

Rapid Probe of the Nicotine Spectra by High-Resolution Rotational Spectroscopy

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Table S1. Measured rotational transitions of conformer *trans-a* of nicotine.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'_T	F'	I''_T	F''	$\nu_{\text{obs}} / \text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{cal}} / \text{MHz}$						
5	0	5	4	0	4	0	5	0	4	5636.575	-0.002						
						2	7	2	6	5636.588	-0.001						
						1	6	1	5	5636.627	-0.001						
						2	6	2	5	5636.666	-0.001						
						2	5	2	4	5636.681	-0.002						
5	1	5	4	1	4	2	7	2	6	5567.533	-0.000						
						1	6	1	5	5567.548	0.002						
						1	5	1	4	5567.560	0.004						
						2	6	2	5	5567.601	-0.002						
						1	4	1	3	5567.623	0.003						
						2	5	2	4	5567.635	0.002						
						2	4	2	3	5567.645	-0.000						
5	1	4	4	1	3	2	3	2	2	5720.137	-0.006						
						0	5	0	4	5720.185	-0.005						
						1	5	1	4	5720.212	-0.003						
						2	6	2	5	5720.231	-0.004						
						2	7	2	6	5720.243	-0.002						
						1	6	1	5	5720.270	-0.002						
						5	2	4	4	2	3	2	4	2	3	5644.786	-0.003
1	6	1	5	5644.803	-0.002												
1	5	1	4	5644.859	-0.004												
2	3	2	2	5644.875	0.003												
2	7	2	6	5644.884	0.005												
0	5	0	4	5644.893	0.006												
2	5	2	4	5644.961	-0.003												
2	6	2	5	5645.047	0.006												
1	4	1	3	5645.047	-0.002												
5	2	3	4	2	2							1	4	1	3	5654.111	0.000
						2	6	2	5	5654.123	0.002						
						2	5	2	4	5654.215	0.004						
						0	5	0	4	5654.239	-0.000						
						2	7	2	6	5654.247	0.001						
						1	5	1	4	5654.267	0.006						
						1	6	1	5	5654.343	0.001						
						2	4	2	3	5654.357	0.002						
						6	0	6	5	0	5	0	6	0	5	6758.825	0.001
												2	8	2	7	6758.832	-0.000
1	6	1	5	6758.858	0.001												
1	7	1	6	6758.886	-0.001												
2	5	2	4	6758.902	-0.003												
1	5	1	4	6758.904	-0.005												
2	7	2	6	6758.923	0.001												
2	6	2	5	6758.964	0.002												
6	1	6	5	1	5							2	8	2	7	6679.835	0.001
												1	7	1	6	6679.850	0.000
						2	7	2	6	6679.888	-0.000						
						1	5	1	4	6679.902	-0.000						
						2	6	2	5	6679.915	0.001						
6	1	5	5	1	4	0	6	0	5	6862.879	-0.000						
						1	6	1	5	6862.899	0.001						
						2	8	2	7	6862.917	-0.002						
						2	6	2	5	6862.932	-0.003						

Table S1. (continued)

