

The Microwave Spectrum of Neurotransmitter Serotonin

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Table S1. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the conformer GPh-out/anti of serotonin.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'	F'	I''	F''	$V_{\text{obs.}}$	$V_{\text{obs.}} - V_{\text{cal.}}$
4	0	4	3	0	3	2	6	2	5	4029.3403	-0.0081
						2	5	2	4	4029.5790	-0.0030
						2	3	2	2	4029.4722	-0.0039
						1	5	1	4	4029.4071	-0.0030
5	0	5	4	0	4	2	7	2	6	4910.5332	0.0005
						2	6	2	5	4910.7049	0.0002
						2	5	2	4	4910.7638	0.0019
						2	4	2	3	4910.6234	-0.0003
						1	6	1	5	4910.5781	0.0002
						1	4	1	3	4910.7140	0.0022
5	1	5	4	1	4	2	7	2	6	4852.7957	0.0023
						2	6	2	5	4852.9102	0.0008
						2	5	2	4	4852.9700	0.0001
						2	3	2	2	4852.8605	-0.0017
						1	6	1	5	4852.8441	0.0026
5	1	5	4	0	4	1	4	1	3	4852.9220	0.0055
						2	7	2	6	4956.1518	0.0007
						2	6	2	5	4956.3643	-0.0010
						2	5	2	4	4956.4228	0.0011
						1	6	1	5	4956.1977	0.0021
						1	5	1	4	4956.1634	-0.0013
6	0	6	5	0	5	1	4	1	3	4956.3721	-0.0002
						0	5	0	4	4956.1700	0.0000
						2	8	2	7	5794.9490	0.0024
						2	6	2	5	5795.1088	0.0010
						2	5	2	4	5795.0212	0.0042
						1	7	1	6	5794.9822	0.0020
						1	6	1	5	5794.9592	0.0021
6	1	6	5	1	5	2	8	2	7	5768.0535	0.0019
						2	7	2	6	5768.1450	-0.0007
						2	6	2	5	5768.1878	0.0003
						1	7	1	6	5768.0887	0.0029
6	1	6	5	0	5	2	8	2	7	5813.6704	0.0005
						2	7	2	6	5813.8053	-0.0010
						2	6	2	5	5813.8483	0.0010
						2	5	2	4	5813.7378	0.0002
						1	7	1	6	5813.7029	-0.0006
						1	6	1	5	5813.6840	0.0035
						1	5	1	4	5813.8181	0.0036
						0	6	0	5	5813.6915	-0.0027
7	0	7	6	0	6	2	9	2	8	6686.5768	-0.0001
						2	8	2	7	6686.6620	-0.0018
						2	7	2	6	6686.6926	-0.0018
						2	6	2	5	6686.6396	0.0073
						1	6	1	5	6686.6716	0.0000
7	1	7	6	1	6	2	9	2	8	6675.1753	0.0001
						2	8	2	7	6675.2487	-0.0031
						2	7	2	6	6675.2819	-0.0006
						2	5	2	4	6675.2156	0.0009
						1	7	1	6	6675.1883	0.0046
						0	7	0	6	6675.2007	-0.0005
7	1	7	6	0	6	2	9	2	8	6693.8979	-0.0007
						2	8	2	7	6693.9912	-0.0002
						2	7	2	6	6694.0230	0.0010
						2	6	2	5	6693.9528	-0.0004

						2	5	2	4	6693.9373	0.0020
						1	8	1	7	6693.9237	-0.0005
						1	7	1	6	6693.9103	0.0032
						1	6	1	5	6694.0018	0.0027
						0	7	0	6	6693.9213	-0.0005
8	0	8	7	0	7	2	10	2	9	7582.7751	-0.0046
						2	9	2	8	7582.8482	0.0022
						2	8	2	7	7582.8663	-0.0032
						1	9	1	8	7582.7965	-0.0032
						1	8	1	7	7582.7847	-0.0021
8	1	8	7	0	7	2	10	2	9	7585.5433	-0.0030
						2	9	2	8	7585.6099	-0.0047
						2	8	2	7	7585.6346	-0.0036
						2	6	2	5	7585.5806	0.0034
						1	9	1	8	7585.5625	-0.0038
						1	8	1	7	7585.5533	0.0000
						1	7	1	6	7585.6194	-0.0021

Table S2. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the conformer GPy-out/anti of serotonin.

