	0	12	12	0	7856.0010	-0.0010
14	12	2	13	11	2	7920.7307	-0.0029

Table S12. Linelist for sevoflurane dimer (homochiral),  $^{13}\text{C}$  (acceptor, isopropyl) species. RMS error for the fit is 10.7 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
5	4	1	4	3	1	2664.4354	-0.0031
8	1	7	7	0	7	2928.1784	-0.0030
6	4	2	5	3	2	3004.3426	0.0101
7	3	4	6	2	4	3065.5786	-0.0170
7	3	5	6	2	5	3070.4636	0.0168
8	2	6	7	1	6	3096.6662	-0.0019
6	5	1	5	4	1	3280.0284	0.0008
7	4	3	6	3	3	3344.1677	-0.0059
9	2	7	8	1	7	3430.4253	0.0008
6	6	0	5	5	0	3555.6868	0.0005
7	5	2	6	4	2	3619.9380	-0.0029
8	4	4	7	3	4	3683.9142	-0.0115
7	6	1	6	5	1	3895.6073	-0.0021
8	5	3	7	4	3	3959.8354	0.0012
9	4	5	8	3	5	4023.5428	0.0035
9	4	6	8	3	6	4023.9384	-0.0039
13	1	12	12	2	10	4089.0345	-0.0120
11	2	9	10	1	9	4101.8192	-0.0229
7	7	0	6	6	0	4171.2674	-0.0015
8	6	2	7	5	2	4235.5218	-0.0025
9	5	4	8	4	4	4299.6957	-0.0009
10	4	6	9	3	6	4362.9443	-0.0044
10	4	7	9	3	7	4363.7638	0.0150
8	7	1	7	6	1	4511.1868	-0.0020
9	6	3	8	5	3	4575.4251	-0.0012
10	5	5	9	4	5	4639.5197	0.0042
11	4	7	10	3	7	4702.0525	-0.0173
11	4	8	10	3	8	4703.5447	0.0023
13	1	12	12	0	12	4760.9882	0.0022
12	3	10	11	2	10	4783.5692	-0.0039
8	8	0	7	7	0	4786.8490	-0.0015
9	7	2	8	6	2	4851.1005	-0.0013
10	6	4	9	5	4	4915.3076	-0.0017
13	2	12	12	1	12	4975.0676	-0.0149
11	5	7	10	4	7	4979.2963	-0.0054
12	4	9	11	3	9	5043.3514	0.0050
14	2	12	13	1	12	5125.2255	0.0102
10	7	3	9	6	3	5191.0014	-0.0036
11	6	5	10	5	5	5255.1651	-0.0016
12	5	8	11	4	8	5319.0279	0.0149
9	9	0	8	8	0	5402.4469	0.0158
10	8	2	9	7	2	5466.6627	-0.0129
15	1	14	14	0	14	5517.3780	0.0133
11	7	4	10	6	4	5530.8913	-0.0032
12	6	7	11	5	6	5594.9851	-0.0053
13	5	8	12	4	8	5658.5349	0.0017
13	5	9	12	4	9	5658.6394	-0.0088
15	2	14	14	1	14	5704.1943	0.0284
14	4	10	13	3	10	5716.5540	0.0250
15	3	12	14	2	12	5727.5136	0.0208
10	9	1	9	8	1	5742.3371	-0.0042
11	8	3	10	7	3	5806.5786	0.0018
12	7	5	11	6	5	5870.7658	0.0000
13	6	7	12	5	7	5934.7706	-0.0011
14	5	9	13	4	9	5997.9703	-0.0100
14	5	10	13	4	10	5998.1864	-0.0098
10	10	0	9	9	0	6018.0045	-0.0056
12	8	4	11	7	4	6146.4662	-0.0005
16	3	14	15	2	14	6172.8549	0.0291
17	2	15	16	1	15	6175.9673	-0.0130

13	7	6	12	6	6	6210.6170	0.0032
14	6	8	13	5	8	6274.5061	0.0056
19	1	18	18	2	17	6308.7584	-0.0185
15	5	11	14	4	11	6337.6452	-0.0019
11	10	1	10	9	1	6357.9342	0.0194
17	3	14	16	2	14	6382.3273	0.0060
16	4	13	15	3	13	6403.6296	0.0377
12	9	3	11	8	3	6422.1442	0.0010
13	8	5	12	7	5	6486.3431	0.0006
14	7	7	13	6	7	6550.4349	0.0017
15	6	10	14	5	9	6614.1718	0.0065
11	11	0	10	10	0	6633.5839	-0.0039
16	5	12	15	4	12	6676.9868	-0.0072
12	10	2	11	9	2	6697.8128	-0.0007
13	9	4	12	8	4	6762.0295	-0.0011
14	8	6	13	7	6	6826.2040	0.0033
15	7	8	14	6	8	6890.2362	0.0185
16	6	11	15	5	11	6953.7674	-0.0020
12	11	1	11	10	1	6973.4837	-0.0022
13	10	3	12	9	3	7037.7079	0.0026
18	4	14	17	3	14	7056.1834	-0.0015
14	9	5	13	8	5	7101.9093	0.0031
15	8	7	14	7	7	7166.0398	0.0025
16	7	9	15	6	9	7229.9352	-0.0254
19	3	17	18	2	17	7230.4397	-0.0256
12	12	0	11	11	0	7249.1587	-0.0055
17	6	12	16	5	12	7293.2786	-0.0023
13	11	2	12	10	2	7313.3751	-0.0030
14	10	4	13	9	4	7377.5882	0.0000
15	9	6	14	8	6	7441.7587	-0.0084
16	8	8	15	7	8	7505.8657	0.0174
17	7	10	16	6	10	7569.6585	0.0038
13	12	1	12	11	1	7589.0536	-0.0014
14	11	3	13	10	3	7653.2648	0.0013
19	5	15	18	4	15	7694.3869	-0.0233
15	10	5	14	9	5	7717.4612	0.0006
16	9	7	15	8	7	7781.6135	0.0025
17	8	9	16	7	9	7845.6301	0.0011
13	13	0	12	12	0	7864.7334	-0.0054
18	7	11	17	6	11	7909.2914	-0.0004
14	12	2	13	11	2	7928.9382	-0.0017
15	11	4	14	10	4	7993.1384	-0.0020

Table S13. Linelist for sevoflurane dimer (homochiral),  $^{13}\text{C}$  (acceptor, fluoromethoxy) species. RMS error for the fit is 10.8 kHz.

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
8	1	7	7	0	7	2936.2395	-0.0093
6	5	1	5	4	1	3270.4425	-0.0017
11	0	11	10	1	9	3443.6886	-0.0068
7	5	2	6	4	2	3610.4205	-0.0032
12	1	11	11	2	9	3753.3910	-0.0088
13	2	11	12	3	9	3807.0327	-0.0035
7	6	1	6	5	1	3883.8748	0.0007
8	5	3	7	4	3	3950.3672	-0.0113
9	4	6	8	3	6	4016.7643	-0.0015
10	3	7	9	2	7	4066.4551	0.0107
11	2	9	10	1	9	4099.3546	-0.0126
7	7	0	6	6	0	4157.3097	-0.0024
8	6	2	7	5	2	4223.8540	-0.0026
9	5	4	8	4	4	4290.3025	0.0070
10	4	6	9	3	6	4355.5321	0.0053
10	4	7	9	3	7	4356.6715	0.0310
8	7	1	7	6	1	4497.2973	-0.0038
9	6	3	8	5	3	4563.8192	-0.0043
10	5	5	9	4	5	4630.1744	0.0166
8	8	0	7	7	0	4770.7380	-0.0032
12	3	10	11	2	10	4782.3315	-0.0181
9	7	2	8	6	2	4837.2773	-0.0051
10	6	4	9	5	4	4903.7668	-0.0009
19	5	15	18	6	13	4965.7372	-0.0110
12	4	9	11	3	9	5036.4239	-0.0079
10	7	3	9	6	3	5177.2489	-0.0033
11	6	5	10	5	5	5243.6815	0.0009
13	4	10	12	3	10	5376.4166	-0.0205
9	9	0	8	8	0	5384.1676	-0.0015
10	8	2	9	7	2	5450.7008	-0.0033
14	3	12	13	2	12	5477.0630	0.0048
11	7	4	10	6	4	5517.2044	-0.0011
12	6	6	11	5	6	5583.5616	0.0093
15	3	12	14	2	12	5713.5149	-0.0133
10	9	1	9	8	1	5724.1433	-0.0055
12	7	5	11	6	5	5857.1402	0.0029
13	6	7	12	5	7	5923.3915	0.0198
10	10	0	9	9	0	5997.5912	-0.0045
11	9	2	10	8	2	6064.1196	-0.0027
13	7	6	12	6	6	6197.0459	0.0049
14	6	8	13	5	8	6263.1558	0.0295
11	10	1	10	9	1	6337.5584	-0.0112
12	9	3	11	8	3	6404.0841	-0.0033
13	8	5	12	7	5	6470.5481	-0.0191
14	7	7	13	6	7	6536.9152	0.0052
11	11	0	10	10	0	6611.0192	-0.0017
12	10	2	11	9	2	6677.5350	-0.0025
14	8	6	13	7	6	6810.4899	0.0046
15	7	8	14	6	8	6876.7529	0.0164
12	11	1	11	10	1	6950.9824	-0.0059
13	10	3	12	9	3	7017.4977	0.0000
19	3	16	18	2	16	7026.7925	-0.0124
18	4	14	17	3	14	7041.5278	0.0147
18	4	15	17	3	15	7080.8937	0.0004
14	9	5	13	8	5	7083.9844	0.0025
15	8	7	14	7	7	7150.3867	0.0091
16	7	9	15	6	9	7216.5428	0.0305
12	12	0	11	11	0	7224.4392	-0.0054
13	11	2	12	10	2	7290.9485	-0.0013
18	5	13	17	4	13	7343.2495	-0.0161

14	10	4	13	9	4	7357.4485	0.0006
15	9	6	14	8	6	7423.9105	0.0050
16	8	8	15	7	8	7490.2506	0.0114
13	12	1	12	11	1	7564.4014	-0.0035
14	11	3	13	10	3	7630.9021	-0.0015
16	9	7	15	8	7	7763.8123	0.0037
17	8	9	16	7	9	7830.0832	0.0190
13	13	0	12	12	0	7837.8617	-0.0050
14	12	2	13	11	2	7904.3465	-0.0125
15	11	4	14	10	4	7970.8345	-0.0139

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Table S14. Linelist for sevoflurane dimer (homochiral),  $^{13}\text{C}$  (acceptor, perfluoro) species. RMS error for the fit is 10.0 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
4	4	0	3	3	0	2321.5607	0.0027
5	4	1	4	3	1	2661.3839	-0.0020
5	5	0	4	4	0	2936.2929	-0.0182
6	4	2	5	3	2	3001.1896	0.0010
8	2	7	7	1	7	3180.2277	0.0131
6	5	1	5	4	1	3276.1459	0.0035
6	6	0	5	5	0	3551.0617	-0.0010
7	5	2	6	4	2	3615.9630	0.0005
10	1	9	9	0	9	3645.4438	-0.0104
8	4	4	7	3	4	3680.6308	0.0172
8	4	5	7	3	5	3680.7901	0.0101
7	6	1	6	5	1	3890.8908	-0.0011
8	5	3	7	4	3	3955.7650	0.0013
11	2	10	10	1	9	4055.0166	-0.0070
13	0	13	12	1	11	4079.3154	0.0124
13	1	12	12	2	10	4088.3535	0.0006
7	7	0	6	6	0	4165.8106	-0.0028
8	6	2	7	5	2	4230.7144	0.0009
11	2	10	10	1	10	4247.3766	-0.0149
9	5	4	8	4	4	4295.5385	0.0022
12	1	11	11	0	11	4379.4019	0.0084
8	7	1	7	6	1	4505.6353	-0.0039
9	6	3	8	5	3	4570.5228	0.0003
10	5	5	9	4	5	4635.2688	0.0009
13	1	12	12	0	12	4751.3693	0.0092
8	8	0	7	7	0	4780.5575	-0.0054
9	7	2	8	6	2	4845.4538	-0.0047
10	6	4	9	5	4	4910.3131	-0.0004
11	5	6	10	4	6	4974.9593	0.0152
9	8	1	8	7	1	5120.3753	-0.0090
10	7	3	9	6	3	5185.2699	0.0015
11	6	5	10	5	5	5250.0837	0.0030
12	5	7	11	4	7	5314.5622	0.0152
14	2	13	13	1	13	5330.4738	-0.0100
13	4	10	12	3	10	5379.3655	-0.0114
9	9	0	8	8	0	5395.3012	-0.0100
10	8	2	9	7	2	5460.1819	-0.0181
11	7	4	10	6	4	5525.0653	0.0000
12	6	6	11	5	6	5589.8177	0.0015
10	9	1	9	8	1	5735.1268	-0.0007
11	8	3	10	7	3	5800.0092	0.0016
16	2	14	15	1	14	5816.3637	0.0123
12	7	5	11	6	5	5864.8512	0.0063
13	6	7	12	5	7	5929.5150	0.0031
10	10	0	9	9	0	6010.0525	-0.0057
15	4	11	14	3	11	6050.0629	0.0080
11	9	2	10	8	2	6074.9358	-0.0024
12	8	4	11	7	4	6139.8083	0.0037
13	7	6	12	6	6	6204.6096	0.0071
14	6	9	13	5	9	6269.1818	0.0203
11	10	1	10	9	1	6349.8667	-0.0020
17	3	14	16	2	14	6382.3273	0.0096
16	4	12	15	3	12	6385.9326	-0.0056
12	9	3	11	8	3	6414.7422	0.0004
13	8	5	12	7	5	6479.5940	0.0060
14	7	7	13	6	7	6544.3397	0.0065
15	6	9	14	5	9	6608.7406	-0.0045
11	11	0	10	10	0	6624.8008	-0.0031
18	1	17	17	0	17	6653.7364	-0.0200
12	10	2	11	9	2	6689.6736	-0.0001

18	3	15	17	2	15	6710.0253	-0.0125
13	9	4	12	8	4	6754.5422	0.0063
14	8	6	13	7	6	6819.3736	0.0190
15	7	8	14	6	8	6884.0355	0.0044
16	6	10	15	5	10	6948.2302	-0.0303
12	11	1	11	10	1	6964.5723	-0.0356
13	10	3	12	9	3	7029.4724	0.0007
14	9	5	13	8	5	7094.3238	0.0052
15	8	7	14	7	7	7159.1087	0.0078
16	7	9	15	6	9	7223.6957	0.0058
12	12	0	11	11	0	7239.5469	-0.0011
23	1	22	22	2	20	7294.9244	-0.0195
13	11	3	12	10	3	7304.4052	-0.0010
14	10	4	13	9	4	7369.2639	0.0028
15	9	6	14	8	6	7434.0947	0.0072
16	8	8	15	7	8	7498.8348	0.0118
17	7	10	16	6	10	7563.2904	-0.0123
13	12	1	12	11	1	7579.3395	-0.0053
18	6	13	17	5	13	7627.0496	-0.0179
14	11	3	13	10	3	7644.1987	0.0011
15	10	5	14	9	5	7709.0473	0.0070
16	9	7	15	8	7	7773.8475	0.0077
17	8	9	16	7	9	7838.5243	0.0078
13	13	0	12	12	0	7854.2923	0.0016
18	7	11	17	6	11	7902.8755	0.0132
14	12	2	13	11	2	7919.1333	-0.0024
15	11	4	14	10	4	7983.9831	0.0022

Table S15. Linelist for sevoflurane dimer (homochiral),  $^{13}\text{C}$  (donor, fluoromethoxy) species. RMS error for the fit is 10.0 kHz.