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'_T	F'	I''_T	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{cal}}/\text{MHz}$
6	1	5	5	1	4	1	7	1	6	6862.944	-0.001
6	2	5	5	2	4	1	7	1	6	6772.964	-0.002
						2	4	2	3	6772.997	-0.006
						1	6	1	5	6773.002	-0.004
						2	6	2	5	6773.059	-0.004
						2	7	2	6	6773.104	-0.004
6	2	4	5	2	3	2	7	2	6	6789.214	0.003
						1	5	1	4	6789.218	0.003
						2	6	2	5	6789.262	0.004
						2	8	2	7	6789.315	0.005
						1	7	1	6	6789.340	0.005
6	3	4	5	3	3	2	5	1	4	6777.407	-0.003
						1	7	2	6	6777.436	-0.002
						2	8	2	7	6777.547	-0.002
						2	7	1	6	6777.727	-0.002
6	3	3	5	3	2	1	6	0	5	6777.763	0.009
						2	5	1	4	6777.660	0.000
						1	7	2	6	6777.684	-0.004
						2	8	2	7	6777.799	-0.002
						2	6	1	5	6777.859	-0.001
						2	7	1	6	6777.976	-0.003
						1	5	2	4	6777.995	-0.000
6	4	3	5	4	2	2	5	2	4	6776.401	0.001
						1	7	1	6	6776.471	0.002
						1	6	1	5	6776.569	0.000
						2	8	2	7	6776.652	-0.000
						2	6	2	5	6776.821	0.000
						2	7	2	6	6776.977	0.000
						1	5	1	4	6777.013	0.000
6	4	2	5	4	1	2	5	2	4	6776.401	0.000
						1	7	1	6	6776.471	0.001
						1	6	1	5	6776.569	-0.001
						2	8	2	7	6776.652	-0.002
						2	6	2	5	6776.821	-0.000
						2	7	2	6	6776.977	-0.000
						1	5	1	4	6777.013	-0.001
7	0	7	6	0	6	0	7	0	6	7878.400	0.001
						2	9	2	8	7878.411	0.001
						1	7	1	6	7878.424	0.000
						1	8	1	7	7878.475	0.001
						2	6	2	5	7878.481	-0.001
						1	6	1	5	7878.495	0.001
						2	8	2	7	7878.508	0.000
						2	7	2	6	7878.567	0.003
7	1	7	6	1	6	2	9	2	8	7791.502	0.000
						1	7	1	6	7791.511	0.000
						1	8	1	7	7791.520	0.000
						0	7	0	6	7791.541	0.000
						2	8	2	7	7791.548	-0.000
						1	6	1	5	7791.557	-0.001
						2	7	2	6	7791.572	-0.000
7	1	6	6	1	5	2	5	2	4	8004.755	-0.003
						0	7	0	6	8004.778	-0.001

Table S1. (continued)

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'_T	F'	I''_T	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{cal}}/\text{MHz}$
7	1	6	6	1	5	1	7	1	6	8004.792	-0.002
						2	9	2	8	8004.805	-0.003
						2	8	2	7	8004.812	-0.002
7	2	6	6	2	5	1	8	1	7	8004.836	-0.000
						1	8	1	7	7900.628	-0.005
						0	7	0	6	7900.648	-0.006
						2	7	2	6	7900.699	-0.002
7	2	5	6	2	4	2	8	2	7	7900.722	-0.006
						2	8	2	7	7926.479	0.008
						2	7	2	6	7926.483	0.009
						1	6	1	5	7926.490	0.010
						1	7	1	6	7926.550	-0.004
						0	7	0	6	7926.556	-0.003
						2	9	2	8	7926.566	0.006
2	5	2	4	7926.577	0.006						
7	3	5	6	3	4	1	8	1	7	7907.823	0.001
						1	7	1	6	7907.886	0.001
						2	7	2	6	7907.935	-0.000
						2	8	2	7	7908.010	0.001
7	3	4	6	3	3	2	6	2	5	7908.379	0.004
						1	8	1	7	7908.386	0.001
						1	7	1	6	7908.454	0.002
						2	7	2	6	7908.496	0.001
						2	8	2	7	7908.572	0.001
						1	8	2	7	7906.782	-0.000
7	4	4	6	4	3	2	6	1	5	7906.806	0.005
						1	8	2	7	7906.782	-0.004
7	4	3	6	4	2	2	6	1	5	7906.805	0.001
						2	6	1	5	7906.805	0.001
8	0	8	7	0	7	0	8	0	7	8995.005	0.003
						2	6	2	5	8995.010	0.004
						2	10	2	9	8995.016	0.004
						1	8	1	7	8995.022	0.002
						1	9	1	8	8995.086	0.002
						2	7	2	6	8995.094	0.003
						1	7	1	6	8995.110	0.003
						2	9	2	8	8995.126	0.008
						2	8	2	7	8995.190	0.003
						2	8	2	7	8902.467	0.003
						1	9	1	8	8902.476	-0.007
0	8	0	7	8902.486	-0.008						
8	1	8	7	1	7	2	6	2	5	8902.498	-0.008
						2	9	2	8	8902.508	0.001
						2	7	2	6	8902.524	0.006
						2	8	2	7	8902.533	0.002
						2	8	2	7	8902.533	0.002
						2	6	2	5	9145.711	0.002
						0	8	0	7	9145.723	-0.001
						1	8	1	7	9145.737	0.001
						2	10	2	9	9145.748	0.001
						2	7	2	6	9145.754	0.002
						2	9	2	8	9145.760	0.000
1	9	1	8	9145.780	0.001						
2	8	2	7	9145.789	0.001						

