Supplementary Material (ESI) for PCCP

Conformational Study of 2-Phenylethylamine by Molecular-Beam Fourier Transform Microwave Spectroscopy

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Supplementary information

Tables of observed rotational frequencies for the four conformers of 2-phenylethylamine observed in this work.

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Table S1. Measured rotational transitions (in MHz) of conformer GI of Phenylethylamine.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
2	1	2	1	0	1	1	0	6191.7825	-0.0021
						2	1	6191.2362	0.0037
						3	2	6191.3415	-0.0012
						1	1	6190.7785	0.0012
						2	2	6191.6372	0.0018
2	2	0	1	1	1	1	0	11025.3162	0.0019
						2	1	11024.9633	0.0013
						3	2	11025.2649	-0.0024
						1	1	11025.6404	0.0014
						2	2	11024.8329	0.0009
2	2	1	1	1	0	1	0	10900.2861	-0.0005
						2	1	10900.2861	-0.0005
						3	2	10900.4479	-0.0028
						1	1	10900.9671	0.0034
						2	2	10900.0188	-0.0002
2	1	1	1	0	1	1	0	6552.1460	-0.0010
						2	1	6551.3596	0.0036
						3	2	6551.6203	0.0005
						1	1	6551.1415	0.0018
2	2	0	1	1	0	1	0	10904.9970	-0.0004
						2	1	10904.9970	-0.0004
						3	2	10905.1618	-0.0007
						2	2	10904.7304	0.0033
2	2	1	1	1	1	2	1	11020.2534	-0.0004
						3	2	11020.5527	-0.0030
						1	1	11020.9271	0.0017
						2	2	11020.1220	-0.0019
3	1	3	2	0	2	2	1	8051.6010	0.0028
						3	2	8051.4836	0.0001
						4	3	8051.5043	0.0021
						2	2	8050.9235	0.0023
						3	3	8051.9211	0.0024
3	1	2	2	0	2	2	1	8772.0634	-0.0006
						3	2	8771.7328	-0.0015
						4	3	8771.9113	-0.0010
						2	2	8771.3867	-0.0003
						3	3	8772.1676	-0.0020
3	2	1	2	1	1	2	1	12842.3957	-0.0013
						3	2	12842.1668	-0.0015
						4	3	12842.3146	-0.0020
3	2	2	2	1	2	2	1	13179.2493	0.0017
						3	2	13178.7932	0.0008
						4	3	13179.0837	-0.0014
4	1	3	3	0	3	3	2	11059.6230	0.0007
						4	3	11059.3952	-0.0012
						5	4	11059.5423	-0.0001
						3	3	11059.0039	-0.0017
						4	4	11059.8499	-0.0034
4	2	3	3	1	3	3	2	15396.9595	0.0035
						4	3	15396.6259	0.0009
						5	4	15396.8577	0.0002
						3	3	15396.3958	0.0020

Table S1. (continued)

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
4	2	2	3	1	2	4	3	14746.5377	-0.0056
4						3	2	14746.6778	-0.0027
4						5	4	14746.6359	0.0025
4						3	3	14746.3289	-0.0042
5	0	5	4	1	4	4	3	8347.9652	0.0038
5						5	4	8347.9652	0.0038
5						6	5	8347.9387	-0.0030
5	1	4	4	0	4	4	3	13423.0521	-0.0012
5						5	4	13422.8676	-0.0000
5						6	5	13423.0011	0.0004
5						4	4	13422.4541	-0.0024
5						5	5	13423.3417	-0.0006
5	2	4	4	1	4	4	3	17674.1090	0.0024
5						5	4	17673.8522	0.0021
5						6	5	17674.0444	0.0022
5	2	3	4	1	3	4	3	16636.2949	-0.0002
5						5	4	16636.2079	-0.0035
5						6	5	16636.2684	0.0012
5						4	4	16635.9044	0.0001
6	1	5	5	0	5	5	4	15872.7873	-0.0017
6						6	5	15872.6210	-0.0001
6						7	6	15872.7534	0.0034

Table S2. Measured rotational transitions (in MHz) of conformer GII of Phenylethylamine.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
2	1	1	1	0	1	1	0	6486.8756	-0.00117
						2	1	6486.4018	-0.00052
						3	2	6486.8898	-0.00050
						1	1	6487.6299	-0.00040
						2	2	6486.1017	0.00082
2	2	0	1	1	0	1	0	10823.6745	-0.00224
						2	1	10825.2172	-0.00335
						3	2	10824.4924	0.00004
						2	2	10824.7887	0.00365
2	2	1	1	1	1	1	0	10930.4355	-0.00058
						2	1	10929.0978	0.00136
						3	2	10929.5114	0.00108
						1	1	10928.5948	0.00059
						2	2	10929.8320	-0.00126
2	2	1	2	1	1	1	1	6663.1801	-0.00222
						2	2	6664.9130	0.00038
						3	3	6663.7991	-0.00113
3	1	2	2	0	2	2	1	8675.5368	-0.00152
						3	2	8674.7849	-0.00411
						4	3	8675.3854	-0.00324
						2	2	8675.9932	-0.00042
						3	3	8674.4979	0.00152
3	2	1	2	1	1	2	1	12754.8335	0.00005
						3	2	12755.9567	0.00074
						4	3	12755.2495	0.00487
						2	2	12756.0662	0.00470
						3	3	12755.1632	-0.00326
3	2	2	2	1	2	2	1	13062.4966	0.00049
						3	2	13061.7725	0.00170
						4	3	13062.2379	0.00074
3	2	2	3	1	2	2	2	6502.8860	-0.00132
						3	3	6504.0920	-0.00005
						4	4	6503.2054	0.00574
4	1	4	3	1	3	3	2	7870.9470	0.00221
						4	3	7870.8925	-0.00100
						5	4	7870.9037	-0.00032
						3	3	7870.3936	0.00171
						4	4	7871.3029	-0.00024
4	0	4	3	0	3	3	2	8057.2041	0.00067
						4	3	8057.2964	-0.00252
						5	4	8057.2432	0.00116
						3	3	8057.5495	-0.00053
						4	4	8057.0393	-0.00283
4	1	3	3	1	2	3	2	8305.2340	0.00316
						4	3	8305.2658	0.00034
						5	4	8305.3043	0.00045
4	1	3	3	0	3	3	2	10924.4440	-0.00150
						4	3	10923.6224	0.00028
						5	4	10924.2944	-0.00162
						3	3	10924.7908	-0.00127
						4	4	10923.3671	0.00175
4	3	2	4	2	2	3	3	11333.1645	-0.00035
						4	4	11333.6249	-0.00253
						5	5	11333.2576	-0.00188