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
5	4	1	4	3	1	2656.0235	0.0210
5	5	0	4	4	0	2929.2763	-0.0013
6	4	2	5	3	2	2995.8940	0.0084
7	3	5	6	2	5	3064.0895	-0.0152
6	5	1	5	4	1	3269.1849	-0.0015
8	3	6	7	2	6	3405.1198	-0.0110
7	5	2	6	4	2	3609.0813	-0.0038
14	3	12	13	4	10	3806.7175	0.0081
7	6	1	6	5	1	3882.3618	-0.0025
8	5	3	7	4	3	3948.9657	-0.0005
7	7	0	6	6	0	4155.6534	0.0167
8	6	2	7	5	2	4222.2656	0.0018
9	5	4	8	4	4	4288.8224	0.0014
12	2	10	11	1	10	4436.9011	0.0034
8	7	1	7	6	1	4495.5364	-0.0034
9	6	3	8	5	3	4562.1488	-0.0028
10	5	5	9	4	5	4628.6385	0.0002
11	4	7	10	3	7	4693.8758	0.0159
11	4	8	10	3	8	4695.0345	0.0051
12	3	9	11	2	9	4737.3623	0.0198
9	7	2	8	6	2	4835.4355	-0.0015
16	2	14	15	3	12	4851.1003	-0.0066
11	5	6	10	4	6	4968.4152	0.0105
12	4	8	11	3	8	5032.8067	0.0298
12	4	9	11	3	9	5034.8039	-0.0003
9	8	1	8	7	1	5108.7143	0.0008
10	7	3	9	6	3	5175.3199	-0.0053
11	6	5	10	5	5	5241.8665	-0.0053
9	9	0	8	8	0	5381.9887	-0.0025
10	8	2	9	7	2	5448.6120	0.0052
14	3	11	13	2	12	5474.1143	-0.0095
15	1	14	14	0	14	5491.4698	0.0159
11	7	4	10	6	4	5515.1984	-0.0027
12	6	6	11	5	6	5581.6906	-0.0010
10	9	1	9	8	1	5721.8832	-0.0018
11	8	3	10	7	3	5788.5070	0.0146
12	7	5	11	6	5	5855.0596	-0.0014
13	6	7	12	5	7	5921.4775	0.0027
10	10	0	9	9	0	5995.1659	-0.0007
15	4	12	14	3	12	6054.4373	-0.0081
11	9	2	10	8	2	6061.7717	-0.0015
12	8	4	11	7	4	6128.3662	-0.0016
20	0	20	19	1	18	6150.6504	-0.0002
13	7	6	12	6	6	6194.9005	-0.0001
14	6	9	13	5	9	6261.2200	0.0050
11	10	1	10	9	1	6335.0517	-0.0028
12	9	3	11	8	3	6401.6514	-0.0032
13	8	5	12	7	5	6468.2299	-0.0008
17	3	15	16	2	15	6510.0670	-0.0214
14	7	8	13	6	8	6534.7179	0.0027
15	6	9	14	5	9	6600.9086	0.0131
11	11	0	10	10	0	6608.3363	-0.0043
12	10	2	11	9	2	6674.9346	-0.0023
17	4	14	16	3	14	6734.9862	-0.0183
14	8	6	13	7	6	6808.0791	0.0012
15	7	8	14	6	8	6874.5077	0.0085
16	6	10	15	5	10	6940.5284	0.0154
12	11	1	11	10	1	6948.2301	0.0080
13	10	3	12	9	3	7014.8117	-0.0010
14	9	5	13	8	5	7081.3896	0.0009

15	8	7	14	7	7	7147.9102	0.0041
16	7	9	15	6	9	7214.2727	0.0255
12	12	0	11	11	0	7221.5106	-0.0025
13	11	2	12	10	2	7288.0973	-0.0005
14	10	4	13	9	4	7354.6772	-0.0030
16	8	8	15	7	8	7487.7137	0.0021
13	12	1	12	11	1	7561.3866	-0.0008
18	6	13	17	5	13	7619.5221	-0.0165
14	11	3	13	10	3	7627.9646	-0.0023
15	10	5	14	9	5	7694.5371	-0.0009
16	9	7	15	8	7	7761.0694	-0.0008
17	8	9	16	7	9	7827.4544	-0.0361
13	13	0	12	12	0	7834.6805	-0.0036
14	12	2	13	11	2	7901.2536	-0.0021
19	6	14	18	5	14	7958.8946	-0.0148
15	11	5	14	10	5	7967.8294	0.0011

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Table S16. Linelist for sevoflurane dimer (homochiral),  $^{13}\text{C}$  (donor, isopropyl) species. RMS error for the fit is 10.8 kHz.

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
4	4	0	3	3	0	2324.6274	0.0008
5	3	2	4	2	2	2388.7822	0.0040
6	3	3	5	2	3	2728.0578	-0.0276
13	5	8	12	6	6	2909.4909	0.0052
8	1	7	7	0	7	2929.5692	0.0061
6	4	2	5	3	2	3004.9404	0.0032
11	1	11	10	2	9	3202.8759	-0.0108
8	3	6	7	2	5	3404.1030	0.0229
8	3	5	7	2	5	3404.4681	-0.0198
6	6	0	5	5	0	3555.7871	0.0000
7	5	2	6	4	2	3620.5361	-0.0048
8	4	4	7	3	4	3685.0078	-0.0209
7	6	1	6	5	1	3895.9561	-0.0016
8	5	3	7	4	3	3960.6829	0.0009
7	7	0	6	6	0	4171.3635	-0.0021
8	6	2	7	5	2	4236.1185	-0.0017
9	5	4	8	4	4	4300.7970	0.0043
10	4	6	9	3	6	4364.5348	-0.0230
16	3	14	15	4	12	4484.4576	0.0247
8	7	1	7	6	1	4511.5344	0.0014
9	6	3	8	5	3	4576.2699	0.0000
10	5	5	9	4	5	4640.8670	0.0068
8	8	0	7	7	0	4786.9424	-0.0008
17	3	15	16	4	13	4824.4939	-0.0267
9	7	2	8	6	2	4851.6903	-0.0032
16	2	14	15	3	12	4860.5836	0.0093
10	6	4	9	5	4	4916.3966	-0.0041
11	5	6	10	4	6	4980.8757	0.0070
14	2	13	13	1	12	5017.3674	-0.0137
17	2	16	16	3	14	5032.3209	0.0219
12	4	9	11	3	9	5045.4480	0.0123
9	8	1	8	7	1	5127.1022	-0.0038
10	7	3	9	6	3	5191.8422	-0.0021
11	6	5	10	5	5	5256.5073	0.0012
12	5	8	11	4	8	5320.8565	0.0005
13	4	10	12	3	10	5385.5469	0.0164
9	9	0	8	8	0	5402.5138	-0.0056
17	1	16	16	2	14	5424.5744	-0.0063
10	8	2	9	7	2	5467.2618	-0.0012
11	7	4	10	6	4	5531.9819	0.0004
18	2	16	17	3	14	5574.6210	-0.0108
20	4	16	19	5	14	5584.5497	-0.0166
12	6	6	11	5	6	5596.5784	0.0001
17	0	17	16	1	16	5724.8214	-0.0034
10	9	1	9	8	1	5742.6758	-0.0014
16	2	14	15	1	14	5825.2883	-0.0067
12	7	5	11	6	5	5872.1016	0.0011
13	6	7	12	5	7	5936.6090	0.0005
10	10	0	9	9	0	6018.0898	-0.0046
11	9	2	10	8	2	6082.8361	0.0067
12	8	4	11	7	4	6147.5514	0.0020
13	7	6	12	6	6	6212.1994	0.0028
14	6	8	13	5	8	6276.5878	0.0010
15	5	10	14	4	10	6339.8667	0.0005
11	10	1	10	9	1	6358.2459	-0.0005
12	9	3	11	8	3	6422.9731	-0.0009
17	2	16	16	1	16	6442.2373	0.0191
13	8	5	12	7	5	6487.6832	0.0103
18	2	16	17	1	16	6536.5212	-0.0243
14	7	7	13	6	7	6552.2674	0.0030

15	6	9	14	5	9	6616.5035	0.0015
11	11	0	10	10	0	6633.6646	-0.0034
16	5	11	15	4	11	6679.1754	-0.0213
16	5	12	15	4	12	6679.8208	-0.0222
12	10	2	11	9	2	6698.3911	-0.0016
13	9	4	12	8	4	6763.1116	0.0025
14	8	6	13	7	6	6827.7844	0.0055
15	7	8	14	6	8	6892.2650	-0.0325
16	6	10	15	5	10	6956.3303	-0.0111
12	11	1	11	10	1	6973.8097	-0.0037
13	10	3	12	9	3	7038.5369	0.0050
19	3	16	18	2	16	7043.6078	-0.0084
14	9	5	13	8	5	7103.2358	0.0036
15	8	7	14	7	7	7167.8731	0.0094
16	7	9	15	6	9	7232.2950	0.0052
12	12	0	11	11	0	7249.2392	-0.0008
17	6	11	16	5	11	7296.1054	0.0141
13	11	2	12	10	2	7313.9521	-0.0011
14	10	4	13	9	4	7378.6679	0.0054
15	9	6	14	8	6	7443.3450	0.0040
16	8	8	15	7	8	7507.9275	0.0046
17	7	10	16	6	10	7572.2360	0.0025
13	12	2	12	11	2	7589.3755	-0.0028
18	6	12	17	5	12	7635.7440	0.0086
14	11	3	13	10	3	7654.0855	-0.0004
24	2	22	23	3	20	7671.3698	0.0148
15	10	5	14	9	5	7718.7851	0.0027
20	4	16	19	3	16	7721.8455	0.0253
16	9	7	15	8	7	7783.4368	0.0041
17	8	9	16	7	9	7847.9597	0.0074
18	7	11	17	6	11	7912.1200	-0.0008
14	12	2	13	11	2	7929.5083	-0.0024
21	2	20	20	1	20	7931.2778	0.0027
15	11	4	14	10	4	7994.2105	0.0001

Table S17. Linelist for sevoflurane dimer (homochiral),  $^{13}\text{C}$  (donor, perfluoro 2) species. RMS error for the fit is 10.4 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
5	4	1	4	3	1	2662.0735	-0.0031
9	1	8	8	2	6	2709.7582	-0.0296
7	2	6	6	1	6	2830.3256	0.0009
5	5	0	4	4	0	2937.1505	-0.0025
6	4	3	5	3	3	3001.9140	-0.0206
10	1	9	9	2	7	3057.6865	0.0000
6	5	1	5	4	1	3277.0180	0.0007
6	6	0	5	5	0	3552.0685	-0.0195
7	5	2	6	4	2	3616.8604	-0.0091
10	2	8	9	1	8	3763.6903	-0.0312
7	6	1	6	5	1	3891.9488	-0.0016
8	5	3	7	4	3	3956.7024	0.0012
13	1	12	12	2	10	4089.0345	-0.0342
7	7	0	6	6	0	4167.0170	-0.0050
8	6	2	7	5	2	4231.8021	-0.0024
9	5	4	8	4	4	4296.5073	0.0058
8	7	1	7	6	1	4506.9029	0.0217
9	6	3	8	5	3	4571.6462	0.0009
10	5	6	9	4	6	4636.2586	-0.0105
11	4	8	10	3	8	4700.8123	-0.0019
8	8	0	7	7	0	4781.9485	-0.0065
9	7	2	8	6	2	4846.7269	-0.0065
10	6	4	9	5	4	4911.4661	-0.0006
11	5	7	10	4	7	4975.9755	-0.0041
9	8	1	8	7	1	5121.8034	-0.0063
10	7	3	9	6	3	5186.5735	-0.0020
11	6	5	10	5	5	5251.2634	0.0015
10	8	2	9	7	2	5461.6602	0.0017
11	7	4	10	6	4	5526.4010	-0.0026
12	6	6	11	5	6	5591.0335	0.0108
10	9	1	9	8	1	5736.7262	-0.0102
11	8	3	10	7	3	5801.4960	-0.0026
12	7	5	11	6	5	5866.2178	0.0045
13	6	7	12	5	7	5930.7522	0.0123
10	10	0	9	9	0	6011.8115	-0.0056
11	9	2	10	8	2	6076.5765	-0.0037
12	8	4	11	7	4	6141.3273	-0.0001
13	7	6	12	6	6	6206.0048	0.0056
14	6	9	13	5	8	6270.4110	0.0077
11	10	1	10	9	1	6351.6552	-0.0057
12	9	3	11	8	3	6416.4153	-0.0012
13	8	5	12	7	5	6481.1448	0.0029
14	7	7	13	6	7	6545.7637	0.0080
15	6	9	14	5	9	6610.0252	0.0236
11	11	0	10	10	0	6626.7395	-0.0067
12	10	2	11	9	2	6691.4966	-0.0025
13	9	4	12	8	4	6756.2423	-0.0006
14	8	6	13	7	6	6820.9407	0.0023
15	7	8	14	6	8	6885.4878	0.0111
19	2	17	18	1	17	6896.0397	0.0047
12	11	1	11	10	1	6966.5782	-0.0053
13	10	3	12	9	3	7031.3295	-0.0005
15	8	7	14	7	7	7160.7201	0.0072
16	7	10	15	6	9	7225.1725	0.0174
12	12	0	11	11	0	7241.6700	-0.0038
13	11	2	12	10	2	7306.4124	-0.0026
14	10	4	13	9	4	7371.1515	-0.0004
15	9	6	14	8	6	7435.8602	0.0033
16	8	8	15	7	8	7500.4682	0.0071
17	7	10	16	6	10	7564.8042	0.0208

13	12	1	12	11	1	7581.4993	-0.0046
14	11	3	13	10	3	7646.2363	-0.0032
15	10	5	14	9	5	7710.9642	0.0009
16	9	7	15	8	7	7775.6535	0.0146
13	13	0	12	12	0	7856.5944	-0.0052
18	7	11	17	6	11	7904.3472	-0.0062
14	12	2	13	11	2	7921.3243	-0.0037
15	11	4	14	10	4	7986.0535	-0.0020

Table S18. Linelist for sevoflurane dimer (homochiral),  $^{13}\text{C}$  (donor, perfluoro) species. RMS error for the fit is 6.56 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
5	5	0	4	4	0	2936.5786	0.0091
7	3	4	6	2	4	3063.5429	0.0010
6	5	1	5	4	1	3276.3639	-0.0073
6	6	0	5	5	0	3551.3804	-0.0013
7	5	2	6	4	2	3616.1617	-0.0011
7	6	1	6	5	1	3891.1808	-0.0007
8	5	3	7	4	3	3955.9353	-0.0014
11	2	9	10	1	9	4100.3620	0.0149
7	7	0	6	6	0	4166.1907	-0.0023
8	6	2	7	5	2	4230.9757	0.0018
9	5	4	8	4	4	4295.6767	-0.0075
12	2	10	11	1	10	4437.8866	-0.0059
8	7	1	7	6	1	4505.9904	0.0011
9	6	3	8	5	3	4570.7573	0.0027
10	5	5	9	4	5	4635.3726	-0.0215
11	4	8	10	3	8	4699.9396	0.0023
8	8	0	7	7	0	4780.9957	-0.0075
9	7	2	8	6	2	4845.7798	0.0004
10	6	4	9	5	4	4910.5168	-0.0018
11	5	6	10	4	6	4975.0437	-0.0094
9	8	1	8	7	1	5120.7959	0.0007
10	7	3	9	6	3	5185.5629	0.0024
11	6	5	10	5	5	5250.2485	-0.0118
9	9	0	8	8	0	5395.8179	0.0055
10	8	2	9	7	2	5460.5830	0.0016
14	3	12	13	2	12	5468.5264	0.0034
11	7	4	10	6	4	5525.3287	-0.0006
10	9	1	9	8	1	5735.5967	-0.0022
11	8	3	10	7	3	5800.3650	0.0050
12	7	5	11	6	5	5865.0823	0.0002
10	10	0	9	9	0	6010.6080	-0.0120
11	9	2	10	8	2	6075.3852	0.0048
12	8	4	11	7	4	6140.1310	0.0025
13	7	6	12	6	6	6204.8146	0.0002
11	10	1	10	9	1	6350.3999	-0.0010
12	9	3	11	8	3	6415.1608	0.0062
13	8	5	12	7	5	6479.8895	0.0054
14	7	8	13	6	8	6544.5020	-0.0195
11	11	0	10	10	0	6625.4220	-0.0044
12	10	3	11	9	3	6690.1795	0.0032
13	9	4	12	8	4	6754.9176	-0.0022
14	8	6	13	7	6	6819.6250	0.0009
12	11	1	11	10	1	6965.2007	0.0000
13	10	3	12	9	3	7029.9511	0.0061
14	9	5	13	8	5	7094.6830	0.0087
15	8	7	14	7	7	7159.3412	-0.0037
12	12	0	11	11	0	7240.2255	-0.0057
13	11	2	12	10	2	7304.9724	0.0029
14	10	4	13	9	4	7369.7148	0.0094
15	9	6	14	8	6	7434.4221	0.0064
13	12	1	12	11	1	7579.9979	-0.0004
14	11	3	13	10	3	7644.7371	0.0056
15	10	5	14	9	5	7709.4641	0.0080
16	9	7	15	8	7	7774.1395	-0.0020
13	13	0	12	12	0	7855.0279	-0.0066
14	12	2	13	11	2	7919.7608	0.0011
15	11	4	14	10	4	7984.4892	0.0035

Table S19. Linelist for sevoflurane dimer (homochiral),  $^{18}\text{O}$  (donor) species. RMS error for the fit is 9.78 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
8	5	4	7	4	4	3949.0625	-0.0078
7	7	0	6	6	0	4160.1250	-0.0073
9	5	5	8	4	5	4287.9625	-0.0000
8	7	2	7	6	1	4499.0875	-0.0018
9	6	4	8	5	4	4563.0125	-0.0133
10	6	4	9	5	4	4901.9375	0.0024
10	8	3	9	7	2	5451.9625	-0.0075
11	8	4	10	7	3	5790.8875	0.0036
12	7	5	11	6	5	5854.7750	0.0081
10	10	1	9	9	1	6001.9875	0.0010
11	9	3	10	8	2	6065.9000	0.0038
12	8	5	11	7	5	6129.8125	-0.0042
13	7	7	12	6	6	6193.6625	0.0168
14	6	9	13	5	9	6257.3000	0.0003
12	9	4	11	8	3	6404.8375	0.0125
13	8	5	12	7	5	6468.7250	0.0059
11	11	1	10	10	0	6615.9000	-0.0158
13	9	5	12	8	4	6743.7375	0.0017
14	8	7	13	7	7	6807.6125	0.0033
15	7	8	14	6	8	6871.3250	0.0041
12	11	1	11	10	1	6954.8250	-0.0109
13	10	4	12	9	4	7018.7500	0.0050
14	9	6	13	8	5	7082.6625	-0.0025
12	12	1	11	11	1	7229.8375	0.0133
13	11	2	12	10	2	7293.7375	-0.0060
13	12	2	12	11	1	7568.7625	0.0137
13	13	1	12	12	0	7843.7875	0.0075
14	12	3	13	11	2	7907.6625	-0.0079

Table S20. Linelist for sevoflurane dimer (homochiral),  $^{18}\text{O}$  (acceptor) species. RMS error for the fit is 9.78 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
8	6	3	7	5	2	4231.3875	0.0142
9	5	5	8	4	5	4296.7500	0.0173
9	6	3	8	5	3	4571.4625	-0.0198
10	5	6	9	4	6	4636.7375	0.0283
11	7	5	10	6	4	5526.2875	-0.0053
12	6	7	11	5	7	5591.5250	0.0067
10	9	2	9	8	1	5735.4875	-0.0013
12	7	5	11	6	5	5866.3250	0.0070
10	10	1	9	9	0	6010.1625	0.0275
11	9	3	10	8	2	6075.6125	-0.0069
12	9	4	11	8	3	6415.7000	-0.0192
14	7	7	13	6	7	6546.3500	0.0034
11	11	1	10	10	0	6624.9125	0.0023
12	10	3	11	9	2	6690.3500	-0.0071
14	8	6	13	7	6	6821.1250	0.0164
15	7	9	14	6	9	6886.3125	-0.0043
12	11	2	11	10	1	6965.0125	0.0109
13	10	4	12	9	4	7030.4250	0.0009
14	9	6	13	8	5	7095.8000	0.0115
15	8	7	14	7	7	7161.1250	0.0309
12	12	1	11	11	0	7239.6750	-0.0087
13	11	3	12	10	3	7305.0750	0.0146
13	12	1	12	11	1	7579.7000	0.0081
14	11	4	13	10	4	7645.1375	0.0164
17	8	9	16	7	9	7841.0875	-0.0036
15	11	5	14	10	5	7985.1875	0.0053

Table S21. Linelist for sevoflurane dimer (heterochiral), parent species. RMS error for the fit is 7.25 kHz.