Table S1. (continued)

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'_T	F'	I''_T	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{cal}}/\text{MHz}$
8	2	7	7	2	6	1	9	1	8	9027.734	-0.009
						2	10	2	9	9027.745	-0.008
						1	8	1	7	9027.753	-0.006
						2	8	2	7	9027.790	-0.007
						1	7	1	6	9027.798	-0.009
						2	9	2	8	9027.804	-0.006
8	3	6	7	3	5	1	9	1	8	9038.475	0.002
						1	8	1	7	9038.524	0.001
						0	8	0	7	9038.532	0.002
						2	8	2	7	9038.542	-0.002
						2	9	2	8	9038.603	0.004
						2	4	2	3	6726.537	-0.002
2	2	0	1	1	0	1	2	2	1	6728.210	-0.001
						1	3	1	2	6728.959	0.002
						0	3	2	2	7916.765	0.002
						1	4	2	3	7917.143	-0.002
						2	4	2	3	7917.144	-0.001
						1	5	2	4	6164.853	-0.002
4	1	3	3	0	3	2	3	1	2	6165.121	-0.000
						2	5	1	4	6165.195	0.002
						2	6	2	5	6166.171	0.001
						0	4	0	3	6166.420	0.000
						1	4	1	3	6166.608	-0.002
						1	6	2	5	7372.997	0.004
5	1	4	4	0	4	2	4	1	3	7373.206	0.003

Table S2. Measured rotational transitions of conformer *trans-b* of nicotine.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'_T	F'	I''_T	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{cal}}/\text{MHz}$
5	0	5	4	0	4	2	7	2	6	5670.978	0.000
						0	5	0	4	5670.999	-0.001
						1	6	1	5	5671.049	-0.001
						2	5	2	4	5671.128	-0.001
5	1	5	4	1	4	2	7	2	6	5602.231	-0.000
						2	6	2	5	5602.268	0.004
						0	5	0	4	5602.313	0.005
						1	6	1	5	5602.328	-0.001
						2	3	2	2	5602.385	0.003
						2	5	2	4	5602.394	0.002
						2	4	2	3	5602.475	0.008
						0	5	0	4	5754.326	0.000
5	1	4	4	1	3	1	5	1	4	5754.346	0.001
						2	7	2	6	5754.378	0.001
						1	6	1	5	5754.395	-0.001
						2	6	2	5	5754.408	-0.006
						2	5	2	4	5754.418	-0.001
						0	5	0	4	5679.257	-0.003
						1	5	1	4	5679.265	-0.002
						2	7	2	6	5679.275	0.001
5	2	4	4	2	3	2	4	2	3	5679.323	-0.005
						1	6	1	5	5679.343	-0.002
						1	4	1	3	5679.423	-0.001
						2	6	2	5	5679.429	-0.001
						2	5	2	4	5679.493	-0.002
						0	5	0	4	5688.677	0.002
						2	7	2	6	5688.689	0.005
						1	6	1	5	5688.693	0.004
6	0	6	5	0	5	2	6	2	5	5688.778	0.003
						2	5	2	4	5688.783	0.003
						2	8	2	7	6800.083	-0.001
						1	6	1	5	6800.089	0.002
						0	6	0	5	6800.102	0.001
						1	7	1	6	6800.167	-0.001
						2	7	2	6	6800.171	0.000
						2	6	2	5	6800.258	-0.000
6	1	6	5	1	5	2	8	2	7	6721.478	0.001
						2	7	2	6	6721.507	0.001
						1	7	1	6	6721.552	-0.000
						2	6	2	5	6721.599	0.001
						2	5	2	4	6721.636	-0.004
						2	4	2	3	6903.812	-0.002
						0	6	0	5	6903.841	-0.002
						2	5	2	4	6903.852	0.000
6	1	5	5	1	4	1	6	1	5	6903.856	-0.001
						2	8	2	7	6903.877	-0.000
						1	7	1	6	6903.895	-0.004
						2	7	2	6	6903.905	-0.002
						2	6	2	5	6903.918	-0.003
						1	7	1	6	6830.650	0.004
						2	6	2	5	6830.669	0.002
						0	6	1	5	6830.681	0.002

Table S2. (continued)

