

**Table 1S.** Assignments of the LIF spectrum of anthranilic acid and comparison with the REMPI results measured by Wu et al.[9]. Frequency of the electronic origin  $\nu_{00} = 28591 \text{ cm}^{-1}$  was subtracted from the LIF frequencies. All frequencies are given in  $\text{cm}^{-1}$ .

$\nu - \nu_{00}$	$I/I_{00}$ [%]	FWHM	assignment	$\Sigma \nu_{\text{fund}}$	$\Delta \nu$	classification	REMPI, Wu et al. [9]
<b>0.0</b>	<b>100</b>	<b>1.63</b>	<b>00</b>	<b>0.0</b>	<b>0.0</b>		
97.0	2	1.45	dimer	97.0	0.0		
153.8	1	1.09	dimer	154.0	0.2		
156.3	1	2.33					
<b>161.5</b>	<b>3</b>	<b>1.57</b>	<b><math>2 \times \nu_{1A}</math></b>	<b>161.5</b>	<b>0.0</b>	$10b_0^2 \gamma(\text{ring})$	
<b>219.0</b>	<b>2</b>	<b>1.57</b>	<b><math>2 \times \nu_{2A}</math></b>	<b>219.0</b>	<b>0.0</b>	$\gamma(-\text{COOH})_0^2$ torsion	$220 = A_0^2 \gamma(-\text{COOH})$ torsion
222.4	2	3.22					
239.4	1	3.30					
<b>253.1</b>	<b>89</b>	<b>1.60</b>	<b><math>\nu_{1S}</math></b>	<b>253.1</b>	<b>0.0</b>	$\beta(-\text{COOH})$	$254 = B_0^1 \beta(-\text{COOH})$
255.9	4	2.13	dimer				
310.2	2	1.26	dimer	313.7	3.5		
<b>354.5</b>	<b>36</b>	<b>1.47</b>	<b><math>\nu_{2S}</math></b>	<b>354.5</b>	<b>0.0</b>	$\beta(-\text{NH}_2)$	$355 = C_0^1 \beta(-\text{NH}_2)$
<b>379.4</b>	<b>13</b>	<b>1.45</b>	<b><math>2 \times \nu_{3A}</math></b>	<b>379.4</b>	<b>0.0</b>	$10a_0^2 \gamma(\text{ring})$	$379 = 10b_0^2 \gamma(\text{ring})$
386.6	1	1.14	dimer	386.7	0.2		
400.7	3	2.34	dimer	397.9	-2.8		
409.2	5	2.23	$\nu_{1S} + 2 \times \nu_{1A}$	414.6	5.4		
<b>418.4</b>	<b>102</b>	<b>1.57</b>	<b><math>\nu_{3S}</math></b>	<b>418.4</b>	<b>0.0</b>	$\beta(-\text{COOH}),$ $\beta(-\text{NH}_2), \beta(\text{ring})$	$418 = D_0^1 \beta(-\text{COOH}),$ $\beta(-\text{NH}_2), \beta(\text{ring})$
441.8	2	1.40	dimer	443.7	1.9		
443.9	1	1.32	dimer				
456.1	2	1.68	dimer	454.9	-1.2		
471.3	3	1.25	$\nu_{1S} + 2 \times \nu_{2A}$	472.1	0.8		
498.3	2	1.72		500.7	2.4		
<b>501.7</b>	<b>13</b>	<b>1.40</b>	<b><math>\nu_{4S}</math></b>	<b>501.7</b>	<b>0.0</b>	$9b, \beta(-\text{COOH}) \beta(-\text{NH}_2),$	
507.4	60	1.52	$2 \times \nu_{1S}$	506.2	-1.2		$506 = B_0^2$
514.6	1	1.51	dimer	511.9	-2.7		
538.8	4	3.41	dimer	539.1	0.3		