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}$ (MHz)	OMC (MHz)
6	1	6	5	1	5	2029.1711	-0.0022
4	3	2	3	2	1	2036.7691	-0.0003
4	3	1	3	2	2	2038.7845	0.0001
6	0	6	5	0	5	2044.1596	-0.0021
6	2	5	5	2	4	2055.1560	-0.0012
6	4	3	5	4	2	2058.2159	0.0038
6	3	4	5	3	3	2058.7290	-0.0001
6	3	3	5	3	2	2059.3575	-0.0010
6	2	4	5	2	3	2067.8897	0.0005
5	2	4	4	1	3	2072.3052	-0.0012
6	1	5	5	1	4	2078.4006	0.0008
6	1	6	5	0	5	2110.8623	-0.0049
5	2	3	4	1	4	2168.6103	0.0043
19	9	11	19	8	12	2257.0254	0.0000
18	9	9	18	8	10	2258.5710	0.0028
17	9	8	17	8	9	2259.8826	0.0024
16	9	7	16	8	8	2260.9835	-0.0025
15	9	6	15	8	7	2261.9112	0.0018
14	9	5	14	8	6	2262.6727	0.0008
13	9	4	13	8	5	2263.2959	0.0019
12	9	3	12	8	4	2263.7927	-0.0016
11	9	2	11	8	3	2264.1909	0.0005
10	9	1	10	8	2	2264.4941	-0.0038
9	9	0	9	8	1	2264.7283	-0.0032
4	4	1	3	3	0	2304.3665	0.0048
7	0	7	6	1	6	2313.5929	-0.0002
20	0	20	19	5	15	2328.0917	0.0175
7	1	7	6	1	6	2366.2103	-0.0022
5	3	3	4	2	2	2377.2711	-0.0015
7	0	7	6	0	6	2380.2956	-0.0029
5	3	2	4	2	3	2383.3598	0.0031
9	2	8	8	3	5	2386.3270	-0.0023
6	2	5	5	1	4	2394.4204	-0.0028
7	2	6	6	2	5	2396.7062	-0.0010
7	6	2	6	6	1	2400.7829	-0.0007
7	5	3	6	5	2	2401.0797	-0.0017
7	4	4	6	4	3	2401.6136	-0.0143
7	4	3	6	4	2	2401.6696	0.0087
7	3	5	6	3	4	2402.2645	0.0004
7	3	4	6	3	3	2403.6675	0.0000
7	2	5	6	2	4	2416.0948	0.0011
7	1	6	6	1	5	2422.9748	0.0007
7	1	7	6	0	6	2432.9131	-0.0048
8	1	7	7	2	6	2476.8023	0.0061
9	2	7	8	3	6	2499.7464	0.0057
10	3	8	9	4	5	2502.8979	0.0001
24	10	14	24	9	15	2517.1608	0.0060
23	10	13	23	9	14	2519.3836	0.0012
22	10	12	22	9	13	2521.3433	0.0032
21	10	11	21	9	12	2523.0548	0.0029
20	10	10	20	9	11	2524.5428	0.0023
19	10	9	19	9	10	2525.8305	0.0033
18	10	8	18	9	9	2526.9336	0.0020
17	10	7	17	9	8	2527.8751	0.0026
16	10	6	16	9	7	2528.6701	0.0028
15	10	5	15	9	6	2529.3326	0.0002
14	10	4	14	9	5	2529.8855	0.0024
13	10	3	13	9	4	2530.3367	0.0030
12	10	2	12	9	3	2530.7003	0.0031
11	10	1	11	9	2	2530.9900	0.0039

6	2	4	5	1	5	2544.7716	0.0076
11	4	7	10	5	6	2584.1693	0.0349
8	0	8	7	1	7	2662.6347	-0.0009
8	1	8	7	1	7	2702.8432	-0.0036
10	2	9	9	3	6	2710.4201	-0.0089
7	2	6	6	1	5	2712.7240	-0.0066
8	0	8	7	0	7	2715.2523	-0.0027
6	3	3	5	2	4	2729.4956	0.0042
13	6	8	12	7	5	2732.3776	-0.0046
8	2	7	7	2	6	2737.8149	-0.0020
8	7	2	7	7	1	2743.7039	-0.0009
8	6	2	7	6	1	2743.9688	-0.0020
8	5	4	7	5	3	2744.4128	-0.0001
8	4	5	7	4	4	2745.2080	-0.0012
8	4	4	7	4	3	2745.2983	-0.0009
8	3	6	7	3	5	2745.8611	0.0001
8	3	5	7	3	4	2748.6618	0.0337
8	1	8	7	0	7	2755.4604	-0.0057
8	2	6	7	2	5	2765.0029	0.0004
8	1	7	7	1	6	2766.5525	-0.0003
25	11	15	25	10	16	2785.5428	0.0064
24	11	13	24	10	14	2787.3975	0.0015
23	11	12	23	10	13	2789.0415	0.0001
22	11	11	22	10	12	2790.4914	0.0013
21	11	10	21	10	11	2791.7597	0.0003
20	11	9	20	10	10	2792.8689	0.0036
19	11	8	19	10	9	2793.8223	-0.0006
18	11	7	18	10	8	2794.6450	-0.0015
17	11	7	17	10	8	2795.3551	0.0053
16	11	6	16	10	7	2795.9471	0.0020
15	11	5	15	10	6	2796.4429	-0.0017
14	11	4	14	10	5	2796.8589	-0.0004
13	11	3	13	10	4	2797.1999	0.0000
12	11	1	12	10	2	2797.4691	-0.0067
11	3	9	10	4	6	2845.8146	-0.0025
9	1	8	8	2	7	2847.8920	0.0055
10	2	8	9	3	7	2873.3239	0.0100
11	3	8	10	4	7	2877.8230	-0.0001
5	5	1	4	4	0	2913.7705	0.0021
7	2	5	6	1	6	2931.7082	0.0239
6	4	3	5	3	2	2989.8940	-0.0025
6	4	2	5	3	3	2990.2277	0.0020
9	0	9	8	1	8	3009.2096	-0.0014
11	2	10	10	3	7	3027.2406	-0.0103
8	2	7	7	1	6	3027.5673	-0.0062
9	1	9	8	1	8	3039.0912	-0.0028
9	0	9	8	0	8	3049.4189	-0.0032
7	3	5	6	2	4	3049.6326	-0.0019
26	12	15	26	11	16	3053.4097	0.0044
25	12	13	25	11	14	3055.0111	0.0107
24	12	12	24	11	13	3056.4225	0.0027
23	12	11	23	11	12	3057.6841	0.0064
22	12	10	22	11	11	3058.7924	0.0052
21	12	9	21	11	10	3059.7619	0.0009
20	12	8	20	11	9	3060.6143	0.0034
19	12	7	19	11	8	3061.3513	0.0029
18	12	6	18	11	7	3061.9864	0.0024
17	12	5	17	11	6	3062.5297	0.0018
16	12	4	16	11	5	3062.9894	-0.0002
15	12	3	15	11	4	3063.3799	0.0017
14	12	2	14	11	3	3063.7214	0.0194
13	12	1	13	11	2	3063.9700	0.0011
12	12	1	12	11	2	3064.1880	0.0017

7	3	4	6	2	5	3078.0038	0.0021
9	2	8	8	2	7	3078.4331	-0.0020
9	1	9	8	0	8	3079.2990	-0.0061
9	8	1	8	8	0	3086.6232	0.0001
9	7	2	8	7	1	3086.8688	-0.0005
9	6	3	8	6	2	3087.2459	0.0003
9	5	5	8	5	4	3087.8746	0.0022
9	4	6	8	4	5	3088.9672	-0.0004
9	4	5	8	4	4	3089.1810	-0.0013
9	3	7	8	3	6	3089.4523	-0.0006
9	3	6	8	3	5	3094.4192	-0.0002
9	1	8	8	1	7	3108.9063	-0.0008
9	2	7	8	2	6	3114.1410	0.0010
15	7	8	14	8	7	3152.6334	0.0266
12	3	10	11	4	7	3187.2231	-0.0079
10	1	9	9	2	8	3219.2676	0.0046
12	3	9	11	4	8	3239.0308	0.0049
11	2	9	10	3	8	3251.6231	0.0083
6	5	2	5	4	1	3256.6863	0.0020
13	4	10	12	5	7	3274.8267	-0.0002
13	4	9	12	5	8	3281.2509	-0.0254
25	13	13	25	12	14	3323.5852	0.0034
24	13	11	24	12	12	3324.6976	0.0009
23	13	10	23	12	11	3325.6870	0.0007
22	13	9	22	12	10	3326.5633	0.0026
21	13	8	21	12	9	3327.3328	0.0034
20	13	7	20	12	8	3328.0043	0.0025
19	13	6	19	12	7	3328.5874	0.0010
18	13	5	18	12	6	3329.0923	0.0007
17	13	4	17	12	5	3329.5258	0.0007
16	13	3	16	12	4	3329.8978	0.0036
15	13	2	15	12	3	3330.2087	0.0028
14	13	1	14	12	2	3330.4589	-0.0078
7	4	4	6	3	3	3332.1644	-0.0015
7	4	4	6	3	3	3332.1644	-0.0015
7	4	3	6	3	4	3333.1587	0.0013
12	2	11	11	3	8	3335.0655	-0.0143
9	2	8	8	1	7	3339.4479	-0.0078
10	0	10	9	1	9	3353.2982	-0.0012
10	1	10	9	1	9	3374.9843	-0.0027
8	3	6	7	2	5	3379.3985	-0.0032
10	0	10	9	0	9	3383.1784	-0.0040
10	1	10	9	0	9	3404.8645	-0.0054
10	2	9	9	2	8	3418.5178	-0.0012
10	9	1	9	9	0	3429.5373	0.0008
10	8	2	9	8	1	3429.7675	-0.0026
8	3	5	7	2	6	3429.9223	-0.0002
10	7	4	9	7	3	3430.1055	0.0005
10	6	4	9	6	3	3430.6188	0.0000
10	5	6	9	5	5	3431.4819	0.0067
10	3	8	9	3	7	3432.9516	-0.0070
10	4	6	9	4	5	3433.3670	-0.0004
10	3	7	9	3	6	3441.2159	0.0006
10	1	9	9	1	8	3449.8104	-0.0012
10	2	8	9	2	7	3463.0271	0.0008
6	6	0	5	5	1	3523.1676	0.0006
13	3	11	12	4	8	3526.2979	-0.0057
11	1	10	10	2	9	3589.8364	0.0056
24	14	10	24	13	11	3592.4991	0.0033
23	14	9	23	13	10	3593.2993	0.0055
16	6	11	16	3	14	3593.7510	-0.0226
22	14	8	22	13	9	3593.9991	-0.0010
21	14	7	21	13	8	3594.6250	0.0025

20	14	6	20	13	7	3595.1705	0.0024
19	14	5	19	13	6	3595.6448	0.0012
18	14	4	18	13	5	3596.0570	0.0014
17	14	3	17	13	4	3596.4107	0.0004
16	14	2	16	13	3	3596.7121	-0.0012
7	5	3	6	4	2	3599.5498	0.0059
13	3	10	12	4	9	3606.0641	0.0075
13	2	12	12	3	9	3632.1653	-0.0118
14	4	10	13	5	9	3632.9801	0.0472
12	2	10	11	3	9	3633.8703	0.0081
10	2	9	9	1	8	3649.0584	-0.0093
8	4	5	7	3	4	3673.7062	-0.0014
8	4	4	7	3	5	3676.1926	0.0001
11	0	11	10	1	10	3695.1343	-0.0021
9	3	7	8	2	6	3703.8466	-0.0056
11	1	11	10	1	10	3710.5644	-0.0047
11	0	11	10	0	10	3716.8203	-0.0035
11	1	11	10	0	10	3732.2516	-0.0050
9	2	7	8	1	8	3741.7796	0.0123
11	2	10	10	2	9	3758.0349	-0.0021
11	10	2	10	10	1	3772.4445	0.0005
11	9	2	10	9	1	3772.6691	-0.0002
11	8	3	10	8	2	3772.9766	-0.0003
11	7	4	10	7	3	3773.4199	0.0001
11	6	6	10	6	5	3774.1010	-0.0004
11	5	7	10	5	6	3775.2267	-0.0092
11	5	6	10	5	5	3775.2626	-0.0031
11	3	9	10	3	8	3776.2857	-0.0010
11	4	8	10	4	7	3777.0174	0.0000
11	4	7	10	4	6	3777.9275	-0.0013
9	3	6	8	2	7	3786.5290	0.0039
11	1	10	10	1	9	3789.0802	-0.0065
11	3	8	10	3	7	3789.1445	0.0025
11	2	9	10	2	8	3811.2585	-0.0009
14	3	12	13	4	9	3861.9862	-0.0087
19	15	5	19	14	6	3862.5860	0.0013
18	15	3	18	14	4	3862.9212	-0.0074
17	15	2	17	14	3	3863.2281	0.0021
15	15	0	15	14	1	3863.7073	0.0089
7	6	2	6	5	1	3866.0900	0.0013
8	5	4	7	4	3	3942.3050	0.0089
11	2	10	10	1	9	3957.2843	-0.0089
12	1	11	11	2	10	3958.4540	0.0048
14	3	11	13	4	10	3979.4991	0.0051
15	4	11	14	5	10	3987.5327	0.0054
9	4	6	8	3	5	4014.0461	-0.0010
13	2	11	12	3	10	4019.1414	0.0061
9	4	5	8	3	6	4019.5134	-0.0004
12	0	12	11	1	11	4035.0812	-0.0020
16	5	11	15	6	10	4045.1141	-0.0026
12	1	12	11	1	11	4045.8866	-0.0020
12	0	12	11	0	11	4050.5138	-0.0022
12	1	12	11	0	11	4061.3187	-0.0028
12	2	11	11	2	10	4096.9692	-0.0016
12	10	2	11	10	1	4115.5656	0.0008
12	9	3	11	9	2	4115.8529	-0.0006
12	8	4	11	8	3	4116.2518	0.0022
12	7	5	11	7	4	4116.8222	0.0002
12	6	6	11	6	5	4117.7061	-0.0008
12	5	8	11	5	7	4119.1676	-0.0006
12	5	7	11	5	6	4119.2393	0.0035
12	3	10	11	3	9	4119.3422	-0.0005
12	4	9	11	4	8	4121.2797	0.0003