Table S2. (Continued)

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
5	1	5	4	1	4	4	3	9831.8817	0.00078
						5	4	9831.8664	-0.00150
						6	5	9831.8612	0.00021
						4	4	9831.3760	-0.00328
5	0	5	4	0	4	4	3	10043.3729	0.00006
						5	4	10043.4718	-0.00073
						6	5	10043.3979	-0.00037
						5	5	10043.2738	0.00118
5	1	4	4	1	3	4	3	10373.6222	-0.00021
						5	4	10373.6574	-0.00294
						6	5	10373.6733	0.00313
						5	5	10372.7293	-0.00042
5	1	4	4	0	4	4	3	13240.8663	0.00178
						5	4	13239.9847	0.00118
						6	5	13240.7250	0.00085

Table S3. Measured rotational transitions (in MHz) of conformer AI of Phenylethylamine.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
1	1	0	0	0	0	0	1	5253.8622	-0.0032
						2	1	5253.5976	-0.0005
						1	1	5253.4225	0.0029
2	1	1	1	0	1	1	0	6969.1469	0.0024
						2	1	6968.2218	-0.0009
						3	2	6968.3609	0.0008
3	1	2	2	0	2	2	1	8729.1759	-0.0012
						3	2	8729.0712	-0.0010
						4	3	8729.0291	0.0006
4	1	3	3	0	3	4	3	10537.8025	-0.0022
						5	4	10537.6819	0.0013
5	1	4	4	0	4	4	3	12397.6048	0.0033
						5	4	12397.7647	0.0014
						6	5	12397.5890	-0.0033
6	1	5	5	0	5	5	4	14313.1292	0.00353
						6	5	14313.3340	-0.0017
						7	6	14313.1292	-0.0023

Table S4. Measured rotational transitions (in MHz) of conformer AII of Phenylethylamine.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
1	1	0	0	0	0	2	1	5216.5712	0.0008
						1	1	5215.6850	0.0030
						0	1	5217.8990	-0.0042
2	1	1	1	0	1	1	0	6928.9583	-0.0020
						2	1	6927.1716	0.0022
						3	2	6928.0929	-0.0018
						1	1	6928.0269	-0.0038
2	2	0	1	1	0	1	0	13847.8948	-0.0034
						2	1	13849.4663	-0.0034
						3	2	13848.9988	-0.0000
2	2	1	1	1	1	1	0	13938.9180	0.0055
						2	1	13937.0003	-0.0012
						3	2	13937.9132	-0.0031
						2	2	10514.8801	0.0012
						3	3	10514.7294	0.0053
3	1	2	2	0	2	2	1	8685.8421	0.0034
						3	2	8684.5648	0.0026
						4	3	8685.4406	-0.0034
4	1	4	3	1	3	3	2	6300.1242	0.0027
						5	4	6300.0402	0.0009
						4	3	6300.1150	-0.0009
4	0	4	3	0	3	3	2	6467.0914	-0.0005
						4	3	6467.1120	-0.0007
						5	4	6467.0622	0.0002
4	1	3	3	1	2	3	2	6661.5541	-0.0000
						4	3	6661.6509	0.0013
						5	4	6661.6109	0.0029
4	1	3	3	0	3	3	2	10491.0144	0.0051
						4	3	10489.8519	-0.0013
						5	4	10490.7382	-0.0003
5	1	5	4	1	4	4	3	7872.0101	-0.0020
						5	4	7872.0101	-0.0020
						6	5	7871.9594	-0.0009
5	0	5	4	0	4	4	3	8071.0299	0.0009
						5	4	8071.0715	-0.0003
						6	5	8071.0141	0.0007
5	1	4	4	0	4	4	3	12347.5116	-0.0006
						5	4	12346.3905	-0.0014
						6	5	12347.2989	-0.0008
6	1	6	5	1	5	5	4	9441.9516	0.0006
						6	5	9441.9516	0.0006
						7	6	9441.9122	-0.0008
6	0	6	5	0	5	5	4	9666.6764	0.0002
						6	5	9666.7346	0.0003
						7	6	9666.6674	-0.0003