<b>542.9</b>	<b>22</b>	<b>1.47</b>	<b><math>\nu_{5S}</math></b>	<b>542.9</b>	<b>0.0</b>	$6a \beta(\text{ring})$	$544 = 6a_0^1 \beta(\text{ring})$
545.5	2	1.42					
562.3	3	1.56					
573.3	1	1.69	$\nu_{2S} + 2 \times \nu_{2A}$	573.5	0.2		
582.7	4	1.38	$\nu_{3S} + 2 \times \nu_{1A}$	579.9	-3.8		
<b>594.6</b>	<b>34</b>	<b>1.53</b>	<b><math>\nu_{6S}</math></b>	<b>594.6</b>	<b>0.0</b>	$6b \beta(\text{ring}), \beta(\text{C=O})$	$595 = A_0^2 10b_0^2$ (*) <i>too large intensity for this combination</i>
602.7	18	1.44	$\nu_{1S} + \nu_{2S}$	607.6	4.9	<i>anharmonicity</i>	$602 = B_0^1 C_0^1$ or $16b_0^2 \gamma(\text{ring})$
<b>609.2</b>	<b>2</b>	<b>1.35</b>	<b><math>2 \times \nu_{4A}</math></b>	<b>609.2</b>	<b>0.0</b>	$16b_0^2 \gamma(\text{ring})$	
631.8	12	1.67	$\nu_{1S} + 2 \times \nu_{3A}$	632.5	0.7		$632 = 6b_0^1 \beta(\text{ring})$ (*)
636.9	2	1.68	$\nu_{3S} + 2 \times \nu_{2A}$	637.4	0.5		
653.9	1	1.38	dimer	653.1	-0.8		
661.5	3	1.29	$2 \times \nu_{1S} + 2 \times \nu_{1A}$	667.7	6.2		
666.6	2	1.72					
670.9	87	1.61	$\nu_{1S} + \nu_{3S}$	671.6	0.7		$672 = B_0^1 D_0^1$
701.5	2	2.04	dimer	698.8	-2.7		
706.8	5	1.53	$2 \times \nu_{2S}$	709.0	2.2		
<b>713.1</b>	<b>31</b>	<b>1.47</b>	<b><math>\nu_{7S}</math></b>	<b>713.1</b>	<b>0.0</b>	$\beta(\text{O-C=O}),$ $1 \nu(\text{ring})$	$713 = C_0^2$ (*) <i>too large intensity for this overtone</i>
728.4	3	1.52	$2 \times \nu_{1S} + 2 \times \nu_{2A}$	725.2	-3.2		

$\nu - \nu_{00}$	$I/I_{00}$ [%]	FWHM	assignment	$\Sigma \nu_{\text{fund}}$	$\Delta \nu$	classification	REMPLI, Wu et al. [9]
732.3	2	1.15	$\nu_{2S}+2\nu_{3A}$	733.9	1.6		
753.1	8	2.42	$\nu_{1S}+\nu_{4S}$	754.8	1.7		
761.5	34	1.42	$3\nu_{1S}$	759.4	-2.1		$762 = B_0^3$
764.9	2	2.00	$\nu_{1S}+\nu_{2S}+2\nu_{1A}$	763.7	-1.2		
772.5	32	1.33	$\nu_{2S}+\nu_{3S}$	772.9	0.4		$772 = C_0^1 D_0^1$
783.3	1	1.00					
795.8	21	1.44	$\nu_{1S}+\nu_{5S}$	796.0	0.2		$797 = B_0^1 6a_0^1$
799.5	22	1.74	$\nu_{3S}+2\nu_{3A}$	797.8	-1.7		
820.6	3	2.42	$\nu_{1S} + \nu_{2S} + 2\nu_{2A}$	826.6	6.0		
827.3	8	1.82	$\nu_{1S}+\nu_{3S}+2\nu_{1A}$	833.0	5.7		
835.0	56	1.67	$2\nu_{3S}$	836.9	1.9		<i>overlapping</i>
<b>839.1</b>	<b>40</b>	<b>1.54</b>	<b><math>2\nu_{5A}</math></b>	<b>839.1</b>	<b>0.0</b>	$16a_0^2 \gamma(\text{ring})$	$839 = D_0^2$