12	4	8	11	4	7	4122.9619	0.0002
27	16	12	27	15	13	4125.1755	0.0022
26	16	11	26	15	12	4125.9440	0.0025
12	1	11	11	1	10	4126.6532	-0.0024
23	16	8	23	15	9	4127.7305	-0.0739
22	16	6	22	15	7	4128.2984	0.0023
21	16	5	21	15	6	4128.7610	0.0298
20	16	4	20	15	5	4129.1123	-0.0025
7	7	0	6	6	1	4132.5654	0.0013
12	3	9	11	3	8	4138.2214	0.0013
10	3	7	9	2	8	4149.3124	0.0071
12	2	10	11	2	9	4158.5348	0.0005
15	3	13	14	4	10	4193.0450	-0.0045
8	6	3	7	5	2	4208.9782	0.0004
12	2	11	11	1	10	4265.1670	-0.0103
9	5	5	8	4	4	4284.8636	-0.0055
9	5	4	8	4	5	4285.0172	0.0069
16	4	13	15	5	10	4314.4005	-0.0019
13	1	12	12	2	11	4324.0782	0.0034
11	3	9	10	2	8	4335.9230	-0.0085
10	4	7	9	3	6	4352.5338	-0.0002
15	3	12	14	4	11	4359.5202	0.0086
10	4	6	9	3	7	4363.4290	0.0007
13	0	13	12	1	12	4373.5277	-0.0009
13	1	13	12	1	12	4380.9915	-0.0021
13	0	13	12	0	12	4384.3324	-0.0016
13	1	13	12	0	12	4391.7967	-0.0024
22	17	6	22	16	7	4395.2716	-0.0018
21	17	4	21	16	5	4395.6487	0.0006
20	17	3	20	16	4	4395.9819	0.0027
19	17	2	19	16	3	4396.2641	-0.0065
14	2	12	13	3	11	4406.4166	0.0097
13	2	12	12	2	11	4435.3148	-0.0025
13	12	1	12	12	0	4458.2370	0.0001
13	11	2	12	11	1	4458.4527	-0.0015
13	10	3	12	10	2	4458.7307	0.0006
13	9	4	12	9	3	4459.0925	-0.0012
13	8	6	12	8	5	4459.5925	-0.0016
13	7	7	12	7	6	4460.3186	-0.0010
13	6	8	12	6	7	4461.4428	0.0009
13	3	11	12	3	10	4462.0329	-0.0013
13	1	12	12	1	11	4462.5926	-0.0039
13	5	9	12	5	8	4463.2803	-0.0021
13	5	8	12	5	7	4463.4240	-0.0010
13	4	10	12	4	9	4465.6546	-0.0007
13	4	9	12	4	8	4468.5850	0.0004
8	7	1	7	6	2	4475.4856	0.0003
13	3	10	12	3	9	4488.3110	0.0010
13	2	11	12	2	10	4504.6145	-0.0013
16	3	14	15	4	11	4517.9895	-0.0066
11	3	8	10	2	9	4519.9376	0.0093
19	7	13	18	8	10	4534.7789	0.0164
9	6	3	8	5	4	4551.8086	-0.0019
13	2	12	12	1	11	4573.8291	-0.0100
10	5	6	9	4	5	4627.1601	-0.0018
10	5	5	9	4	6	4627.5320	0.0021
12	3	10	11	2	9	4644.0043	-0.0104
17	4	14	16	5	11	4659.7219	0.0008
14	1	13	13	2	12	4685.9210	0.0034
11	4	8	10	3	7	4688.3350	-0.0011
11	4	7	10	3	8	4708.4155	0.0170
14	0	14	13	1	13	4710.8281	-0.0003
14	1	14	13	1	13	4715.9277	-0.0009

14	0	14	13	0	13	4718.2991	0.0056
14	1	14	13	0	13	4723.3927	-0.0009
8	8	1	7	7	0	4741.9608	0.0009
16	3	13	15	4	12	4745.8479	0.0082
18	5	13	17	6	12	4746.1286	-0.0014
14	2	13	13	2	12	4773.0874	-0.0018
15	2	13	14	3	12	4794.5528	0.0032
14	1	13	13	1	12	4797.1581	-0.0020
14	13	2	13	13	1	4801.1197	-0.0009
14	12	2	13	12	1	4801.3327	-0.0039
14	11	3	13	11	2	4801.6024	-0.0011
14	10	4	13	10	3	4801.9389	-0.0051
14	9	5	13	9	4	4802.3940	-0.0005
14	8	6	13	8	5	4803.0156	-0.0010
14	7	8	13	7	7	4803.9206	-0.0004
14	3	12	13	3	11	4804.2748	-0.0010
14	6	9	13	6	8	4805.3270	0.0048
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14	2	13	13	1	12	4884.3240	-0.0078
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12	3	9	11	2	10	4900.1227	0.0115
13	3	11	12	2	10	4947.5035	-0.0112
11	5	7	10	4	6	4969.0299	-0.0006
11	5	6	10	4	7	4969.8895	0.0002
15	1	14	14	2	13	5043.5579	0.0028
15	0	15	14	1	14	5047.2802	-0.0003
15	0	15	14	0	14	5052.3815	0.0007
12	4	8	11	3	9	5055.0751	0.0017
15	1	15	14	0	14	5055.8330	0.0002
9	8	1	8	7	2	5084.8772	-0.0009
15	2	14	14	2	13	5110.3141	-0.0010
15	1	14	14	1	13	5130.7242	-0.0025
17	3	14	16	4	13	5137.8151	-0.0009
18	3	16	17	4	13	5142.7669	-0.0061
15	14	1	14	14	0	5143.9877	-0.0070
15	13	2	14	13	1	5144.2095	-0.0013
15	12	3	14	12	2	5144.4712	-0.0004
15	11	4	14	11	3	5144.7945	-0.0009
15	10	5	14	10	4	5145.2090	-0.0012
15	9	6	14	9	5	5145.7602	-0.0007
15	3	13	14	3	12	5145.9913	-0.0023
15	8	8	14	8	7	5146.5236	0.0001
15	7	8	14	7	7	5147.6355	0.0001
15	6	10	14	6	9	5149.3743	0.0165
15	5	11	14	5	10	5152.0776	-0.0027
15	5	10	14	5	9	5152.6093	0.0001
15	4	12	14	4	11	5154.5212	-0.0009
10	7	4	9	6	3	5161.2405	-0.0027
15	4	11	14	4	10	5162.1802	-0.0002
16	2	14	15	3	13	5182.3467	0.0059
15	3	12	14	3	11	5190.1095	-0.0004
15	2	13	14	2	12	5192.4155	-0.0030
15	2	14	14	1	13	5197.4803	-0.0066
11	6	6	10	5	5	5237.1732	0.0081
14	3	12	13	2	11	5247.1629	-0.0117
13	3	10	12	2	11	5291.4684	0.0181
12	5	8	11	4	7	5310.2680	-0.0017

12	5	7	11	4	8	5312.1112	0.0035
19	4	16	18	5	13	5344.5397	-0.0030
13	4	10	12	3	9	5347.9049	-0.0037
9	9	1	8	8	0	5351.3536	-0.0009
16	0	16	15	1	15	5383.1223	0.0025
16	1	16	15	1	15	5385.4392	0.0016
16	0	16	15	0	15	5386.5739	0.0021
16	1	16	15	0	15	5388.8905	0.0008
16	1	15	15	2	14	5396.9575	0.0012
13	4	9	12	3	10	5404.3173	0.0021
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20	5	16	19	6	13	5437.9778	-0.0104
19	3	17	18	4	14	5438.9784	-0.0070
16	2	15	15	2	14	5447.0355	-0.0012
19	4	15	18	5	14	5453.3038	-0.0001
20	5	15	19	6	14	5455.7664	-0.0017
16	1	15	15	1	14	5463.7147	-0.0017
16	15	2	15	15	1	5486.8576	-0.0007
16	3	14	15	3	13	5487.1228	-0.0041
16	13	3	15	13	2	5487.3305	-0.0022
16	12	4	15	12	3	5487.6423	-0.0021
16	11	5	15	11	4	5488.0312	-0.0018
16	10	6	15	10	5	5488.5320	-0.0005
16	9	7	15	9	6	5489.1976	0.0000
16	8	8	15	8	7	5490.1206	-0.0003
16	7	10	15	7	9	5491.4707	0.0011
16	6	10	15	6	9	5493.5867	-0.0150
16	5	12	15	5	11	5496.7601	0.0004
16	5	11	15	5	10	5497.7052	-0.0003
16	4	13	15	4	12	5498.8623	-0.0007
11	7	4	10	6	5	5504.0422	-0.0023
16	4	12	15	4	11	5510.4571	-0.0002
16	2	15	15	1	14	5513.7944	-0.0024
18	3	15	17	4	14	5534.4847	0.0021
16	3	13	15	3	12	5540.8503	0.0000
15	3	13	14	2	12	5543.8507	-0.0120
17	2	15	16	3	14	5568.4948	0.0047
12	6	6	11	5	7	5579.6450	-0.0097
13	5	9	12	4	8	5650.5732	-0.0174
13	5	8	12	4	9	5654.2525	-0.0007
14	4	11	13	3	10	5669.6856	-0.0055
10	9	1	9	8	2	5694.2672	-0.0008
14	3	11	13	2	12	5695.2421	0.0164
17	0	17	16	1	16	5718.5268	0.0028
17	1	17	16	1	16	5720.0732	0.0036
17	0	17	16	0	16	5720.8467	0.0049
17	1	17	16	0	16	5722.3912	0.0037
17	1	16	16	2	15	5746.4151	0.0005
14	4	10	13	3	11	5757.2584	0.0384
11	8	3	10	7	4	5770.6494	-0.0014
17	2	16	16	2	15	5783.3061	0.0000
21	5	17	20	6	14	5787.2388	-0.0077
17	1	16	16	1	15	5796.4938	-0.0012
17	3	15	16	3	14	5827.6291	-0.0021
17	16	1	16	16	0	5829.7086	-0.0020
17	15	2	16	15	1	5829.9284	-0.0017
17	14	3	16	14	2	5830.1845	-0.0008
17	12	5	16	12	4	5830.8569	-0.0006
17	11	6	16	11	5	5831.3189	-0.0003
17	10	7	16	10	6	5831.9143	-0.0004
17	9	8	16	9	7	5832.7029	-0.0065
17	2	16	16	1	15	5833.3868	0.0002
17	8	10	16	8	9	5833.8148	-0.0004

17	7	11	16	7	10	5835.4354	0.0013
17	6	12	16	6	11	5837.9322	-0.0048
17	6	11	16	6	10	5838.0196	-0.0013
16	3	14	15	2	13	5838.5612	-0.0098
17	5	13	16	5	12	5841.6078	-0.0008
17	4	14	16	4	13	5843.0238	-0.0002
17	5	12	16	5	11	5843.2311	0.0002
12	7	6	11	6	5	5846.7630	-0.0012
17	4	13	16	4	12	5859.8751	-0.0006
17	2	15	16	2	14	5873.2732	-0.0029
17	3	14	16	3	13	5890.8366	-0.0026
13	6	8	12	5	7	5921.8084	-0.0025
13	6	7	12	5	8	5921.9386	0.0062
19	3	16	18	4	15	5934.6813	-0.0012
18	2	16	17	3	15	5951.7085	0.0007
10	10	1	9	9	0	5960.7485	0.0005
15	4	12	14	3	11	5985.1128	-0.0076
14	5	10	13	4	9	5989.5904	-0.0017
14	5	9	13	4	10	5996.4677	0.0018
11	9	2	10	8	3	6037.1669	-0.0004
18	0	18	17	1	17	6053.6301	0.0064
18	1	18	17	1	17	6054.6547	0.0065
18	0	18	17	0	17	6055.1767	0.0073
18	1	18	17	0	17	6056.2021	0.0083
18	1	17	17	2	16	6092.4316	0.0030
15	3	12	14	2	13	6112.2669	0.0206
12	8	4	11	7	5	6113.4785	-0.0022
15	4	11	14	3	12	6115.1223	-0.0021
18	2	17	17	2	16	6119.1826	0.0010
18	1	17	17	1	16	6129.3204	0.0003
17	3	15	16	2	14	6132.4094	-0.0078
18	2	17	17	1	16	6156.0739	0.0007
18	3	16	17	3	15	6167.4779	-0.0009
18	17	2	17	17	1	6172.5488	-0.0022
18	16	2	17	16	1	6172.7706	-0.0030
18	15	3	17	15	2	6173.0274	-0.0007
18	14	4	17	14	3	6173.3355	0.0100
18	13	5	17	13	4	6173.6802	0.0001
18	12	6	17	12	5	6174.1139	0.0004
18	11	7	17	11	6	6174.6587	0.0012
18	10	8	17	10	7	6175.3609	0.0003
18	9	10	17	9	9	6176.3014	-0.0001
18	8	11	17	8	10	6177.6136	0.0002
18	7	11	17	7	10	6179.5414	-0.0019
18	6	13	17	6	12	6182.4991	-0.0003
18	6	12	17	6	11	6182.6583	0.0000
18	5	14	17	5	13	6186.6013	0.0007
18	4	15	17	4	14	6186.9093	0.0002
18	5	13	17	5	12	6189.2787	-0.0002
13	7	7	12	6	6	6189.3768	-0.0001
18	4	14	17	4	13	6210.4514	0.0031
18	2	16	17	2	15	6210.8458	-0.0030
18	3	15	17	3	14	6239.6854	-0.0052
14	6	9	13	5	8	6263.7034	-0.0046
14	6	8	13	5	9	6263.9856	0.0043
16	4	13	15	3	12	6293.8543	-0.0193
11	10	1	10	9	2	6303.6552	-0.0002
15	5	11	14	4	10	6326.7335	0.0001
19	2	17	18	3	16	6330.8212	-0.0004
20	3	17	19	4	16	6337.1229	-0.0047
15	5	10	14	4	11	6338.9857	0.0030
12	9	3	11	8	4	6380.0439	0.0000
19	0	19	18	1	18	6388.5225	0.0099

19	1	19	18	1	18	6389.1982	0.0100
19	0	19	18	0	18	6389.5457	0.0086
19	1	19	18	0	18	6390.2210	0.0084
18	3	16	17	2	15	6426.6138	-0.0062
19	1	18	18	2	17	6435.5843	0.0025
19	2	18	18	2	17	6454.7263	0.0027
13	8	6	12	7	5	6456.2518	-0.0009
19	1	18	18	1	17	6462.3371	0.0022
16	4	12	15	3	13	6479.5947	0.0064
19	2	18	18	1	17	6481.4793	0.0027
19	3	17	18	3	16	6506.6609	0.0002
19	18	1	18	18	0	6515.3793	0.0005
19	17	2	18	17	1	6515.6024	-0.0025
19	16	3	18	16	2	6515.8599	-0.0003
19	15	4	18	15	3	6516.1534	-0.0002
19	14	5	18	14	4	6516.4971	-0.0006
19	13	6	18	13	5	6516.9093	-0.0004
19	12	7	18	12	6	6517.4133	-0.0016
19	11	8	18	11	7	6518.0480	-0.0025
19	10	9	18	10	8	6518.8738	-0.0004
19	9	11	18	9	10	6519.9782	-0.0004
19	8	12	18	8	11	6521.5225	0.0008
19	7	13	18	7	12	6523.7961	0.0073
19	6	14	18	6	13	6527.2521	-0.0002
19	6	13	18	6	12	6527.5404	-0.0010
19	5	15	18	5	14	6531.6938	-0.0016
14	7	8	13	6	7	6531.8537	0.0015
19	5	14	18	5	13	6535.9652	0.0001
16	3	13	15	2	14	6542.8006	0.0192
19	2	17	18	2	16	6546.5881	-0.0047
23	5	18	22	6	17	6548.4814	-0.0114
19	4	15	18	4	14	6562.0415	-0.0031
11	11	0	10	10	1	6570.1398	-0.0002
19	3	16	18	3	15	6587.1033	-0.0057
17	4	14	16	3	13	6596.0391	-0.0083
15	6	10	14	5	9	6605.1954	-0.0024
15	6	9	14	5	10	6605.7712	-0.0021
22	4	18	21	5	17	6623.4142	-0.0127
12	10	3	11	9	2	6646.5508	0.0000
23	4	20	22	5	17	6658.5332	0.0017
16	5	12	15	4	11	6661.3134	0.0007
16	5	11	15	4	12	6682.1658	-0.0002
20	2	18	19	3	17	6704.9128	-0.0041
19	3	17	18	2	16	6722.4291	-0.0026
13	9	4	12	8	5	6722.8867	-0.0013
20	0	20	19	1	19	6723.2686	0.0118
20	1	20	19	1	19	6723.7129	0.0128
20	0	20	19	0	19	6723.9450	0.0127
20	1	20	19	0	19	6724.3886	0.0130
21	3	18	20	4	17	6740.4266	-0.0084
20	1	19	19	2	18	6776.4545	0.0026
20	2	19	19	2	18	6789.9946	0.0040
20	1	19	19	1	18	6795.5992	0.0055
14	8	6	13	7	7	6798.9484	-0.0014
20	2	19	19	1	18	6809.1384	0.0061
20	3	18	19	3	17	6845.1821	-0.0023
17	4	13	16	3	14	6852.3385	0.0014
20	19	2	19	19	1	6858.1954	0.0025
20	18	2	19	18	1	6858.4233	0.0000
20	17	3	19	17	2	6858.6778	-0.0027
20	16	4	19	16	3	6858.9723	0.0003
20	15	5	19	15	4	6859.3074	-0.0010
20	14	6	19	14	5	6859.7021	-0.0021

