

The conformational landscape of the volatile anesthetic sevoflurane

SUPPLEMENTARY INFORMATION

Alberto Lesarri,^{a*} Alicia Vega-Toribio,^a Richard D. Suenram,^b Dale J. Brugh,^c

Jens-Uwe Grabow^d

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^a*Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, Calle Doctor Mergelina, s/n, E-47011 Valladolid, Spain*

^b*Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA-22904, USA*

^c*Department of Chemistry, Ohio Wesleyan University, 61 S. Sandusky St., Delaware, OH 43015, USA*

^d*Institut für Physikalische Chemie & Elektrochemie, Lehrgebiet A, Gottfried-Wilhelm-Leibniz Universität Hannover, Callinstrasse 3A, D-30167 Hannover, Germany*

Table S1. Observed rotational transitions (obs.) and residuals (obs.-calc.) for the parent species of sevoflurane (in MHz).

J'	K' ₋₁	K' ₊₁	J''	K'' ₋₁	K'' ₊₁	obs.	obs.-calc.
6	3	4	5	2	3	9074.7637	0.0015
5	4	2	4	3	1	9117.0469	0.0001
6	3	3	5	4	2	9179.8809	0.0012
5	1	4	4	0	4	9552.1260	0.0029
6	3	3	5	3	2	9870.1455	0.0000
5	5	1	4	4	0	9937.4775	0.0017
5	5	0	4	4	0	9964.7002	0.0015
5	5	1	4	4	1	9998.9248	0.0014
5	5	0	4	4	1	10026.1484	0.0021
6	6	1	5	5	0	12003.7717	-0.0015
6	6	0	5	5	0	12014.9863	-0.0015
6	6	1	5	5	1	12030.9943	-0.0018
6	6	0	5	5	1	12042.2089	-0.0018
10	2	9	9	2	8	13093.1797	0.0001
10	1	9	9	2	8	13093.1797	0.0002
10	2	9	9	1	8	13093.1797	-0.0010
10	1	9	9	1	8	13093.1797	-0.0009
7	4	3	6	3	3	13102.1033	-0.0027
7	5	2	6	4	2	13127.4442	-0.0014
7	6	1	6	5	1	13559.9525	-0.0017
11	0	11	10	0	10	13583.8359	-0.0017
11	1	11	10	0	10	13583.8359	-0.0017
11	1	11	10	1	10	13583.8359	-0.0017
11	0	11	10	1	10	13583.8359	-0.0017
7	7	1	6	6	0	14056.6191	0.0015
7	7	0	6	6	0	14061.0186	-0.0004
7	7	1	6	6	1	14067.8330	0.0008
7	7	0	6	6	1	14072.2334	-0.0002
11	2	10	10	2	9	14295.6113	-0.0004
11	2	10	10	1	9	14295.6113	-0.0005
11	1	10	10	2	9	14295.6113	-0.0004
11	1	10	10	1	9	14295.6113	-0.0005
10	3	7	9	4	6	14522.2412	0.0003
10	4	7	9	4	6	14522.7012	0.0002
10	3	7	9	3	6	14525.1807	0.0010
10	4	7	9	3	6	14525.6406	0.0008
12	0	12	11	0	11	14786.3564	0.0000
12	1	12	11	0	11	14786.3564	0.0000
12	0	12	11	1	11	14786.3564	0.0000
12	1	12	11	1	11	14786.3564	0.0000
12	2	11	11	2	10	15498.0625	-0.0010
12	1	11	11	2	10	15498.0625	-0.0010
12	2	11	11	1	10	15498.0625	-0.0011
12	1	11	11	1	10	15498.0625	-0.0011
13	0	13	12	0	12	15988.8701	0.0000
13	1	13	12	0	12	15988.8701	0.0000
13	0	13	12	1	12	15988.8701	0.0000
13	1	13	12	1	12	15988.8701	0.0000
12	6	6	11	7	5	18934.5781	0.0000
18	0	18	17	0	17	22001.3374	0.0011
18	1	18	17	1	17	22001.3374	0.0011