<b>840.9</b>	<b>35</b>	<b>1.35</b>	<b><math>\nu_{8S}</math></b>	<b>840.9</b>	<b>0.0</b>	12 $\beta(\text{ring})$	<i>overlapping</i>
846.5	23	1.34	$\nu_{1S}+\nu_{6S}$	847.7	1.2		
853.7	3	1.04	$2\nu_{1S}+\nu_{2S}$	860.7	7.0		
857.2	2	1.03	$\nu_{4S}+\nu_{2S}$	856.2	-1.0		
860.5	1	1.59	$2\nu_{1S}+\nu_{2S}$	860.7	0.2		
864.5	2	1.62	$\nu_{1S}+2\nu_{4A}$	862.3	-2.2		
879.6	2	1.05	$\nu_{4S}+2\nu_{3A}$	881.1	1.4		
882.2	4	2.36	<b>dimer</b>				
885.5	6	2.07	$2\nu_{1S}+2\nu_{3A}$	885.6	0.1		$884 = 19a_0^1 \beta(\text{ring}) (*)$
888.7	2	1.65	$\nu_{1S}+ \nu_{3S}+2\nu_{2A}$	890.5	1.8		
897.8	13	2.72	$\nu_{2S}+\nu_{5S}$	897.4	-0.4		
919.7	10	1.31	$\nu_{3S}+\nu_{4S}$	920.1	0.4		
921.6	4	1.34	$\nu_{5S}+2\nu_{3A}$	922.3	0.6		
924.7	53	1.27	$2\nu_{1S}+\nu_{3S}$	924.7	0.0		$923 = B_0^2 D_0^1$
945.3	4	1.23					
947.9	7	2.06	$\nu_{2S}+\nu_{6S}$	949.1	1.2		
953.1	3	2.53	$\nu_{1S}+\nu_{5S}+2\nu_{1A}$	957.4	4.3		
			$2\nu_{2S}+ \nu_{1S}$	962.1	9.0	<i>anharmonicity</i>	
960.7	26	1.26	$\nu_{3S}+\nu_{5S}$	961.3	0.6		$961 = B_0^1 C_0^2 (*)$ <i>overlapping,</i> <i>too large intensity</i> <i>overlapping</i>
966.5	29	1.23	$\nu_{1S}+\nu_{7S}$	966.2	-0.3		
977.9	1	2.97	<b>dimer</b>	981.2	3.3		
986.7	2	0.98	$\nu_{1S}+\nu_{2S}+2\nu_{3A}$	987.0	0.3		$988 = C_0^1 6b_0^1 (*)$
1005.0	4	1.52	$2\nu_{1S}+\nu_{4S}$	1007.9	2.9		
1012.5	28	1.38	$\nu_{3S}+\nu_{6S}$	1013.0	0.5		$1013 = B_0^4 (*)$ <i>overlapping</i> <i>too large intensity for this</i> <i>combination</i> <i>overlapping,</i>
1016.5	10	1.08	$4\nu_{1S}$	1012.5	-4.0	<i>anharmonicity</i>	
1020.5	12	1.72	$\nu_{3S}+\nu_{1S}+\nu_{2S}$	1026.1	5.5		
1050.5	16	2.00	$2\nu_{1S}+\nu_{5S}$	1049.1	-1.4		$1050 = C_0^3 (*)$ <i>too large</i> <i>intensity,</i> <i>discrepancy <math>\Delta \nu = 16\text{cm}^{-1}</math></i>
			$\nu_{1S}+\nu_{3S}+2\nu_{3A}$	1051.0	0.5		
1060.5	3	1.41	$3\nu_{2S}$	1063.5	3.0		
1067.7	2	1.26	$\nu_{2S}+\nu_{7S}$	1067.5	-0.1		
1079.6	2	1.24	$2\nu_{1S}+\nu_{3S}+2\nu_{1A}$	1086.1	6.5		
1087.0	30	1.60	$\nu_{1S}+2\nu_{3S}$	1090.0	3.0		<i>overlapping</i>
1091.6	25	1.37	$\nu_{1S}+2\nu_{5A}$	1092.2	0.6		$1092 = B_0^1 D_0^2 (*)$
1094.2	34	2.11	$\nu_{1S}+\nu_{8S}$	1094.1	-0.2		<i>overlapping</i>