20	13	7	19	13	6	6860.1781	-0.0017
20	12	9	19	12	8	6860.7632	-0.0012
20	11	10	19	11	9	6861.5019	0.0000
20	10	10	19	10	9	6862.4591	-0.0003
20	9	11	19	9	10	6863.7453	-0.0007
20	8	13	19	8	12	6865.5468	-0.0005
20	7	13	19	7	12	6868.2224	0.0010
20	6	15	19	6	14	6872.1968	-0.0014
20	6	14	19	6	13	6872.7024	-0.0036
20	4	17	19	4	16	6873.4692	-0.0039
15	7	8	14	6	9	6874.1634	-0.0084
20	5	16	19	5	15	6876.8348	-0.0044
20	2	18	19	2	17	6880.7533	-0.0024
20	5	15	19	5	14	6883.4213	-0.0034
18	4	15	17	3	14	6892.1076	-0.0094
12	11	1	11	10	2	6913.0403	-0.0002
20	4	16	19	4	15	6914.3585	-0.0064
20	3	17	19	3	16	6932.8591	-0.0083
16	6	11	15	5	10	6946.1454	-0.0026
16	6	10	15	5	11	6947.2924	-0.0023
13	10	3	12	9	4	6989.4267	-0.0005
17	5	13	16	4	12	6992.4621	-0.0019
20	3	18	19	2	17	7021.0245	0.0011
17	5	12	16	4	13	7026.5352	0.0013
23	4	19	22	5	18	7027.2674	-0.0200
21	0	21	20	1	20	7057.9172	0.0152
21	1	21	20	1	20	7058.2067	0.0151
21	0	21	20	0	20	7058.3593	0.0141
21	1	21	20	0	20	7058.6491	0.0141
14	9	6	13	8	5	7065.6879	-0.0006
21	2	19	20	3	18	7073.4494	-0.0038
21	1	20	20	2	19	7115.5638	0.0077
21	1	20	20	1	19	7129.1022	0.0074
21	2	20	20	1	19	7138.5794	0.0037
15	8	8	14	7	7	7141.5509	-0.0011
22	3	19	21	4	18	7143.1299	-0.0201
12	12	0	11	11	1	7179.5289	-0.0017
19	4	16	18	3	15	7182.8447	-0.0042
21	3	19	20	3	18	7183.0768	0.0012
21	20	1	20	20	0	7200.9860	-0.0067
21	19	2	20	19	1	7201.2254	-0.0028
21	18	3	20	18	2	7201.4862	-0.0019
21	17	4	20	17	3	7201.7786	-0.0004
21	16	5	20	16	4	7202.1098	-0.0005
21	15	6	20	15	5	7202.4915	-0.0023
21	14	7	20	14	6	7202.9486	0.0019
21	13	8	20	13	7	7203.4906	-0.0015
21	12	9	20	12	8	7204.1638	-0.0007
21	11	10	20	11	9	7205.0141	-0.0004
21	10	11	20	10	10	7206.1208	0.0003
21	9	13	20	9	12	7207.6086	-0.0004
21	8	14	20	8	13	7209.6987	0.0013
21	7	15	20	7	14	7212.7979	0.0262
21	2	19	20	2	18	7213.7197	-0.0010
16	7	9	15	6	10	7216.2842	-0.0005
21	6	16	20	6	15	7217.3328	-0.0014
21	6	15	20	6	14	7218.1965	-0.0008
21	5	17	20	5	16	7221.9624	-0.0020
21	5	16	20	5	15	7231.7999	-0.0058
18	4	14	17	3	15	7235.1618	0.0078
13	11	3	12	10	2	7255.9287	-0.0013
21	4	17	20	4	16	7266.9500	-0.0097
21	3	18	20	3	17	7276.7720	-0.0085

17	6	12	16	5	11	7286.3773	-0.0024
17	6	11	16	5	12	7288.5572	0.0012
21	3	19	20	2	18	7323.3463	0.0032
14	10	5	13	9	4	7332.2764	-0.0012
18	5	13	17	4	14	7372.7894	0.0006
22	0	22	21	1	21	7392.4984	0.0189
22	1	22	21	1	21	7392.6841	0.0161
22	0	22	21	0	21	7392.7908	0.0217
22	1	22	21	0	21	7392.9752	0.0175
15	9	7	14	8	6	7408.4295	-0.0032
22	2	20	21	3	19	7436.3105	-0.0038
22	1	21	21	2	20	7453.3326	0.0044
22	2	21	21	2	20	7459.9196	0.0095
22	1	21	21	1	20	7462.8168	0.0076
20	4	17	19	3	16	7469.2095	-0.0034
22	2	21	21	1	20	7469.3997	0.0087
16	8	9	15	7	8	7484.0373	-0.0003
22	3	20	21	3	19	7520.3745	0.0006
13	12	1	12	11	2	7522.4228	-0.0002
22	20	2	21	20	1	7544.0257	0.0070
22	19	3	21	19	2	7544.2799	-0.0022
22	18	4	21	18	3	7544.5722	-0.0016
22	17	5	21	17	4	7544.9022	0.0004
22	16	6	21	16	5	7545.2769	0.0005
22	15	7	21	15	6	7545.7121	0.0004
22	2	20	21	2	19	7545.9349	-0.0017
22	14	9	21	14	8	7546.2266	-0.0002
22	13	10	21	13	9	7546.8503	0.0011
22	12	11	21	12	10	7547.6188	0.0008
22	11	12	21	11	11	7548.5855	-0.0062
22	10	12	21	10	11	7549.8601	-0.0010
22	9	13	21	9	12	7551.5720	-0.0009
22	8	14	21	8	13	7553.9802	-0.0024
22	7	16	21	7	15	7557.5151	-0.0057
22	7	15	21	7	14	7557.6028	-0.0033
22	4	19	21	4	18	7557.8713	-0.0034
17	7	11	16	6	10	7558.0722	-0.0073
17	7	10	16	6	11	7558.1691	0.0068
22	6	17	21	6	16	7562.6443	-0.0065
22	6	16	21	6	15	7564.0696	-0.0044
22	5	18	21	5	17	7566.9853	-0.0058
22	5	17	21	5	16	7581.2388	-0.0096
14	11	4	13	10	3	7598.8017	-0.0017
22	3	19	21	3	18	7618.6839	-0.0112
22	4	18	21	4	17	7619.2826	-0.0148
18	6	13	17	5	12	7625.6468	-0.0013
18	6	12	17	5	13	7629.6031	-0.0024
19	4	15	18	3	16	7629.7248	0.0051
22	3	20	21	2	19	7630.0065	0.0103
19	5	15	18	4	14	7640.4322	-0.0039
15	10	5	14	9	6	7675.0913	-0.0020
19	5	14	18	4	15	7721.8439	-0.0007
23	0	23	22	1	22	7727.0328	0.0223
23	0	23	22	0	22	7727.1927	-0.0064
23	1	23	22	0	22	7727.3451	0.0236
17	4	14	16	1	15	7741.8830	0.0105
16	9	8	15	8	7	7751.1042	-0.0027
21	4	18	20	3	17	7752.3287	0.0031
13	13	1	12	12	0	7788.9176	-0.0020
23	1	22	22	2	21	7790.1239	0.0080
23	2	21	22	3	20	7793.7640	-0.0047
23	2	22	22	2	21	7794.6598	0.0093
23	1	22	22	1	21	7796.7116	0.0138

23	2	22	22	1	21	7801.2448	0.0124
17	8	9	16	7	10	7826.3827	-0.0015
23	3	21	22	3	20	7857.1359	0.0049
14	12	3	13	11	2	7865.3048	-0.0008
23	2	21	22	2	20	7877.8288	0.0006
23	22	2	22	22	1	7886.5646	0.0180
23	21	2	22	21	1	7886.7851	-0.0086
23	20	3	22	20	2	7887.0591	-0.0025
23	19	4	22	19	3	7887.3606	0.0053
23	18	5	22	18	4	7887.6790	-0.0026
23	17	6	22	17	5	7888.0471	-0.0026
23	16	7	22	16	6	7888.4702	-0.0014
23	15	8	22	15	7	7888.9629	-0.0002
23	14	9	22	14	8	7889.5452	-0.0013
23	13	10	22	13	9	7890.2536	0.0007
23	12	11	22	12	10	7891.1245	-0.0028
23	11	12	22	11	11	7892.2369	0.0000
23	10	13	22	10	12	7893.6825	-0.0031
23	9	15	22	9	14	7895.6410	-0.0020
23	8	16	22	8	15	7898.4009	0.0005
23	4	20	22	4	19	7899.0999	-0.0048
18	7	12	17	6	11	7899.5878	-0.0081
23	7	17	22	7	16	7902.4443	-0.0079
23	7	16	22	7	15	7902.6002	-0.0044
23	6	18	22	6	17	7908.1212	-0.0084
23	6	17	22	6	16	7910.4064	-0.0043
23	5	19	22	5	18	7911.8258	-0.0042
23	5	18	22	5	17	7931.8445	-0.0094
24	3	21	23	4	20	7940.8210	-0.0328
23	3	21	22	2	20	7941.1941	0.0036
15	11	4	14	10	5	7941.6544	-0.0004
20	5	16	19	4	15	7955.2268	-0.0039
23	3	20	22	3	19	7958.4914	-0.0126
19	6	14	18	5	13	7963.6227	0.0010
19	6	13	18	5	14	7970.5429	-0.0034
23	4	19	22	4	18	7970.8354	-0.0161

Table S22. Linelist for sevoflurane dimer (heterochiral),  $^{13}\text{C}$  (acceptor, perfluoro) species. RMS error for the fit is 10.7 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
6	1	6	5	1	5	2025.1508	-0.0035
6	0	6	5	0	5	2040.1035	-0.0041
6	2	4	5	2	3	2063.6806	0.0194
6	1	5	5	1	4	2074.1722	0.0005
7	1	7	6	1	6	2361.5326	0.0008
7	0	7	6	0	6	2375.5960	-0.0010
7	2	6	6	2	5	2391.9156	0.0241
7	3	5	6	3	4	2397.4130	0.0057
7	3	4	6	3	3	2398.8183	0.0231
7	2	5	6	2	4	2411.1293	-0.0114
7	1	6	6	1	5	2418.0607	0.0041
8	1	8	7	1	7	2697.5261	0.0194
8	0	8	7	0	7	2709.8929	-0.0161
8	2	7	7	2	6	2732.3311	0.0082
8	3	6	7	3	5	2740.3069	-0.0017
8	3	5	7	3	4	2743.0511	0.0054
8	2	6	7	2	5	2759.3276	0.0022
8	1	7	7	1	6	2760.9528	-0.0019
9	1	9	8	1	8	3033.0898	-0.0065
9	0	9	8	0	8	3043.4336	0.0027
9	2	8	8	2	7	3072.2645	-0.0020
9	7	2	8	7	1	3080.6373	0.0018
9	6	3	8	6	2	3081.0143	0.0055
9	5	5	8	5	4	3081.6097	-0.0212
9	4	6	8	4	5	3082.6974	-0.0209
9	3	7	8	3	6	3083.2137	0.0072
9	1	8	8	1	7	3102.6459	0.0069
9	2	7	8	2	6	3107.7519	0.0076
10	1	10	9	1	9	3368.3244	-0.0091
10	0	10	9	0	9	3376.5415	-0.0016
10	3	8	9	3	7	3426.0110	-0.0086
10	3	7	9	3	6	3434.1882	-0.0006
10	1	9	9	1	8	3442.8912	0.0057
10	2	8	9	2	7	3455.9223	0.0020
11	1	11	10	1	10	3703.2500	-0.0110
11	0	11	10	0	10	3709.5282	-0.0050
11	2	10	10	2	9	3750.5304	-0.0007
11	7	4	10	7	3	3765.7914	-0.0049
11	6	6	10	6	5	3766.4713	-0.0014
11	3	9	10	3	8	3768.6582	0.0001
11	4	8	10	4	7	3769.3752	0.0064
11	4	7	10	4	6	3770.2665	-0.0005
11	3	8	10	3	7	3781.3833	0.0021
11	2	9	10	2	8	3803.4582	0.0049
12	1	12	11	1	11	4037.9222	-0.0043
12	0	12	11	0	11	4042.5745	0.0025
12	2	11	11	2	10	4088.8128	0.0107
12	9	3	11	9	2	4107.5511	0.0095
12	7	5	11	7	4	4108.4854	-0.0172
12	3	9	11	3	8	4129.7494	0.0305
12	2	10	11	2	9	4150.0430	0.0045
13	1	13	12	1	12	4372.3488	-0.0290
13	2	12	12	2	11	4426.4870	-0.0018
13	10	3	12	10	2	4449.7239	-0.0022
13	7	7	12	7	6	4451.2980	-0.0058
13	6	7	12	6	6	4452.4302	0.0089
13	1	12	12	1	11	4453.7685	0.0081
13	5	8	12	5	7	4454.3798	-0.0044
13	4	10	12	4	9	4456.6021	-0.0038
13	4	9	12	4	8	4459.5037	0.0097

13	3	10	12	3	9	4479.0541	-0.0128
13	2	11	12	2	10	4495.4490	0.0069
14	1	14	13	1	13	4706.6344	-0.0248
14	0	14	13	0	13	4709.0210	-0.0171
14	8	6	13	8	5	4793.3102	-0.0002
14	7	8	13	7	7	4794.2114	0.0034
14	6	9	13	6	8	4795.6010	0.0027
14	5	9	13	5	8	4798.1264	0.0038
14	4	11	13	4	10	4800.3461	0.0022
14	4	10	13	4	9	4805.1191	-0.0040
14	2	12	13	2	11	4839.4541	-0.0123
15	1	15	14	1	14	5040.8155	0.0058
15	0	15	14	0	14	5042.4696	0.0004
15	2	14	14	2	13	5100.1725	-0.0038
15	1	14	14	1	13	5120.6234	-0.0078
15	11	4	14	11	3	5134.4114	0.0059
15	7	9	14	7	8	5137.2262	0.0027
15	5	11	14	5	10	5141.6116	-0.0248
15	5	10	14	5	9	5142.1612	0.0052
15	4	12	14	4	11	5144.0991	0.0228
15	3	12	14	3	11	5179.4198	0.0164
16	1	16	15	1	15	5374.8543	-0.0067
16	0	16	15	0	15	5376.0284	0.0243
16	2	15	15	2	14	5436.2498	0.0039
16	1	15	15	1	14	5452.9796	-0.0028
16	3	14	15	3	13	5476.1098	-0.0010
16	8	8	15	8	7	5479.0216	0.0007
16	7	10	15	7	9	5480.3602	0.0010
16	5	12	15	5	11	5485.6235	0.0119
16	5	11	15	5	10	5486.5420	0.0011
16	4	13	15	4	12	5487.7290	0.0065
16	4	12	15	4	11	5499.1628	-0.0004
16	2	14	15	2	13	5522.6408	-0.0164
17	1	17	16	1	16	5708.8457	0.0065
17	0	17	16	0	16	5709.6339	0.0157
17	2	16	16	2	15	5771.8648	0.0002
17	1	16	16	1	15	5785.1169	0.0017
17	3	15	16	3	14	5815.9528	0.0007
17	8	9	16	8	8	5822.0348	0.0174
17	6	12	16	6	11	5826.1041	-0.0032
17	6	11	16	6	10	5826.1892	-0.0003
17	4	14	16	4	13	5831.1688	-0.0237
17	4	13	16	4	12	5847.8320	0.0032
17	2	15	16	2	14	5861.5153	-0.0101
18	0	18	17	0	17	6043.3034	0.0133
18	2	17	17	2	16	6107.0947	0.0048
18	3	16	17	3	15	6155.1530	0.0118
18	10	9	17	10	8	6162.9013	0.0204
18	9	9	17	9	8	6163.8153	0.0006
18	8	11	17	8	10	6165.1174	0.0008
18	7	12	17	7	11	6167.0243	-0.0014
18	4	14	17	4	13	6197.6540	0.0109
18	2	16	17	2	15	6198.4955	0.0092
18	3	15	17	3	14	6226.8996	0.0018
19	1	19	18	1	18	6376.6739	0.0243
19	0	19	18	0	18	6376.9879	-0.0144
19	2	18	18	2	17	6441.9791	-0.0027
19	10	9	18	10	8	6505.7162	0.0181
19	9	10	18	9	9	6506.8031	0.0090
19	8	12	18	8	11	6508.3233	-0.0019
19	7	13	18	7	12	6510.5856	0.0109
19	6	13	18	6	12	6514.2836	-0.0118
19	4	16	18	4	15	6517.2132	-0.0100