J'	K' ₋₁	K' ₊₁	J''	K'' ₋₁	K'' ₊₁	I'	F'	I''	F''	V _{obs.}	V _{obs.} -V _{cal.}
5	0	5	4	0	4	2	7	2	6	4748.1472	-0.0017
						2	6	2	5	4748.3535	-0.0007
						2	5	2	4	4748.2446	0.0013
						2	4	2	3	4748.1244	0.0022
						1	6	1	5	4748.1156	-0.0007
						1	4	1	3	4748.3277	-0.0008
						0	5	0	4	4748.1641	-0.0014
5	1	5	4	1	4	2	7	2	6	4632.7752	-0.0019
						2	6	2	5	4632.8838	0.0009
						2	3	2	2	4632.7988	0.0000
						1	6	1	5	4632.7225	-0.0003
						1	5	1	4	4632.8402	-0.0003
6	0	6	5	0	5	2	8	2	7	5609.5989	-0.0015
						2	7	2	6	5609.7612	-0.0052
						2	6	2	5	5609.6973	-0.0012
						1	7	1	6	5609.5735	0.0005
						1	6	1	5	5609.6276	-0.0031
						0	6	0	5	5609.6046	0.0014
6	1	6	5	1	5	2	8	2	7	5529.2228	0.0004
						2	7	2	6	5529.3138	0.0015
						2	6	2	5	5529.2440	-0.0051
						2	5	2	4	5529.2168	0.0006
						1	7	1	6	5529.1873	0.0011
						1	6	1	5	5529.2699	0.0030
						1	5	1	4	5529.2998	0.0037
6	1	6	5	0	5	2	8	2	7	5721.6427	0.0002
						2	7	2	6	5721.9092	0.0004
						2	5	2	4	5721.6137	-0.0012
						1	7	1	6	5721.6238	0.0032
						1	5	1	4	5721.8971	0.0077
7	0	7	6	0	6	2	9	2	8	6467.1483	0.0014
						2	8	2	7	6467.2747	0.0024
						2	7	2	6	6467.2302	0.0036
						2	6	2	5	6467.1397	0.0015
						1	8	1	7	6467.1264	0.0023
						1	6	1	5	6467.2587	0.0005

7	1	7	6	0	6	2	9	2	8	6529.0552	-0.0013
						2	8	2	7	6529.2319	-0.0028
						2	7	2	6	6529.1843	-0.0046
						2	5	2	4	6529.0465	-0.0020
						1	8	1	7	6529.0338	-0.0020
						1	6	1	5	6529.2167	-0.0036
						0	7	0	6	6529.0572	0.0021

Table S3. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the conformer GPy-up/anti of serotonin.

J'	K' ₋₁	K' ₊₁	J''	K'' ₋₁	K'' ₊₁	I'	F'	I''	F''	V _{obs.}	V _{obs.} -V _{cal.}
4	1	3	3	1	2	2	6	2	5	4276.8052	-0.0008
						1	4	1	3	4276.8751	0.0041
						0	4	0	3	4276.8182	-0.0033
5	0	5	4	0	4	2	7	2	6	4750.2987	-0.0046
						2	6	2	5	4750.4823	-0.0033
						2	5	2	4	4750.5261	-0.0016
5	1	5	4	1	4	1	6	1	5	4750.3267	-0.0066
						2	7	2	6	4639.3068	0.0007
						2	6	2	5	4639.4003	0.0006
						2	5	2	4	4639.4611	0.0025
						2	3	2	2	4639.3756	0.0010
5	1	4	4	1	3	1	6	1	5	4639.3529	0.0003
						2	7	2	6	5299.7206	0.0006
						2	5	2	4	5299.8578	0.0006
						2	3	2	2	5299.6945	-0.0038
						1	5	1	4	5299.7472	-0.0031
5	1	5	4	0	4	0	5	0	4	5299.7065	0.0062
						2	7	2	6	4925.8136	0.0023
						1	6	1	5	4925.8209	-0.0012
						1	4	1	3	4926.1648	0.0039
6	0	6	5	0	5	2	7	2	6	5611.4363	0.0001
						2	6	2	5	5611.4628	-0.0013
						1	6	1	5	5611.3069	0.0073
						1	5	1	4	5611.4504	0.0046
						0	6	0	5	5611.3034	0.0048
6	1	6	5	1	5	2	8	2	7	5535.8395	0.0028
						2	7	2	6	5535.9192	0.0012
						2	6	2	5	5535.9596	0.0039
						2	4	2	3	5535.8841	-0.0020
						1	7	1	6	5535.8698	0.0030
6	1	6	5	0	5	2	8	2	7	5711.3431	-0.0016
						2	7	2	6	5711.5828	-0.0009
						2	6	2	5	5711.6022	0.0003
						1	7	1	6	5711.3569	0.0013
						1	5	1	4	5711.5915	-0.0030
						0	6	0	5	5711.3389	-0.0037
7	1	7	6	1	6	2	9	2	8	6423.6507	-0.0026
						2	8	2	7	6423.7162	-0.0085
						1	7	1	6	6423.6585	-0.0040
7	1	7	6	0	6	2	9	2	8	6523.7123	-0.0001
						2	8	2	7	6523.8709	-0.0014
						2	6	2	5	6523.7382	-0.0004
						1	8	1	7	6523.7271	0.0034
						1	6	1	5	6523.8787	-0.0029
8	1	8	7	0	7	2	7	2	6	7359.3353	0.0019
						1	9	1	8	7359.3209	0.0035

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