1100.4	8	1.28	$2\nu_{1S}+\nu_{6S}$	1100.8	0.4		
1109.2	2	2.56	$\nu_{1S}+\nu_{2S}+\nu_{4S}$	1109.3	0.1		
<b>1118.9</b>	<b>7</b>	<b>1.66</b>	<b><math>\nu_{11S}</math></b>	<b>1118.9</b>	<b>0.0</b>	$\beta_{\text{as}}(\text{NH}_2), \nu(\text{C-OH}),$ $\beta(\text{ring})$	

$\nu - \nu_{00}$	$I/I_{00}$ [%]	FWHM	assignment	$\Sigma \nu_{\text{fund}}$	$\Delta \nu$	classification	REMPL, Wu et al. [9]
1125.0	4	1.50	$\nu_{3S}+2\times\nu_{2S}$	1127.4	2.4		
1130.9	31	1.20	$\nu_{3S}+\nu_{7S}$	1131.5	0.6		$1130 = C_0^2 D_0^1 (*)$ too large intensity for this combination
1136.8	3	2.15	$\nu_{5S}+\nu_{6S}$	1137.4	0.6		
1141.8	13	2.17	$\nu_{5S}+\nu_{6S}$	1137.5	-4.3		$1140 = B_0^2 6b_0^1 (*)$
			$3\times\nu_{1S}+2\times\nu_{3A}$	1138.8	-3.1		
1145.3	5	1.95	$\nu_{5S}+\nu_{1S}+\nu_{2S}$	1150.5	5.2		
1167.8	2	1.23	$4\times\nu_{1S}+2\times\nu_{1A}$	1173.9	6.1		
1170.9	5	1.67	$\nu_{1S}+\nu_{3S}+\nu_{4S}$	1173.2	2.4		
1174.6	8	2.21	$\nu_{1S}+\nu_{5S}+2\times\nu_{3A}$	1175.4	0.8		
1178.6	26	1.59	$3\times\nu_{1S}+\nu_{3S}$	1177.8	-0.8		$1178 = 6a_0^1 6b_0^1 (*)$
1188.9	5	1.63	$2\times\nu_{6S}$	1189.1	0.3		
			$2\times\nu_{3S}+\nu_{2S}$	1191.4	2.5		
1192.7	10	1.40	$2\times\nu_{3S}+\nu_{2S}$	1191.4	-1.3		
			$\nu_{2S}+2\times\nu_{5A}$	1193.6	0.9		
1194.7	7	1.19	$\nu_{2S}+\nu_{8S}$	1195.4	0.7		
			$\nu_{6S}+\nu_{1S}+\nu_{2S}$	1202.2	7.5		
1199.7	10	1.59	$\nu_{1S}+\nu_{2S}+\nu_{6S}$	1202.2	2.5		
1206.5	13	1.66	$2\times\nu_{1S}+2\times\nu_{2S}$	1205.4	-1.1		
1213.6	19	1.61	$\nu_{1S}+\nu_{3S}+\nu_{5S}$	1214.4	0.8		
1220.9	30	2.26	$2\times\nu_{1S}+\nu_{7S}$	1219.3	-1.5		$1218 = B_0^2 C_0^2 (*)$ too large intensity for this combination
<b>1229.9</b>	<b>10</b>	<b>1.59</b>	<b><math>\nu_{1SS}</math></b>	<b>1229.9</b>	<b>0.0</b>	$\beta(\text{O-H}),$ $\nu(\text{C-COOH})$	
1233.7	3	1.58	$2\times\nu_{1S}+\nu_{2S}+2\times\nu_{3A}$	1241.1	6.5		
			$\nu_{2S}+2\times\nu_{3A}+\nu_{4S}$	1235.6	1.9		
1239.5	9	1.49	$2\times\nu_{1S}+\nu_{2S}+2\times\nu_{3A}$	1240.1	0.6		
1250.7	12	1.95	$3\times\nu_{3S}$	1255.3	4.6	<i>anharmonicity</i>	<i>overlapping</i>
1257.8	30	1.72	$\nu_{3S}+2\times\nu_{5A}$	1257.6	-0.2		$1258 = D_0^3 (*)$
			$\nu_{5S}+\nu_{7S}$	1255.9	-1.8		<i>overlapping</i>
1260.0	19	1.31	$\nu_{3S}+\nu_{8S}$	1259.4	-0.6		<i>overlapping</i>