19	5	15	18	5	14	6518.4275	-0.0067
19	5	14	18	5	13	6522.6132	-0.0182
19	4	15	18	4	14	6548.4780	-0.0036
19	3	16	18	3	15	6573.6623	0.0084
20	1	20	19	1	19	6710.5168	0.0094
20	0	20	19	0	19	6710.7366	-0.0056
20	2	19	19	2	18	6776.5990	0.0001
20	1	19	19	1	18	6782.2527	0.0044
20	3	18	19	3	17	6831.5430	0.0017
20	9	12	19	9	11	6849.8490	-0.0139
20	8	13	19	8	12	6851.6471	-0.0032
20	7	13	19	7	12	6854.3067	0.0034
20	2	18	19	2	17	6867.1876	0.0069
20	4	16	19	4	15	6900.0538	0.0016
21	0	21	20	0	20	7044.5085	0.0082
21	2	20	20	2	19	7110.9982	0.0032
21	1	20	20	1	19	7115.0795	-0.0111
21	3	19	20	3	18	7168.7852	0.0010
21	9	13	20	9	12	7193.0160	-0.0107
21	8	14	20	8	13	7195.0946	-0.0043
21	2	19	20	2	18	7199.5235	-0.0081
21	5	17	20	5	16	7207.2768	-0.0249
21	5	16	20	5	15	7216.9718	-0.0111
21	4	17	20	4	16	7251.9052	-0.0072
21	3	18	20	3	17	7262.0517	0.0007
22	1	22	21	1	21	7378.1656	-0.0011
22	2	21	21	2	20	7445.2222	0.0050
22	1	21	21	1	20	7448.1178	-0.0285
22	3	20	21	3	19	7505.4413	0.0051
22	2	20	21	2	19	7531.1326	0.0106
22	8	15	21	8	14	7538.6754	-0.0028
23	5	18	22	5	17	7915.4905	-0.0093

Table S23. Linelist for sevoflurane dimer (heterochiral),  $^{13}\text{C}$  (acceptor, isopropyl) species. RMS error for the fit is 10.3 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
6	1	6	5	1	5	2025.3953	-0.0082
6	0	6	5	0	5	2040.3921	0.0043
6	2	5	5	2	4	2051.2865	0.0075
6	2	4	5	2	3	2063.8976	0.0087
6	1	5	5	1	4	2074.4376	-0.0041
7	1	7	6	1	6	2361.8216	-0.0030
7	0	7	6	0	6	2375.9450	0.0155
7	2	6	6	2	5	2392.1962	0.0035
7	3	5	6	3	4	2397.6907	-0.0053
7	3	4	6	3	3	2399.0707	-0.0056
7	2	5	6	2	4	2411.4144	0.0111
7	1	6	6	1	5	2418.3784	0.0010
8	1	8	7	1	7	2697.8410	-0.0025
8	0	8	7	0	7	2710.2981	0.0066
8	2	7	7	2	6	2732.6895	0.0192
8	6	2	7	6	1	2738.7906	0.0299
8	3	6	7	3	5	2740.6377	-0.0012
8	2	6	7	2	5	2759.6279	0.0013
8	1	7	7	1	6	2761.3279	-0.0018
9	1	9	8	1	8	3033.4732	-0.0042
9	0	9	8	0	8	3043.8588	-0.0007
9	2	8	8	2	7	3072.6550	-0.0062
9	7	2	8	7	1	3081.0143	0.0055
9	4	5	8	4	4	3083.3154	0.0187
9	3	7	8	3	6	3083.5906	0.0114
9	1	8	8	1	7	3103.0711	-0.0010
9	2	7	8	2	6	3108.0968	0.0073
10	1	10	9	1	9	3368.7531	-0.0056
10	0	10	9	0	9	3377.0111	-0.0028
10	7	3	9	7	2	3423.6012	0.0104
10	5	6	9	5	5	3424.9585	0.0115
10	4	7	9	4	6	3426.3753	0.0095
10	3	7	9	3	6	3434.5715	0.0074
10	1	9	9	1	8	3443.3841	0.0028
10	2	8	9	2	7	3456.3250	0.0092
11	1	11	10	1	10	3703.7321	0.0021
11	0	11	10	0	10	3710.0596	0.0165
11	2	10	10	2	9	3751.0161	-0.0076
11	6	6	10	6	5	3766.9154	-0.0103
11	5	7	10	5	6	3768.0363	-0.0125
11	3	9	10	3	8	3769.1227	0.0031
11	4	7	10	4	6	3770.7364	0.0291
11	3	8	10	3	7	3781.7629	-0.0191
11	1	10	10	1	9	3782.0714	-0.0055
11	2	9	10	2	8	3803.9090	0.0042
12	1	12	11	1	11	4038.4352	-0.0036
12	0	12	11	0	11	4043.1247	0.0059
12	2	11	11	2	10	4089.3033	-0.0415
12	7	5	11	7	4	4109.0014	0.0036
12	6	7	11	6	6	4109.8739	0.0017
12	3	10	11	3	9	4111.5344	-0.0017
12	4	9	11	4	8	4113.3959	-0.0217
12	4	8	11	4	7	4115.0661	0.0036
12	3	9	11	3	8	4130.1471	0.0021
13	1	13	12	1	12	4372.9276	-0.0051
13	0	13	12	0	12	4376.3117	-0.0059
13	2	12	12	2	11	4427.0900	0.0074
13	7	7	12	7	6	4451.8463	0.0074
13	6	7	12	6	6	4452.9404	-0.0130
13	3	11	12	3	10	4453.5870	-0.0073

13	1	12	12	1	11	4454.4605	0.0022
13	5	9	12	5	8	4454.7702	-0.0019
13	5	8	12	5	7	4454.9052	-0.0054
13	4	10	12	4	9	4457.1345	0.0006
13	4	9	12	4	8	4460.0003	0.0017
13	3	10	12	3	9	4479.5247	0.0036
13	2	11	12	2	10	4496.0211	-0.0002
14	1	14	13	1	13	4707.2599	0.0036
14	0	14	13	0	13	4709.6523	-0.0047
14	2	13	13	2	12	4764.2431	-0.0062
14	1	13	13	1	12	4788.4667	0.0096
14	8	6	13	8	5	4793.8882	0.0004
14	7	8	13	7	7	4794.7984	0.0154
14	3	12	13	3	11	4795.2079	-0.0013
14	6	9	13	6	8	4796.1682	-0.0014
14	5	10	13	5	9	4798.4156	0.0037
14	4	11	13	4	10	4800.9236	0.0102
14	3	11	13	3	10	4829.6053	0.0037
14	2	12	13	2	11	4840.1134	-0.0039
15	1	15	14	1	14	5041.4543	0.0062
15	2	14	14	2	13	5100.8840	0.0117
15	11	5	14	11	4	5135.0112	-0.0160
15	8	7	14	8	6	5136.7614	0.0233
15	6	10	14	6	9	5139.5510	0.0077
15	5	11	14	5	10	5142.2494	0.0084
15	5	10	14	5	9	5142.7661	0.0114
15	2	13	14	2	12	5182.6484	-0.0072
16	1	16	15	1	15	5375.5199	-0.0206
16	0	16	15	0	15	5376.6968	0.0007
16	1	15	15	1	14	5453.8447	-0.0011
16	11	5	15	11	4	5477.5951	-0.0158
16	9	7	15	9	6	5478.7614	-0.0027
16	8	8	15	8	7	5479.6826	0.0044
16	7	10	15	7	9	5481.0238	0.0109
16	5	12	15	5	11	5486.2540	-0.0003
16	4	13	15	4	12	5488.3757	-0.0043
16	2	14	15	2	13	5523.4657	-0.0015
16	3	13	15	3	12	5530.0198	-0.0013
17	0	17	16	0	16	5710.3544	0.0070
17	1	16	16	1	15	5786.0130	-0.0056
17	9	8	16	9	7	5821.6013	-0.0182
17	7	11	16	7	10	5824.3213	0.0052
18	1	18	17	1	17	6043.5475	0.0236
18	0	18	17	0	17	6044.0490	-0.0076
18	2	17	17	2	16	6107.9318	-0.0030
18	1	17	17	1	16	6118.2280	0.0012
18	10	8	17	10	7	6163.6219	-0.0007
18	9	9	17	9	8	6164.5524	-0.0017
18	8	11	17	8	10	6165.8471	-0.0054
18	6	13	17	6	12	6170.6989	0.0100
18	6	12	17	6	11	6170.8393	-0.0027
18	4	15	17	4	14	6175.1389	-0.0073
18	5	13	17	5	12	6177.3633	-0.0041
18	4	14	17	4	13	6198.2499	0.0016
18	3	15	17	3	14	6227.6233	-0.0074
19	1	19	18	1	18	6377.4448	-0.0047
19	1	18	18	1	17	6450.6207	0.0027
19	3	17	18	3	16	6494.5417	-0.0153
19	10	9	18	10	8	6506.4773	-0.0024
19	9	10	18	9	9	6507.5785	0.0054
19	8	12	18	8	11	6509.0987	-0.0015
19	7	13	18	7	12	6511.3506	0.0070
19	6	14	18	6	13	6514.7760	0.0030

19	6	13	18	6	12	6515.0624	0.0102
19	5	15	18	5	14	6519.2021	0.0073
19	3	16	18	3	15	6574.4745	0.0025
20	1	20	19	1	19	6711.3591	0.0121
20	10	10	19	10	9	6849.4026	-0.0051
20	9	11	19	9	10	6850.6739	-0.0074
20	8	13	19	8	12	6852.4499	-0.0140
20	4	17	19	4	16	6860.4561	-0.0062
20	5	15	19	5	14	6870.1211	0.0336
20	4	16	19	4	15	6900.7132	0.0062
21	3	19	20	3	18	7169.7938	0.0037
21	8	14	20	8	13	7195.9468	-0.0039
21	5	17	20	5	16	7208.1518	0.0038
21	5	16	20	5	15	7217.7139	-0.0187
21	4	17	20	4	16	7252.5953	-0.0160
22	1	22	21	1	21	7379.0729	-0.0121
22	2	20	21	2	19	7532.4017	0.0060
22	8	15	21	8	14	7539.5523	-0.0155
22	6	17	21	6	16	7548.1514	-0.0075
22	6	16	21	6	15	7549.5275	-0.0064

Table S24. Linelist for sevoflurane dimer (heterochiral),  $^{13}\text{C}$  (acceptor, fluoromethoxy) species. RMS error for the fit is 10.0 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
6	2	4	5	2	3	2064.7496	0.0018
6	1	5	5	1	4	2075.1283	0.0066
7	1	7	6	1	6	2361.2522	-0.0016
7	0	7	6	0	6	2375.3119	-0.0012
7	2	6	6	2	5	2392.3705	0.0024
7	3	5	6	3	4	2398.1384	-0.0232
7	3	4	6	3	3	2399.6711	0.0057
7	2	5	6	2	4	2412.5393	0.0049
7	1	6	6	1	5	2419.0397	-0.0174
8	1	8	7	1	7	2697.1262	-0.0026
8	0	8	7	0	7	2709.4241	0.0022
8	2	7	7	2	6	2732.8010	0.0001
8	4	5	7	4	4	2740.5244	-0.0032
8	3	6	7	3	5	2741.1710	-0.0079
8	3	5	7	3	4	2744.1443	0.0028
8	1	7	7	1	6	2761.9463	0.0017
9	1	9	8	1	8	3032.6002	-0.0065
9	2	8	8	2	7	3072.7256	0.0043
9	7	2	8	7	1	3081.5480	0.0098
9	4	6	8	4	5	3083.7235	-0.0028
9	4	5	8	4	4	3083.9349	-0.0274
9	3	7	8	3	6	3084.1893	0.0056
9	1	8	8	1	7	3103.5456	0.0019
9	2	7	8	2	6	3109.6657	-0.0008
10	1	10	9	1	9	3367.7208	-0.0030
10	0	10	9	0	9	3375.7187	0.0054
10	6	5	9	6	4	3424.7377	0.0077
10	5	6	9	5	5	3425.6277	0.0026
10	1	9	9	1	8	3443.6178	-0.0035
10	2	8	9	2	7	3458.0169	0.0031
11	1	11	10	1	10	3702.5197	-0.0063
11	0	11	10	0	10	3708.5752	0.0007
11	2	10	10	2	9	3750.8620	-0.0006
11	8	3	10	8	2	3766.4713	0.0024
11	4	7	10	4	6	3771.6677	-0.0052
11	3	8	10	3	7	3783.4906	0.0017
11	2	9	10	2	8	3805.6423	0.0002
12	1	12	11	1	11	4037.0623	-0.0018
12	0	12	11	0	11	4041.5219	0.0180
12	2	11	11	2	10	4089.0345	-0.0003
12	6	7	11	6	6	4110.6918	0.0074
12	5	8	11	5	7	4112.2110	-0.0008
12	5	7	11	5	6	4112.2900	0.0019
12	4	9	11	4	8	4114.3827	-0.0022
12	1	11	11	1	10	4118.6289	0.0112
12	2	10	11	2	9	4152.2477	0.0038
13	2	12	12	2	11	4426.5988	-0.0026
13	1	12	12	1	11	4453.5870	0.0040
13	3	10	12	3	9	4482.0329	0.0064
13	2	11	12	2	10	4497.5850	0.0035
14	1	14	13	1	13	4705.5332	-0.0103
14	0	14	13	0	13	4707.7664	-0.0123
14	2	13	13	2	12	4763.5685	-0.0102
14	4	10	13	4	9	4807.3847	-0.0017
14	2	12	13	2	11	4841.4489	-0.0011
15	1	15	14	1	14	5039.5720	0.0016
15	0	15	14	0	14	5041.1137	-0.0032
15	2	14	14	2	13	5099.9980	-0.0008
15	1	14	14	1	13	5119.8586	0.0268
15	10	5	14	10	4	5136.3489	-0.0032

15	3	13	14	3	12	5136.7614	-0.0203
15	9	6	14	9	5	5136.9317	0.0047
15	8	8	14	8	7	5137.7107	-0.0128
15	7	9	14	7	8	5138.8991	0.0139
15	5	10	14	5	9	5144.0991	-0.0146
15	4	11	14	4	10	5154.2703	-0.0290
15	3	12	14	3	11	5183.0153	0.0030
15	2	13	14	2	12	5183.6611	0.0028
16	1	16	15	1	15	5373.4849	-0.0158
16	2	15	15	2	14	5435.8789	-0.0288
16	1	15	15	1	14	5451.9628	0.0007
16	3	14	15	3	13	5477.1764	0.0135
16	11	5	15	11	4	5478.6072	0.0292
16	10	6	15	10	5	5479.1009	0.0018
16	9	7	15	9	6	5479.7947	0.0012
16	8	9	15	8	8	5480.7785	0.0203
16	5	11	15	5	10	5488.7378	0.0011
17	2	16	16	2	15	5771.3687	0.0070
17	1	16	16	1	15	5783.9302	-0.0077
17	3	15	16	3	14	5816.8893	0.0020
17	11	6	16	11	5	5821.2944	0.0068
17	8	10	16	8	9	5823.8974	0.0028
17	7	11	16	7	10	5825.5920	0.0048
17	4	14	16	4	13	5833.2203	-0.0072
17	4	13	16	4	12	5851.4981	-0.0072
17	3	14	16	3	13	5882.5166	-0.0012
18	1	18	17	1	17	6041.1640	-0.0050
18	9	9	17	9	8	6165.7780	0.0096
18	8	10	17	8	9	6167.1470	0.0072
18	7	12	17	7	11	6169.1750	0.0232
18	4	15	17	4	14	6176.4648	0.0021
18	2	16	17	2	15	6198.9092	0.0046
18	4	14	17	4	13	6201.8725	-0.0078
18	3	15	17	3	14	6230.5889	-0.0029
19	1	19	18	1	18	6374.9154	-0.0252
19	0	19	18	0	18	6375.2666	0.0073
19	1	18	18	1	17	6448.2724	-0.0107
19	3	17	18	3	16	6494.2922	0.0065
19	10	9	18	10	8	6507.7325	-0.0006
19	9	10	18	9	9	6508.8996	0.0124
19	8	12	18	8	11	6510.4942	-0.0061
19	7	13	18	7	12	6512.8825	0.0109
19	4	16	18	4	15	6519.2968	0.0048
19	2	17	18	2	16	6533.5106	0.0015
19	4	15	18	4	14	6553.2697	0.0119
19	3	16	18	3	15	6577.1129	-0.0156
20	1	20	19	1	19	6708.7026	0.0167
20	0	20	19	0	19	6708.8983	0.0019
20	2	19	19	2	18	6775.6194	0.0060
20	10	10	19	10	9	6850.7640	0.0078
20	9	11	19	9	10	6852.1105	0.0098
20	8	13	19	8	12	6853.9803	-0.0039
20	5	15	19	5	14	6872.9732	-0.0013
20	4	16	19	4	15	6905.2818	-0.0021
20	3	17	19	3	16	6921.8951	-0.0075
21	1	21	20	1	20	7042.4236	0.0118
21	0	21	20	0	20	7042.5637	0.0136
21	2	20	20	2	19	7109.8584	-0.0009
21	1	20	20	1	19	7113.5992	-0.0004
21	9	12	20	9	11	7195.4360	0.0215
21	8	14	20	8	13	7197.5957	-0.0030
21	2	19	20	2	18	7198.5009	0.0018
21	7	14	20	7	13	7200.8543	-0.0150