18	1	18	17	0	17	22001.3374	0.0011
18	0	18	17	1	17	22001.3374	0.0011
16	4	12	15	4	11	22446.5630	-0.0004
16	4	12	15	5	11	22446.5630	0.0004
16	5	12	15	4	11	22446.5630	-0.0005
16	5	12	15	5	11	22446.5630	0.0003
15	7	9	14	7	8	22691.1660	0.0007
10	5	5	9	4	6	22691.6543	0.0000
15	6	9	14	6	8	22694.8760	0.0013
15	7	9	14	6	8	22695.6953	0.0010
18	2	17	17	2	16	22712.8256	0.0007
18	1	17	17	2	16	22712.8256	0.0007
18	1	17	17	1	16	22712.8256	0.0007
18	2	17	17	1	16	22712.8256	0.0007
17	4	14	16	4	13	22934.5508	-0.0005
17	3	14	16	3	13	22934.5508	-0.0005
17	4	14	16	3	13	22934.5508	-0.0005
17	3	14	16	4	13	22934.5508	-0.0005
19	0	19	18	0	18	23203.8047	-0.0001
19	1	19	18	1	18	23203.8047	-0.0001
19	0	19	18	1	18	23203.8047	-0.0001
19	1	19	18	0	18	23203.8047	-0.0001
15	8	8	14	8	7	23421.2617	-0.0007
18	2	16	17	2	15	23424.5371	-0.0005
18	3	16	17	2	15	23424.5371	-0.0005
18	2	16	17	3	15	23424.5371	-0.0005
17	4	13	16	4	12	23648.2070	-0.0017
17	4	13	16	5	12	23648.2070	-0.0017
17	5	13	16	4	12	23648.2070	-0.0017
17	5	13	16	5	12	23648.2070	-0.0017
20	0	20	19	0	19	24406.2637	-0.0017
20	1	20	19	1	19	24406.2637	-0.0017
20	0	20	19	1	19	24406.2637	-0.0017
20	1	20	19	0	19	24406.2637	-0.0017

Table S2. Observed rotational transitions (obs.) and residuals (obs.-cal.) for the $^{13}\text{C}(1)$ species of sevoflurane (in MHz).

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	obs.	obs.-calc.
8	1	8	7	1	7	9951.7674	-0.0002
8	0	8	7	0	7	9951.7674	-0.0009
9	1	9	8	1	8	11151.2819	-0.0009
9	0	9	8	0	8	11151.2819	-0.0010
9	2	8	8	2	7	11862.4392	-0.0026
9	1	8	8	1	7	11862.4549	0.0031
6	6	1	5	5	0	11985.5189	-0.0013
6	6	0	5	5	1	12023.1997	-0.0015
10	2	9	9	2	8	13061.8283	0.0008
10	1	9	9	1	8	13061.8283	-0.0003
8	5	3	7	5	2	13526.1378	-0.0023
11	0	11	10	0	10	13550.3104	-0.0004
11	1	11	10	1	10	13550.3104	-0.0004
7	6	1	6	5	2	13752.4796	0.0046
7	7	1	6	6	0	14035.1800	-0.0026
7	7	0	6	6	1	14050.4172	-0.0034
12	0	12	11	0	11	14749.8202	0.0004
12	1	12	11	1	11	14749.8202	0.0004
9	5	4	8	5	3	14995.8630	-0.0016
8	7	2	7	6	1	15546.3216	0.0055
13	0	13	12	0	12	15949.3244	0.0007
13	1	13	12	1	12	15949.3244	0.0007
8	8	1	7	7	0	16078.1059	-0.0049
8	8	0	7	7	1	16084.0028	-0.0046
9	8	2	8	7	1	17630.4386	0.0043
9	8	1	8	7	2	17704.6058	0.0055

Table S3. Observed rotational transitions (obs.) and residuals (obs.-cal.) for the $^{13}\text{C}(2)$ species of sevoflurane (in MHz).