1264.1	22	1.63	$\nu_{1S}+\nu_{3S}+\nu_{6S}$	1266.1	2.0		<i>overlapping</i>
1271.5	4	1.32	$5\times\nu_{1S}$	1265.6	-5.9		
1274.3	9	3.13	$2\times\nu_{1S}+\nu_{3S}+\nu_{2S}$	1279.1	4.9		
1277.9	3	1.67					
1296.0	5	1.87					
1304.9	6	1.58	$3\times\nu_{1S}+\nu_{5S}$	1302.2	-2.6		
1308.1	12	2.12	$\nu_{6S}+\nu_{7S}$	1307.7	-0.5		
1317.2	14	3.94	$\nu_{7S}+\nu_{1S}+\nu_{2S}$	1320.7	3.5		
			$\nu_{2S}+\nu_{3S}+\nu_{5S}$	1315.8	-1.4		
1334.3	15	2.08	$\nu_{1S}+2\times\nu_{5S}$	1338.8	4.6		<i>overlapping</i>
			$2\times\nu_{3S}+\nu_{4S}$	1338.6	5.4		
1340.9	35	3.02	$2\times\nu_{1S}+2\times\nu_{3S}$	1343.1	2.2		$1342 = B_0^2 D_0^2$
			$\nu_{3S}+\nu_{5S}+2\times\nu_{3A}$	1340.7	-0.2		<i>overlapping</i>
1345.4	10	1.55	$2\times\nu_{1S}+2\times\nu_{5A}$	1345.4	-0.0		<i>overlapping</i>
1347.7	16	1.82	$2\times\nu_{1S}+\nu_{8S}$	1347.1	-0.5		<i>overlapping</i>
1354.1	6	1.53	$3\times\nu_{1S}+\nu_{6S}$	1353.9	-0.1		
1363.8	5	1.66	$\nu_{2S}+\nu_{3S}+\nu_{6S}$	1367.5	3.7		
			$4\times\nu_{1S}+\nu_{2S}$	1367.0	3.1		
1365.6	4	1.30	$\nu_{2S}+\nu_{3S}+\nu_{6S}$	1367.5	1.9		
1372.4	7	1.35	$2\times\nu_{2S}+\nu_{3S}+\nu_{1S}$	1380.5	8.2		
1377.3	4	1.59	$\nu_{1S}+2\times\nu_{2S}+\nu_{3S}$	1380.5	3.2		
1383.6	43	1.85	$\nu_{1S}+\nu_{3S}+\nu_{7S}$	1384.6	1.0		
			$2\times\nu_{3S}+\nu_{5S}$	1379.7	-3.8		
1389.0	4	1.51	$\nu_{1S}+\nu_{5S}+\nu_{6S}$	1390.6	1.6		

$\nu - \nu_{00}$	$I/I_{00}$ [%]	FWHM	assignment	$\Sigma \nu_{\text{fund}}$	$\Delta \nu$	classification	REMPL, Wu et al. [9]
<b>1395.0</b>	<b>33</b>	<b>2.39</b>	<b><math>\nu_{17S}</math></b>	<b>1395.0</b>	<b>0.0</b>	$\beta(\text{O-H}), \beta(\text{N-H}),$ $\nu(\text{C-O}) \nu(\text{ring})$	
			$\nu_{2S} + \nu_{5S} + \nu_{4S}$	1399.0	4.0		
1398.8	4	1.42	$2 \times \nu_{1S} + \nu_{5S} + \nu_{2S}$	1403.6	4.8		
			$\nu_{3S} + \nu_{6S} + 2 \times \nu_{3A}$	1392.4	-6.4		
			$\nu_{3S} + 2 \times \nu_{3A} + \nu_{1S} + \nu_{2S}$	1400.6	1.8		
			$4 \times \nu_{1S} + 2 \times \nu_{3A}$	1391.9	-8.1		
1404.5	14	1.44	$2 \times \nu_{1S} + \nu_{2S} + \nu_{5S}$	1403.6	-0.9		
1429.0	10	1.32	$2 \times \nu_{3S} + \nu_{6S}$	1431.5	2.4		
			$4 \times \nu_{1S} + \nu_{3S}$	1430.9	1.9		
1431.8	3	0.92	$\nu_{6S} + 2 \times \nu_{5A}$	1433.7	1.9		