21	6	16	20	6	15	7205.5553	-0.0062
21	6	15	20	6	14	7206.5444	-0.0098
21	3	18	20	3	17	7264.7204	-0.0083
22	2	21	21	2	20	7443.9206	-0.0180
22	3	20	21	3	19	7505.4413	-0.0003
22	6	17	21	6	16	7550.3735	-0.0056
22	3	19	21	3	18	7605.4484	-0.0084
23	3	21	22	3	20	7841.3354	-0.0021
23	4	20	22	4	19	7884.8760	-0.0035

Table S25. Linelist for sevoflurane dimer (heterochiral),  $^{13}\text{C}$  (acceptor, perfluoro 2) species. RMS error for the fit is 9.59 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
6	1	6	5	1	5	2024.9887	-0.0163
6	0	6	5	0	5	2039.8976	-0.0017
6	2	5	5	2	4	2050.5866	0.0121
6	2	4	5	2	3	2062.9322	0.0000
6	1	5	5	1	4	2073.4860	-0.0030
7	1	7	6	1	6	2361.3857	0.0046
7	0	7	6	0	6	2375.4603	0.0249
7	2	6	6	2	5	2391.3764	-0.0144
7	4	3	6	4	2	2396.1874	-0.0016
7	3	4	6	3	3	2398.1384	0.0158
7	1	6	6	1	5	2417.3051	-0.0021
8	1	8	7	1	7	2697.3574	-0.0039
8	2	7	7	2	6	2731.7945	0.0142
8	4	5	7	4	4	2738.9412	-0.0021
8	3	6	7	3	5	2739.5990	0.0067
8	3	5	7	3	4	2742.2204	-0.0123
8	2	6	7	2	5	2758.2486	0.0048
8	1	7	7	1	6	2760.1671	0.0017
9	1	9	8	1	8	3032.9634	0.0014
9	0	9	8	0	8	3043.3643	-0.0032
9	3	6	8	3	5	3087.1498	0.0069
9	1	8	8	1	7	3101.8410	-0.0010
9	2	7	8	2	6	3106.5167	0.0069
10	1	10	9	1	9	3368.2138	-0.0002
10	2	9	9	2	8	3411.0926	0.0064
10	7	3	9	7	2	3422.3165	0.0025
10	4	7	9	4	6	3425.0367	0.0022
10	3	8	9	3	7	3425.1346	0.0041
10	4	6	9	4	5	3425.4622	-0.0050
10	1	9	9	1	8	3442.1171	-0.0006
10	2	8	9	2	7	3454.5660	0.0040
11	1	11	10	1	10	3703.1498	-0.0092
11	0	11	10	0	10	3709.5282	0.0024
11	2	10	10	2	9	3749.9241	-0.0048
11	7	4	10	7	3	3764.8456	0.0055
11	6	6	10	6	5	3765.5024	0.0016
11	4	8	10	4	7	3768.3442	0.0067
11	4	7	10	4	6	3769.1941	0.0008
11	3	8	10	3	7	3780.0064	0.0058
11	1	10	10	1	9	3780.7936	-0.0196
11	2	9	10	2	8	3802.0145	0.0105
12	1	12	11	1	11	4037.8552	0.0119
12	0	12	11	0	11	4042.5745	-0.0026
12	6	7	11	6	6	4108.3085	0.0016
12	4	8	11	4	7	4113.3959	0.0253
12	3	9	11	3	8	4128.1271	0.0203
12	2	10	11	2	9	4148.5378	0.0051
13	1	13	12	1	12	4372.3106	-0.0029
13	0	13	12	0	12	4375.7571	0.0096
13	3	11	12	3	10	4451.9445	-0.0144
13	4	10	12	4	9	4455.3626	0.0044
13	4	9	12	4	8	4458.1110	-0.0010
13	3	10	12	3	9	4477.2228	0.0009
13	2	11	12	2	10	4493.9169	0.0007
14	1	14	13	1	13	4706.6344	0.0209
14	2	13	13	2	12	4763.0424	0.0045
14	1	13	13	1	12	4787.3134	-0.0022
14	10	4	13	10	3	4791.0351	-0.0051
14	8	7	13	8	6	4792.0772	-0.0034
14	7	8	13	7	7	4792.9550	-0.0023

14	3	12	13	3	11	4793.4845	-0.0020
14	5	9	13	5	8	4796.7736	0.0006
14	4	11	13	4	10	4798.9999	0.0079
14	4	10	13	4	9	4803.5534	0.0006
14	3	11	13	3	10	4827.0458	-0.0078
14	2	12	13	2	11	4837.9662	0.0067
15	0	15	14	0	14	5042.4696	-0.0218
15	10	5	14	10	4	5133.5089	-0.0100
15	9	6	14	9	5	5134.0485	-0.0046
15	3	13	14	3	12	5134.5134	0.0035
15	6	9	14	6	8	5137.5604	0.0030
15	5	11	14	5	10	5140.1757	-0.0089
15	5	10	14	5	9	5140.6591	-0.0143
15	4	12	14	4	11	5142.6130	-0.0135
15	3	12	14	3	11	5177.1633	-0.0054
15	2	13	14	2	12	5180.4835	0.0012
16	1	16	15	1	15	5374.8543	0.0049
16	0	16	15	0	15	5376.0284	-0.0029
16	2	15	15	2	14	5435.7280	-0.0103
16	3	14	15	3	13	5474.9710	0.0023
16	8	8	15	8	7	5477.5951	0.0031
16	7	10	15	7	9	5478.8917	-0.0070
16	5	11	15	5	10	5484.9042	-0.0091
16	4	13	15	4	12	5486.1851	0.0005
16	4	12	15	4	11	5497.1367	0.0088
16	2	14	15	2	13	5521.3261	0.0082
17	1	17	16	1	16	5708.8457	0.0027
17	0	17	16	0	16	5709.6339	-0.0174
17	2	16	16	2	15	5771.3689	-0.0222
17	1	16	16	1	15	5784.9244	-0.0070
17	3	15	16	3	14	5814.8231	0.0051
17	8	9	16	8	8	5820.4875	0.0020
17	7	11	16	7	10	5822.0348	-0.0189
17	6	12	16	6	11	5824.4894	0.0099
17	6	11	16	6	10	5824.5438	-0.0118
17	4	13	16	4	12	5845.5192	0.0006
17	2	15	16	2	14	5860.3365	0.0022
17	3	14	16	3	13	5876.3013	0.0034
18	11	7	17	11	6	6160.6231	0.0099
18	8	11	17	8	10	6163.4916	0.0126
18	4	14	17	4	13	6195.0459	0.0038
18	2	16	17	2	15	6197.4723	-0.0035
19	1	19	18	1	18	6376.6739	-0.0077
19	0	19	18	0	18	6377.0460	-0.0042
19	2	18	18	2	17	6441.6069	0.0297
19	1	18	18	1	17	6449.4817	0.0016
19	7	13	18	7	12	6508.7714	-0.0038
19	4	16	18	4	15	6515.5017	-0.0013
19	5	14	18	5	13	6520.4390	-0.0194
19	2	17	18	2	16	6532.8131	0.0036
19	4	15	18	4	14	6545.5984	0.0043
20	1	19	19	1	18	6782.0823	0.0077
20	8	12	19	8	11	6849.8003	0.0064
20	6	15	19	6	14	6856.2335	-0.0096
20	2	18	19	2	17	6866.5512	-0.0010
20	5	15	19	5	14	6866.9466	0.0024
20	4	16	19	4	15	6896.9166	0.0085
20	3	17	19	3	16	6916.4426	-0.0170
21	1	21	20	1	20	7044.4046	0.0023
21	1	20	20	1	19	7114.9216	0.0130
21	3	19	20	3	18	7167.7936	-0.0044
21	9	12	20	9	11	7191.1083	0.0040
21	4	18	20	4	17	7199.6650	-0.0161

21	6	15	20	6	14	7201.3092	-0.0153
21	5	17	20	5	16	7205.1452	-0.0052
21	4	17	20	4	16	7248.5656	-0.0022
21	3	18	20	3	17	7259.8846	-0.0050
22	4	19	21	4	18	7540.9172	-0.0056
22	5	18	21	5	17	7549.4103	0.0198
23	2	22	22	2	21	7779.0125	-0.0002
23	3	21	22	3	20	7840.6925	0.0192

Table S26. Linelist for sevoflurane dimer (heterochiral),  $^{13}\text{C}$  (donor, isopropyl) species. RMS error for the fit is 8.82 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
6	1	6	5	1	5	2026.8569	0.0041
6	0	6	5	0	5	2041.8271	-0.0104
6	2	5	5	2	4	2052.7669	0.0006
6	3	3	5	3	2	2056.9303	-0.0082
6	2	4	5	2	3	2065.4165	-0.0036
6	1	5	5	1	4	2075.9626	0.0057
7	1	7	6	1	6	2363.5080	-0.0037
7	2	6	6	2	5	2393.9258	0.0016
7	3	5	6	3	4	2399.4534	0.0065
7	2	5	6	2	4	2413.2071	0.0089
7	1	6	6	1	5	2420.1379	0.0005
8	1	8	7	1	7	2699.7609	-0.0066
8	0	8	7	0	7	2712.1944	-0.0056
8	2	7	7	2	6	2734.6469	0.0022
8	3	6	7	3	5	2742.6402	-0.0002
8	2	6	7	2	5	2761.6915	0.0081
8	1	7	7	1	6	2763.3305	0.0003
9	1	9	8	1	8	3035.6357	-0.0018
9	0	9	8	0	8	3045.9969	-0.0022
9	3	7	8	3	6	3085.8360	0.0055
9	3	6	8	3	5	3090.7459	-0.0004
9	2	7	8	2	6	3110.4091	0.0049
10	1	10	9	1	9	3371.1555	0.0009
10	6	5	9	6	4	3426.5971	-0.0011
10	4	6	9	4	5	3429.3288	0.0018
10	2	8	9	2	7	3458.8880	0.0049
11	1	11	10	1	10	3706.3568	-0.0043
11	2	10	10	2	9	3753.7126	-0.0032
11	8	3	10	8	2	3768.5564	-0.0026
11	6	6	10	6	5	3769.6826	0.0062
11	3	9	10	3	8	3771.8676	0.0006
11	4	8	10	4	7	3772.5904	0.0143
11	3	8	10	3	7	3784.6015	0.0022
11	1	10	10	1	9	3784.7666	0.0010
11	2	9	10	2	8	3806.7175	-0.0013
12	1	12	11	1	11	4041.2988	-0.0065
12	2	11	11	2	10	4092.2700	-0.0026
12	6	7	11	6	6	4112.8624	-0.0123
12	5	7	11	5	6	4114.3827	-0.0117
12	4	9	11	4	8	4116.4261	-0.0043
12	4	8	11	4	7	4118.0979	0.0090
12	1	11	11	1	10	4121.9949	0.0083
12	3	9	11	3	8	4133.2400	0.0049
12	2	10	11	2	9	4153.6052	-0.0011
13	1	13	12	1	12	4376.0324	-0.0023
13	0	13	12	0	12	4379.4025	-0.0004
13	2	12	12	2	11	4430.2306	-0.0142
13	9	4	12	9	3	4453.8666	-0.0052
13	8	5	12	8	4	4454.3798	0.0107
13	7	6	12	7	5	4455.0839	-0.0060
13	6	8	12	6	7	4456.2065	0.0017
13	3	11	12	3	10	4456.8432	0.0130
13	5	9	12	5	8	4458.0418	0.0079
13	5	8	12	5	7	4458.1584	-0.0153
13	2	11	12	2	10	4499.2978	-0.0135
14	0	14	13	0	13	4712.9914	0.0101
14	2	13	13	2	12	4767.6474	0.0027
14	1	13	13	1	12	4791.7981	-0.0021
14	10	4	13	10	3	4796.3417	0.0202
14	9	5	13	9	4	4796.7736	0.0044

14	8	6	13	8	5	4797.4117	0.0244
14	3	12	13	3	11	4798.6910	0.0050
14	6	9	13	6	8	4799.6587	-0.0190
14	4	11	13	4	10	4804.4437	0.0127
14	3	11	13	3	10	4833.2356	0.0036
14	2	12	13	2	11	4843.6395	0.0037
15	1	15	14	1	14	5045.0175	-0.0041
15	2	14	14	2	13	5104.4956	-0.0044
15	1	14	14	1	13	5125.0153	0.0018
15	9	6	14	9	5	5139.7286	-0.0030
15	3	13	14	3	12	5140.0210	-0.0011
15	8	8	14	8	7	5140.4900	0.0006
15	7	9	14	7	8	5141.6116	0.0182
15	4	12	14	4	11	5148.4786	0.0214
15	3	12	14	3	11	5183.8203	-0.0076
15	2	13	14	2	12	5186.3953	-0.0004
16	1	16	15	1	15	5379.3631	0.0128
16	1	15	15	1	14	5457.6400	-0.0001
16	3	14	15	3	13	5480.7785	0.0003
16	10	6	15	10	5	5482.1024	-0.0007
16	7	10	15	7	9	5485.0173	-0.0037
16	5	12	15	5	11	5490.2824	0.0022
16	5	11	15	5	10	5491.2106	0.0017
16	4	13	15	4	12	5492.3993	0.0017
16	4	12	15	4	11	5503.8378	-0.0028
16	2	14	15	2	13	5527.4260	0.0042
17	2	16	16	2	15	5776.7530	0.0008
17	10	7	16	10	6	5825.0824	0.0011
17	9	8	16	9	7	5825.8644	-0.0066
17	8	9	16	8	8	5826.9492	-0.0205
17	5	13	16	5	12	5834.7241	0.0060
17	5	12	16	5	11	5836.3109	-0.0003
17	4	13	16	4	12	5852.8002	-0.0027
17	2	15	16	2	14	5866.5783	-0.0060
17	3	14	16	3	13	5883.7527	-0.0123
18	1	18	17	1	17	6047.8094	0.0026
18	0	18	17	0	17	6048.3284	-0.0067
18	7	12	17	7	11	6172.2803	0.0080
18	6	13	17	6	12	6175.2246	0.0093
18	5	14	17	5	13	6179.2773	-0.0221
18	4	14	17	4	13	6202.9108	-0.0051
18	2	16	17	2	15	6203.8354	-0.0014
18	3	15	17	3	14	6232.2466	0.0009
19	1	19	18	1	18	6381.9743	0.0050
19	0	19	18	0	18	6382.3285	0.0050
19	2	18	18	2	17	6447.4261	-0.0039
19	1	18	18	1	17	6455.1223	-0.0018
19	11	8	18	11	7	6510.4286	0.0154
19	9	10	18	9	9	6512.3275	-0.0014
19	4	16	18	4	15	6522.7529	-0.0284
19	5	15	18	5	14	6523.9844	-0.0005
19	5	14	18	5	13	6528.1723	-0.0079
19	2	17	18	2	16	6539.2757	0.0126
19	4	15	18	4	14	6554.0656	0.0097
19	3	16	18	3	15	6579.3096	0.0004
20	1	20	19	1	19	6716.1074	0.0038
20	2	19	19	2	18	6782.3309	0.0044
20	1	19	19	1	18	6788.0005	0.0027
20	3	18	19	3	17	6837.3581	-0.0049
20	8	12	19	8	11	6857.4798	-0.0002
20	6	14	19	6	13	6864.6019	0.0171
20	2	18	19	2	17	6873.1276	0.0244
20	5	15	19	5	14	6875.1885	-0.0063

20	4	16	19	4	15	6905.9266	-0.0041
20	3	17	19	3	16	6924.7264	-0.0016
21	3	19	20	3	18	7174.8972	0.0052
21	9	12	20	9	11	7199.1517	0.0058
21	2	19	20	2	18	7205.7339	0.0000
21	5	16	20	5	15	7223.1254	0.0048
21	4	17	20	4	16	7258.0986	-0.0002
21	3	18	20	3	17	7268.3120	-0.0047
22	2	21	21	2	20	7451.4778	-0.0234
22	3	20	21	3	19	7511.8370	0.0080
22	2	20	21	2	19	7537.5757	-0.0242
22	8	15	21	8	14	7545.0850	-0.0071
22	6	17	21	6	16	7553.7048	-0.0075
22	6	16	21	6	15	7555.0989	-0.0060