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	obs.	obs.-calc.
6	6	1	5	5	0	12003.2208	0.0000
6	6	0	5	5	1	12041.6066	0.0001
8	5	3	7	5	2	13559.5511	0.0016
7	6	1	6	5	2	13777.4926	0.0006
7	7	1	6	6	0	14055.9567	0.0009
7	7	0	6	6	1	14071.5463	-0.0001
12	0	12	11	0	11	14786.7568	0.0008
12	1	12	11	1	11	14786.7568	0.0008
9	5	4	8	5	3	15027.5891	0.0000
8	7	2	7	6	1	15569.8162	-0.0019
13	0	13	12	0	12	15989.3101	0.0002
13	1	13	12	1	12	15989.3101	0.0002
8	8	1	7	7	0	16101.8792	0.0016
8	8	0	7	7	1	16107.9385	0.0017
9	8	2	8	7	1	17657.5426	-0.0014
9	8	1	8	7	2	17733.6024	0.0001

Table S4. Observed rotational transitions (obs.) and residuals (obs.-calc.) for the $^{13}\text{C}(3)$ species of sevoflurane (in MHz).

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	obs.	obs.-calc.
8	1	8	7	1	7	9954.1761	0.0000
8	0	8	7	0	7	9954.1761	-0.0005
9	1	9	8	1	8	11153.9764	0.0000
9	0	9	8	0	8	11153.9764	0.0000
9	2	8	8	2	7	11865.3804	-0.0035
9	1	8	8	1	7	11865.3934	0.0019
6	6	1	5	5	0	11959.3998	-0.0004
6	6	0	5	5	1	12001.1593	-0.0007
10	2	9	9	2	8	13065.0635	0.0003
10	1	9	9	1	8	13065.0635	-0.0004
11	0	11	10	0	10	13553.5733	0.0002
11	1	11	10	1	10	13553.5733	0.0002
7	6	1	6	5	2	13749.2128	0.0000
7	7	1	6	6	0	14005.1972	-0.0004
7	7	0	6	6	1	14022.5202	0.0002
12	0	12	11	0	11	14753.3662	0.0001
12	1	12	11	1	11	14753.3662	0.0001
9	5	4	8	5	3	15000.6324	0.0001
8	7	2	7	6	1	15512.8481	-0.0008
13	0	13	12	0	12	15953.1549	0.0008
13	1	13	12	1	12	15953.1549	0.0008
8	8	1	7	7	0	16043.8322	0.0003
8	8	0	7	7	1	16050.7070	0.0008
9	8	2	8	7	1	17596.0937	0.0006

Table S5. Observed rotational transitions (obs.) and residuals (obs.-cal.) for the $^{13}\text{C}(4)$ species of sevoflurane (in MHz).

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	obs.	obs.-calc.
8	1	8	7	1	7	9903.7239	-0.0006
8	0	8	7	0	7	9903.7239	-0.0014
9	1	9	8	1	8	11097.3545	0.0000
9	0	9	8	0	8	11097.3545	0.0000
9	2	8	8	2	7	11806.5926	-0.0053
9	1	8	8	1	7	11806.6099	0.0007
6	6	1	5	5	0	11951.4515	-0.0025
6	6	0	5	5	1	11987.2393	-0.0041
10	2	9	9	2	8	13000.0932	-0.0012
10	1	9	9	1	8	13000.0932	-0.0025
8	5	3	7	5	2	13453.4466	-0.0006
11	0	11	10	0	10	13484.6125	0.0003
11	1	11	10	1	10	13484.6125	0.0003
7	7	1	6	6	0	13995.1135	0.0030
7	7	0	6	6	1	14009.4123	0.0020
12	0	12	11	0	11	14678.2376	0.0016
12	1	12	11	1	11	14678.2376	0.0016
9	5	4	8	5	3	14930.2292	0.0026
13	0	13	12	0	12	15871.8573	0.0023
13	1	13	12	1	12	15871.8573	0.0023

Table S6. Observed rotational transitions (obs.) and residuals (obs.-cal.) for the ^{18}O species of sevoflurane (in MHz).