			$2 \times \nu_{1S} + \nu_{5S} + 2 \times \nu_{3A}$	1428.5	-3.2		
1433.7	19	1.90	$\nu_{6S} + \nu_{8S}$	1435.5	1.8		
1438.1	5	1.15					
1440.5	4	1.49					
1442.3	6	1.88	$\nu_{1S} + 2 \times \nu_{6S}$	1442.3	-0.0		
1452.7	10	1.67	$2 \times \nu_{1S} + \nu_{2S} + \nu_{6S}$	1455.3	2.6		
1459.3	21	2.02	$3 \times \nu_{1S} + 2 \times \nu_{2S}$	1468.3	9.0		
1467.6	4	1.22	$\nu_{1S} + 2 \times \nu_{3A} + 2 \times \nu_{3S}$	1469.4	1.8		
			$2 \times \nu_{1S} + \nu_{3S} + \nu_{5S}$	1467.5	-0.0		
1470.9	1	0.89	$\nu_{1S} + 2 \times \nu_{3A} + 2 \times \nu_{5A}$	1471.6	0.8		
1473.4	6	1.76	$\nu_{1S} + 2 \times \nu_{3A} + \nu_{8S}$	1473.5	0.0		
1475.5	8	1.49	$3 \times \nu_{1S} + \nu_{7S}$	1472.4	-3.1		
1478.4	3	1.00	$2 \times \nu_{1S} + 2 \times \nu_{3A} + \nu_{6S}$	1480.2	1.8		
1483.3	5	1.29	$\nu_{1S} + \nu_{15S}$	1483.0	-0.3		
1485.3	10	1.83	$\nu_{3S} + \nu_{2S} + \nu_{7S}$	1486.0	0.7		
1488.6	2	1.64					
1493.5	3	1.45					
1495.8	6	1.74					
1499.3	2	1.55					
1502.8	5	1.91	$\nu_{1S} + 3 \times \nu_{3S}$	1508.4	5.6		
1509.8	17	1.75	$\nu_{1S} + \nu_{3S} + 2 \times \nu_{5A}$	1510.7	0.9		
			$\nu_{1S} + \nu_{7S} + \nu_{5S}$	1509.1	-0.7		
1512.7	17	1.35	$\nu_{1S} + \nu_{3S} + \nu_{8S}$	1512.5	-0.2		
			$\nu_{1S} + \nu_{7S} + \nu_{5S}$	1509.1	-3.6		
1517.6	7	1.28	$2 \times \nu_{1S} + \nu_{3S} + \nu_{6S}$	1519.3	1.7		
1527.4	3	1.63	$3 \times \nu_{1S} + \nu_{3S} + \nu_{2S}$	1532.3	4.8		
			$6 \times \nu_{1S}$	1518.7	-8.7		
1529.7	3	1.42					
1531.9	18	2.61	$\nu_{1S} + \nu_{2S} + \nu_{3S} + \nu_{4S}$	1527.7	-4.2		
			$\nu_{3S} + \nu_{11S}$	1537.3	5.2		
			$3 \times \nu_{1S} + \nu_{2S} + \nu_{3S}$	1532.2	0.3		
1542.0	3	1.56					
1547.6	12	2.01	$2 \times \nu_{3S} + \nu_{7S}$	1550.0	2.3		
1552.2	7	1.22	$\nu_{7S} + 2 \times \nu_{5A}$	1552.2	-0.0		
1554.2	5	1.15	$\nu_{7S} + \nu_{8S}$	1554.0	-0.2		
1557.6	2	1.37	$\nu_{1S} + \nu_{6S} + \nu_{7S}$	1560.8	3.1		

In column 6:  $\Delta \nu = \Sigma \nu_{\text{fund}} - \Delta \nu_{\text{osc}}$

**bold** – fundamental frequencies or overtones  $\nu_0^2$  of out-of-plane vibrations,

*italic* – comments to the assignment

(\*) – indicates discrepancies between the assignment of Wu et al.[8] and the assignment proposed in this work