Table S27. Linelist for sevoflurane dimer (heterochiral),  $^{13}\text{C}$  (donor, fluoromethoxy) species. RMS error for the fit is 10.0 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
6	0	6	5	0	5	2039.7749	0.0069
6	3	3	5	3	2	2055.2707	-0.0096
6	1	5	5	1	4	2074.3539	-0.0203
7	1	7	6	1	6	2361.1021	0.0269
7	0	7	6	0	6	2375.1055	0.0024
7	2	6	6	2	5	2391.8104	-0.0048
7	3	5	6	3	4	2397.4823	-0.0022
7	3	4	6	3	3	2398.9484	0.0101
7	2	5	6	2	4	2411.5715	0.0022
7	1	6	6	1	5	2418.2367	0.0039
8	1	8	7	1	7	2696.9534	0.0015
8	0	8	7	0	7	2709.2542	-0.0041
8	2	7	7	2	6	2732.2010	0.0020
8	6	2	7	6	1	2738.5001	0.0129
8	5	3	7	5	2	2738.9412	0.0009
8	3	6	7	3	5	2740.4017	0.0007
8	3	5	7	3	4	2743.2634	-0.0025
8	2	6	7	2	5	2759.8654	0.0045
8	1	7	7	1	6	2761.0625	-0.0077
9	1	9	8	1	8	3032.4196	-0.0176
9	0	9	8	0	8	3042.6574	0.0218
9	7	2	8	7	1	3080.7049	0.0064
9	3	7	8	3	6	3083.3154	0.0069
9	3	6	8	3	5	3088.4287	-0.0184
9	1	8	8	1	7	3102.6459	-0.0060
9	2	7	8	2	6	3108.3600	0.0034
10	1	10	9	1	9	3367.5494	-0.0165
10	0	10	9	0	9	3375.6253	0.0034
10	2	9	9	2	8	3411.4178	-0.0011
10	5	5	9	5	4	3424.6605	-0.0061
10	4	6	9	4	5	3426.5971	0.0019
10	3	7	9	3	6	3434.6663	0.0086
10	1	9	9	1	8	3442.7517	0.0024
10	2	8	9	2	7	3456.5803	0.0113
11	1	11	10	1	10	3702.3609	-0.0215
11	0	11	10	0	10	3708.4973	-0.0058
11	2	10	10	2	9	3750.1787	-0.0018
11	4	8	10	4	7	3769.5615	0.0053
11	1	10	10	1	9	3781.1796	-0.0042
11	3	8	10	3	7	3782.0060	-0.0152
11	2	9	10	2	8	3804.1048	0.0106
12	1	12	11	1	11	4036.9239	-0.0124
12	2	11	11	2	10	4088.3531	0.0045
12	4	9	11	4	8	4113.1502	-0.0020
12	2	10	11	2	9	4150.6284	0.0017
13	1	13	12	1	12	4371.2579	-0.0186
13	6	8	12	6	7	4452.5885	0.0010
13	1	12	12	1	11	4452.9401	-0.0132
13	5	9	12	5	8	4454.4605	-0.0057
13	4	10	12	4	9	4456.8432	-0.0172
13	4	9	12	4	8	4459.9230	-0.0093
13	3	10	12	3	9	4480.0852	0.0026
13	2	11	12	2	10	4495.9344	0.0036
14	0	14	13	0	13	4707.7664	0.0332
14	2	13	13	2	12	4762.9102	-0.0023
14	1	13	13	1	12	4786.6531	0.0000
14	9	6	13	9	5	4792.8009	-0.0106
14	7	8	13	7	7	4794.3594	-0.0114
14	5	9	13	5	8	4798.4156	0.0036
14	4	11	13	4	10	4800.6304	0.0053

14	4	10	13	4	9	4805.6809	-0.0225
14	3	11	13	3	10	4830.2854	0.0034
14	2	12	13	2	11	4839.7924	-0.0126
15	1	15	14	1	14	5039.4941	0.0037
15	1	14	14	1	13	5119.3841	0.0014
15	8	7	14	8	6	5136.2628	-0.0174
15	7	9	14	7	8	5137.4137	-0.0019
15	6	10	14	6	9	5139.1876	0.0113
15	5	10	14	5	9	5142.5109	-0.0025
15	4	11	14	4	10	5152.3830	-0.0069
15	3	12	14	3	11	5180.6752	0.0057
15	2	13	14	2	12	5182.0594	-0.0023
16	1	15	15	1	14	5451.5619	-0.0078
16	3	14	15	3	13	5475.9025	0.0078
16	10	7	15	10	6	5477.5951	0.0111
16	8	8	15	8	7	5479.2084	0.0020
16	7	10	15	7	9	5480.5832	-0.0012
16	6	10	15	6	9	5482.7860	0.0205
16	5	12	15	5	11	5485.9746	-0.0018
16	2	14	15	2	13	5522.5224	-0.0077
16	3	13	15	3	12	5530.7112	-0.0114
17	0	17	16	0	16	5708.0424	-0.0039
17	2	16	16	2	15	5770.7825	0.0124
17	8	10	16	8	9	5822.2310	-0.0008
17	7	11	16	7	10	5823.8965	0.0104
17	2	15	16	2	14	5861.0835	-0.0021
17	3	14	16	3	13	5879.9681	0.0029
18	1	17	17	1	16	6115.6531	-0.0026
18	3	16	17	3	15	6154.6680	-0.0061
18	6	13	17	6	12	6170.3634	0.0085
18	5	13	17	5	12	6177.3633	0.0095
18	4	14	17	4	13	6199.1422	0.0030
18	3	15	17	3	14	6228.0095	-0.0038
19	8	11	18	8	10	6508.6110	0.0028
19	7	13	18	7	12	6510.9355	0.0106
19	2	17	18	2	16	6532.4935	0.0164
19	4	15	18	4	14	6550.2343	0.0040
20	9	12	19	9	11	6850.1343	0.0027
20	8	13	19	8	12	6851.9624	-0.0099
22	4	19	21	4	18	7542.5611	0.0031
23	1	22	22	1	21	7779.3908	0.0038

Table S28. Linelist for sevoflurane dimer (heterochiral),  $^{13}\text{C}$  (donor, perfluoro) species. RMS error for the fit is 10.7 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
6	1	6	5	1	5	2024.6877	0.0098
6	2	4	5	2	3	2063.4155	0.0254
7	1	7	6	1	6	2360.9709	0.0030
7	0	7	6	0	6	2375.0370	-0.0149
7	2	6	6	2	5	2391.4604	0.0009
7	3	4	6	3	3	2398.4185	-0.0007
7	2	5	6	2	4	2410.8444	0.0000
7	1	6	6	1	5	2417.7238	0.0005
8	1	8	7	1	7	2696.8581	0.0049
8	0	8	7	0	7	2709.2542	-0.0053
8	3	5	7	3	4	2742.6402	0.0100
8	2	6	7	2	5	2758.9709	-0.0320
8	1	7	7	1	6	2760.5529	0.0007
9	1	9	8	1	8	3032.3534	0.0021
9	0	9	8	0	8	3042.6574	-0.0203
9	3	7	8	3	6	3082.6974	-0.0079
9	3	6	8	3	5	3087.6705	-0.0011
9	1	8	8	1	7	3102.1832	0.0264
9	2	7	8	2	6	3107.3976	0.0074
10	1	10	9	1	9	3367.5050	0.0096
10	2	9	9	2	8	3411.0176	-0.0052
10	3	8	9	3	7	3425.4650	0.0036
10	3	7	9	3	6	3433.7171	-0.0005
10	1	9	9	1	8	3442.3125	0.0010
10	2	8	9	2	7	3455.5234	-0.0028
11	0	11	10	0	10	3708.5752	-0.0070
11	2	10	10	2	9	3749.7904	-0.0011
11	7	5	10	7	4	3765.1670	-0.0061
11	6	6	10	6	5	3765.8650	0.0102
11	3	9	10	3	8	3768.0363	-0.0035
11	4	7	10	4	6	3769.6826	0.0006
11	3	8	10	3	7	3780.8910	-0.0035
11	2	9	10	2	8	3802.9996	-0.0095
12	1	12	11	1	11	4036.9239	0.0243
12	0	12	11	0	11	4041.5219	-0.0040
12	2	11	11	2	10	4087.9839	0.0078
12	9	3	11	9	2	4106.8511	-0.0062
12	8	4	11	8	3	4107.2452	-0.0082
12	6	7	11	6	6	4108.7238	0.0146
13	1	13	12	1	12	4371.2579	0.0021
13	0	13	12	0	12	4374.6237	0.0283
13	2	12	12	2	11	4425.5523	-0.0210
13	9	5	12	9	4	4449.3420	-0.0059
13	8	5	12	8	4	4449.8497	0.0013
13	6	7	12	6	6	4451.6933	-0.0066
13	4	10	12	4	9	4455.9201	0.0109
13	4	9	12	4	8	4458.8617	0.0233
13	3	10	12	3	9	4478.5574	-0.0052
13	2	11	12	2	10	4494.8605	-0.0047
14	1	13	13	1	12	4786.6531	-0.0100
14	4	10	13	4	9	4804.4442	0.0009
14	3	11	13	3	10	4828.5965	0.0012
14	2	12	13	2	11	4838.7918	-0.0130
15	1	15	14	1	14	5039.4933	-0.0040
15	2	14	14	2	13	5099.0741	0.0009
15	7	9	14	7	8	5136.4026	0.0124
15	6	10	14	6	9	5138.1242	0.0112
15	5	10	14	5	9	5141.3610	-0.0031
15	2	13	14	2	12	5181.1646	-0.0033
16	0	16	15	0	15	5374.5920	0.0042

16	2	15	15	2	14	5435.0526	0.0067
16	7	10	15	7	9	5479.4772	0.0017
16	5	12	15	5	11	5484.7569	-0.0083
16	5	11	15	5	10	5485.7044	-0.0067
16	2	14	15	2	13	5521.7872	0.0026
16	3	13	15	3	12	5528.8509	-0.0012
17	1	17	16	1	16	5707.3181	-0.0192
17	0	17	16	0	16	5708.1008	-0.0086
17	1	16	16	1	15	5783.7784	0.0257
17	3	15	16	3	14	5814.8835	-0.0039
17	6	11	16	6	10	5825.2883	0.0109
17	2	15	16	2	14	5860.5329	0.0068
17	3	14	16	3	13	5878.0884	-0.0024
18	1	18	17	1	17	6041.1640	-0.0036
18	0	18	17	0	17	6041.6850	-0.0035
18	2	17	17	2	16	6105.6870	-0.0063
18	1	17	17	1	16	6115.8408	0.0112
18	5	13	17	5	12	6175.7870	0.0013
18	4	14	17	4	13	6196.9455	-0.0086
18	2	16	17	2	15	6197.3513	0.0018
19	2	18	18	2	17	6440.4962	0.0094
19	1	18	18	1	17	6448.0803	-0.0160
19	7	13	18	7	12	6509.5485	0.0018
19	3	16	18	3	15	6572.8510	-0.0090
20	1	20	19	1	19	6708.7026	-0.0202
20	8	13	19	8	12	6850.5507	-0.0054
20	2	18	19	2	17	6865.7513	-0.0073
20	5	15	19	5	14	6868.4488	0.0157
20	3	17	19	3	16	6917.8551	-0.0132
21	8	13	20	8	12	7193.9654	0.0067
22	2	20	21	2	19	7529.4449	0.0018
22	8	15	21	8	14	7537.4963	0.0065
23	2	22	22	2	21	7777.4265	0.0058

Table S29. Linelist for sevoflurane dimer (heterochiral),  $^{13}\text{C}$  (donor, perfluoro 2) species. RMS error for the fit is 9.57 kHz.

J'	$K_a'$	$K_c'$	J''	$K_a''$	$K_c''$	$\nu_{obs}$ (MHz)	OMC (MHz)
6	1	6	5	1	5	2025.4605	0.0004
6	2	4	5	2	3	2063.4133	0.0021
7	1	7	6	1	6	2361.8889	-0.0219
7	1	7	6	1	6	2361.8889	-0.0219
7	0	7	6	0	6	2375.9450	-0.0159
7	2	6	6	2	5	2391.9156	-0.0169
7	3	4	6	3	3	2398.6783	0.0054
7	1	6	6	1	5	2417.8702	0.0143
7	1	6	6	1	5	2417.8702	0.0143
8	2	7	7	2	6	2732.3800	-0.0178
8	5	4	7	5	3	2738.7906	-0.0053
8	3	6	7	3	5	2740.2173	-0.0009
8	3	5	7	3	4	2742.8652	0.0010
8	2	6	7	2	5	2758.8855	-0.0013
8	1	7	7	1	6	2760.7922	0.0032
8	1	7	7	1	6	2760.7922	0.0032
9	1	9	8	1	8	3033.6480	0.0076
9	0	9	8	0	8	3044.0376	0.0000
9	2	8	8	2	7	3072.3948	0.0090
9	5	5	8	5	4	3081.5480	0.0071
9	3	7	8	3	6	3083.1052	0.0004
9	1	8	8	1	7	3102.5243	-0.0145
9	2	7	8	2	6	3107.2365	0.0033
10	1	10	9	1	9	3368.9754	0.0088
10	0	10	9	0	9	3377.2614	0.0040
10	2	9	9	2	8	3411.8583	0.0042
10	6	5	9	6	4	3423.6012	0.0075
10	5	5	9	5	4	3424.4290	-0.0068
10	3	8	9	3	7	3425.9293	0.0168
10	3	7	9	3	6	3433.8213	0.0014
10	2	8	9	2	7	3455.3638	0.0000
11	1	11	10	1	10	3703.9749	-0.0106
11	2	10	10	2	9	3750.7786	0.0074
11	7	4	10	7	3	3765.7025	0.0028
11	3	9	10	3	8	3768.5564	0.0028
11	4	8	10	4	7	3769.1930	-0.0076
11	4	7	10	4	6	3770.0625	0.0035
11	1	10	10	1	9	3781.6493	-0.0016
11	2	9	10	2	8	3802.8894	0.0069
12	1	12	11	1	11	4038.7495	0.0057
12	0	12	11	0	11	4043.4780	0.0077
12	9	3	11	9	2	4107.4531	0.0044
12	8	4	11	8	3	4107.8400	0.0067
12	4	9	11	4	8	4112.7261	-0.0064
12	2	10	11	2	9	4149.5014	0.0155
13	1	13	12	1	12	4373.2905	0.0023
13	2	12	12	2	11	4426.8954	0.0044
13	8	6	12	8	5	4450.4597	-0.0068
13	6	8	12	6	7	4452.2502	-0.0092
13	5	9	12	5	8	4454.0415	-0.0054
13	4	10	12	4	9	4456.3867	0.0070
13	3	10	12	3	9	4478.2698	-0.0043
14	1	14	13	1	13	4707.6645	0.0022
14	2	13	13	2	12	4764.0706	-0.0296
14	7	7	13	7	6	4794.0434	-0.0098
14	6	9	13	6	8	4795.4177	0.0053
14	5	10	13	5	9	4797.6173	0.0049
14	4	11	13	4	10	4800.1012	0.0090
14	4	10	13	4	9	4804.6748	0.0094
14	3	11	13	3	10	4828.2031	0.0134

15	1	15	14	1	14	5041.9103	0.0058
15	2	14	14	2	13	5100.7761	0.0037
15	7	9	14	7	8	5137.0412	-0.0031
15	5	11	14	5	10	5141.3610	-0.0032
15	5	10	14	5	9	5141.8565	0.0016
15	4	12	14	4	11	5143.8097	0.0044
15	4	11	14	4	10	5151.0438	0.0035
15	3	12	14	3	11	5178.3773	-0.0086
16	0	16	15	0	15	5377.2328	0.0070
16	3	14	15	3	13	5476.1977	-0.0059
16	9	8	15	9	7	5477.9346	-0.0136
16	7	10	15	7	9	5480.1545	0.0017
16	6	11	15	6	10	5482.1900	0.0098
16	5	11	15	5	10	5486.1851	0.0092
16	4	12	15	4	11	5498.4137	0.0014
16	2	14	15	2	13	5522.5224	-0.0269
16	3	13	15	3	12	5528.3597	-0.0082
17	1	17	16	1	16	5710.1296	0.0147
17	3	15	16	3	14	5816.1220	-0.0038
17	8	9	16	8	8	5821.8133	-0.0035
17	7	11	16	7	10	5823.3902	0.0033
17	5	13	16	5	12	5829.4028	0.0029
17	4	13	16	4	12	5846.8831	-0.0078
17	3	14	16	3	13	5877.6635	-0.0042
18	9	10	17	9	9	6163.6219	0.0053
18	8	11	17	8	10	6164.8852	-0.0042
18	6	12	17	6	11	6169.7781	0.0026
18	3	15	17	3	14	6225.8918	-0.0067
19	1	19	18	1	18	6378.0849	-0.0178
19	2	18	18	2	17	6443.0146	0.0112
19	3	17	18	3	16	6494.0476	0.0064
19	10	10	18	10	9	6505.5106	0.0106
19	8	11	18	8	10	6508.0674	-0.0018
19	7	13	18	7	12	6510.2771	0.0095
19	4	15	18	4	14	6547.1291	-0.0142
19	3	16	18	3	15	6572.7632	-0.0003
20	1	20	19	1	19	6712.0247	-0.0234
20	2	19	19	2	18	6777.7428	0.0173
20	9	12	19	9	11	6849.6206	0.0057
20	3	17	19	3	16	6918.0352	0.0003
21	1	21	20	1	20	7045.9641	-0.0085
21	0	21	20	0	20	7046.1434	0.0077
21	3	18	20	3	17	7261.5232	-0.0045