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	obs.	obs.-calc.
9	1	9	8	1	8	11137.9999	0.0000
6	6	1	5	5	0	11959.7341	0.0036
6	6	0	5	5	1	11995.8520	-0.0073
7	6	1	6	5	2	13714.5825	0.0014
7	7	1	6	6	0	14004.6402	-0.0006
7	7	0	6	6	1	14019.1176	-0.0042
8	8	1	7	7	0	16043.0038	0.0000
8	8	0	7	7	1	16048.5574	-0.0008
9	9	1	8	8	0	18078.4956	0.0027
9	9	0	8	8	1	18080.5599	0.0031

Table S7. Stark effect measurements on sevoflurane, including the applied electric fields (ϵ , in V cm^{-1}), the observed transition frequencies (obs.) and the residuals (obs.-calc.) for the fit of Table 3 (frequencies in MHz).

J'	K'_{-1}	K'_{+1}	M'	J''	K''_{-1}	K''_{+1}	M''	ϵ	obs.	obs.-calc.
4	3	2	0	3	0	3	0	0.00	9540.1611	-0.0010
4	3	2	6	3	0	3	6	5.53	9540.3721	0.0035
4	3	2	6	3	0	3	6	7.79	9540.5576	0.0017
4	3	2	4	3	0	3	4	9.74	9540.4434	0.0019
4	3	2	4	3	0	3	4	11.77	9540.5586	-0.0012
4	3	2	4	3	0	3	4	13.80	9540.6914	-0.0024
4	3	2	2	3	0	3	2	13.80	9540.3076	0.0032
4	3	2	2	3	0	3	2	19.52	9540.4385	-0.0003
4	3	2	2	3	0	3	2	23.50	9540.5518	-0.0014
4	3	2	0	3	0	3	0	39.17	9540.1357	-0.0065
4	3	2	0	3	0	3	0	78.02	9540.0830	-0.0002
4	3	2	0	3	0	3	0	156.24	9539.8477	0.0020
4	4	1	0	3	1	2	0	0.00	9556.0068	0.0039
4	4	1	2	3	1	2	2	78.02	9555.6592	0.0009
4	4	1	0	3	1	2	0	78.02	9556.0557	0.0056
4	4	1	0	3	1	2	0	117.15	9556.1123	0.0028
4	4	1	0	3	1	2	0	156.20	9556.1943	0.0018
6	3	4	0	5	2	3	0	0.00	9074.7627	0.0005
6	3	4	0	5	2	3	0	195.09	9074.8457	0.0040
6	3	4	0	5	2	3	0	234.53	9074.8789	0.0017
6	3	4	0	5	2	3	0	273.19	9074.9180	-0.0003
6	3	3	0	5	4	2	0	0.00	9179.8789	-0.0008
6	3	3	10	5	4	2	10	124.79	9179.6152	-0.0017
6	3	3	8	5	4	2	8	124.79	9179.7109	-0.0030
6	3	3	8	5	4	2	8	156.20	9179.6016	-0.0030
6	3	3	8	5	4	2	8	195.36	9179.4141	0.0014
6	3	3	6	5	4	2	6	156.20	9179.7207	-0.0007
6	3	3	6	5	4	2	6	195.36	9179.6191	-0.0011
6	3	3	6	5	4	2	6	233.98	9179.4922	0.0051
6	3	3	4	5	4	2	4	233.98	9179.6797	-0.0024
6	3	3	4	5	4	2	4	253.39	9179.6426	-0.0026
6	3	3	4	5	4	2	4	292.44	9179.5626	0.0035
6	3	3	2	5	4	2	2	253.39	9179.7598	-0.0021
6	3	3	2	5	4	2	2	391.23	9179.5957	0.0012
6	3	3	2	5	4	2	2	428.72	9179.5352	-0.0003