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'_T	F'	I''_T	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{cal}}/\text{MHz}$
6	2	4	5	2	3	2	4	2	3	6830.685	-0.000
						2	7	2	6	6830.694	-0.001
						1	5	1	4	6830.699	-0.001
6	2	5	5	2	4	2	8	2	7	6814.295	-0.005
						1	7	1	6	6814.345	-0.003
						2	7	2	6	6814.396	-0.002
						2	6	2	5	6814.445	-0.004
6	3	4	5	3	3	2	8	2	7	6818.839	0.001
						2	5	2	4	6818.875	0.001
						1	7	1	6	6818.902	-0.001
						2	7	2	6	6819.016	0.001
6	3	3	5	3	2	2	4	2	3	6819.053	-0.002
						2	8	2	7	6819.095	0.001
						1	7	1	6	6819.156	-0.000
						1	5	1	4	6819.262	0.004
						2	7	2	6	6819.271	0.003
						2	6	2	5	6819.329	0.002
7	0	7	6	0	6	2	9	2	8	7926.513	-0.001
						1	8	1	7	7926.606	-0.001
						2	7	2	6	7926.705	-0.001
7	1	7	6	1	6	2	9	2	8	7840.087	0.001
						1	7	1	6	7840.111	-0.001
						2	8	2	7	7840.115	0.001
						1	8	1	7	7840.147	-0.001
						2	5	2	4	7840.161	0.001
						2	7	2	6	7840.185	-0.001
						2	6	2	5	7840.206	-0.001
7	1	6	6	1	5	2	5	2	4	8052.544	0.001
						0	7	0	6	8052.564	0.000
						1	7	1	6	8052.574	0.001
						2	9	2	8	8052.588	0.000
						1	6	1	5	8052.604	-0.001
						2	8	2	7	8052.618	0.000
						2	7	2	6	8052.637	-0.001
7	2	6	6	2	5	1	7	1	6	7948.831	-0.006
						2	9	2	8	7948.835	-0.002
						2	8	2	7	7948.904	-0.004
						2	7	2	6	7948.943	-0.005
7	2	5	6	2	4	1	8	1	7	7974.793	-0.007
						2	6	2	5	7974.810	-0.000
						2	8	2	7	7974.836	0.004
						1	6	1	5	7974.841	0.002
						0	7	0	6	7974.859	0.002
						2	5	2	4	7974.870	0.002
8	0	8	7	0	7	1	8	1	7	9049.959	0.001
						0	8	0	7	9049.966	0.001
						1	9	1	8	9050.062	-0.001
						2	9	2	8	9050.071	0.006
						2	7	2	6	9050.079	0.008
						2	8	2	7	9050.170	0.000
8	1	8	7	1	7	2	10	2	9	8957.987	0.001
						1	8	1	7	8958.001	-0.005
						0	8	0	7	8958.017	0.001

Table S2. (continued)

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'_T	F'	I''_T	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{cal}}/\text{MHz}$
8	1	8	7	1	7	1	7	1	6	8958.027	-0.002
						1	9	1	8	8958.037	-0.004
						2	6	2	5	8958.045	0.002
						2	8	2	7	8958.077	0.000
						2	7	2	6	8958.086	0.003
8	1	7	7	1	6	2	6	2	5	9200.308	-0.000
						0	8	0	7	9200.323	0.000
						1	8	1	7	9200.332	0.001
						2	10	2	9	9200.341	-0.001
						2	9	2	8	9200.374	0.000
8	2	7	7	2	6	2	8	2	7	9200.400	-0.000
						2	8	2	9	9082.812	-0.009
						1	8	1	7	9082.816	-0.004
						1	9	1	8	9082.845	-0.009
						2	7	2	6	9082.867	0.007
2	2	0	1	1	0	2	8	2	7	9082.903	-0.008
						2	8	2	7	9082.903	-0.008
						2	4	2	3	6690.120	-0.003
						1	3	1	2	6690.518	-0.004
						2	3	2	2	6691.348	0.004
4	1	3	3	0	3	2	4	2	3	6173.339	0.000
						2	3	2	2	6175.659	0.000
						2	6	2	5	6175.917	-0.002
5	1	4	4	0	4	2	5	2	4	7388.045	0.005
						2	7	2	6	7390.724	0.006

Reference 32:

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