

Supplementary Information for

Structural motifs of 2-(2-fluoro-phenyl)-ethylamine conformers

Nitzan Mayorkas,^a Hanan Sachs,^a Markus Schütz,^b Shunichi Ishiuchi,^c Masaaki Fujii,^c Otto Dopfer,^b and Ilana Bar^{,a}*

Table S1. Vibrational transition frequencies^a (cm^{-1}) and intensities (arb. units) as obtained from the measured ionization-loss stimulated Raman and calculated Raman spectra of the five conformers (G2h, G1h, A1h, G1f, A2) of 2-(2-fluoro-phenyl)-ethylamine.

G2h				G1h				A1h			
ILSR		Raman		ILSR		Raman		ILSR		Raman	
Frequenc	Intensit										
3408.5	0.29	3615.6	0.18	3413.5	0.38	3624.3	0.40	3416.7	0.60	3624.2	0.48
3344.2	0.63	3531.1	0.51	3346.3	0.96	3539.1	0.78	3349.2	0.87	3539.9	0.98
3101.2	0.32	3236.2	1.59	3100.9	0.25	3235.2	1.64	3100.2	0.25	3234.2	1.70
3084.3	1.00	3226.2	0.64	3082.6	1.00	3225.8	0.60	3083.4	1.00	3225.2	0.58
3074.6	0.61	3213.5	0.52	3073.0	0.53	3213.1	0.54	3072.8	0.54	3212.2	0.54
3059.3	0.45	3195.7	0.37	3058.9	0.37	3200.0	0.33	3059.5	0.56	3196.0	0.39
2948.4	0.96	3122.9	0.33	3025.7	0.16	3135.2	0.39	3029.4	0.27	3130.0	0.25
2930.6	0.45	3111.7	0.98	2967.3	0.67	3102.7	1.51	2968.2	0.48	3093.1	0.35
2889.6	0.61	3074.1	1.24	2946.2	0.80	3082.0	0.65	2946.9	0.47	3069.9	1.05
2864.7	0.43	3064.8	0.89	2927.1	0.47	3015.5	0.78	2926.5	0.48	3019.4	0.71
1623.8	0.98	1690.1	0.51	2871.2	0.49	1690.0	0.52	2871.6	0.50	1691.6	0.64
1595.3	0.37	1664.7	0.06	1625.2	0.79	1659.7	0.13	1626.5	0.46	1661.6	0.07
1495.0	0.22	1659.9	0.14	1595.3	0.22	1656.2	0.15	1593.9	0.29	1658.7	0.14
1466.6	0.33	1542.2	0.05	1483.7	0.21	1542.6	0.05	1480.5	0.25	1543.6	0.05
1409.3	0.25	1504.3	0.09	1442.8	0.16	1518.3	0.19	1451.0	0.25	1521.3	0.08
1361.6	0.29	1495.7	0.09	1389.3	0.21	1500.2	0.01	1429.1	0.23	1503.1	0.06
1352.0	0.21	1484.0	0.13	1340.4	0.78	1479.7	0.14	1390.4	0.23	1489.3	0.22
1331.4	0.74	1393.6	0.28	1318.5	0.21	1419.3	0.07	1325.1	0.23	1428.3	0.22
1240.7	1.00	1391.0	0.05	1299.5	0.18	1367.4	0.44	1242.7	0.66	1355.2	0.25
1215.4	0.86	1358.5	0.30	1238.2	0.87	1347.6	0.13	1233.3	0.39	1345.8	0.09
1139.0	0.27	1334.0	0.08	1202.0	0.15	1332.0	0.05	1107.5	0.34	1330.2	0.12
1067.5	0.25	1302.9	0.03	1154.8	0.13	1306.3	0.02	1071.7	0.39	1309.3	0.06
1037.3	1.51	1281.0	0.59	1142.1	0.34	1279.6	0.68	1039.3	1.16	1280.9	0.69
989.6	0.31	1245.1	0.49	1110.8	0.34	1229.0	0.14	1020.5	0.50	1260.1	0.06
903.6	0.22	1217.7	0.03	1085.5	0.25	1208.3	0.04	960.0	0.64	1217.3	0.08
868.7	0.61	1174.7	0.11	1054.1	0.31	1174.3	0.13	936.4	0.39	1174.4	0.13
843.4	0.68	1164.1	0.20	1040.0	1.28	1168.7	0.13	767.1	1.10	1164.1	0.08
825.7	0.18	1136.3	0.05	1027.4	0.56	1134.3	0.10	760.9	0.23	1134.1	0.11
778.0	0.53	1095.9	0.10	1016.1	0.37	1117.2	0.14	725.3	0.32	1111.5	0.22
749.5	0.14	1066.1	0.86	912.3	0.22	1068.0	0.74	552.6	0.46	1070.2	0.80
733.5	0.39	1012.2	0.18	877.7	0.66	1047.9	0.12			1048.1	0.16
725.7	0.61	1009.0	0.00	849.5	0.56	1009.4	0.00			1004.9	0.00
590.5	0.31	973.8	0.01	829.1	0.16	976.3	0.00			987.5	0.27
561.8	0.33	929.5	0.07	796.0	0.40	932.9	0.21			968.8	0.10

542.9	0.16	896.5	0.07	736.2	0.60	902.0	0.09		889.7	0.03
		867.8	0.21	726.7	0.90	873.6	0.16		867.5	0.02
		847.2	0.08	586.6	0.34	852.1	0.03		852.1	0.05
		835.5	0.31	558.4	0.49	839.9	0.20		801.0	0.67
		781.1	0.01	528.5	0.15	782.4	0.01		782.9	0.23
		749.6	0.60			756.7	0.42		779.8	0.03
		745.7	0.32			747.1	0.65		742.9	0.30
		600.4	0.15			601.0	0.16		617.0	0.17
		570.1	0.45			569.6	0.43		564.6	0.36
		539.2	0.18			537.7	0.19		545.3	0.23
		492.4	0.09			493.1	0.07		481.7	0.08
		441.1	0.06			445.6	0.03		457.7	0.03
		415.3	0.03			416.9	0.05		338.8	0.20
		346.1	0.09			342.3	0.09		324.3	0.11
		297.6	0.24			282.4	0.27		294.3	0.06
		275.7	0.14			265.9	0.02		245.7	0.13
		202.4	0.30			203.1	0.30		212.5	0.31
		146.8	0.28			144.5	0.31		109.0	0.58
		87.7	1.44			90.0	1.41		96.2	1.13
		55.4	2.31			43.2	2.60		60.2	0.90

G2f				A2			
ILSR		Raman		ILSR		Raman	
Frequency	Intensity	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
3408.1	0.38	3616.3	0.16	3412.8	0.27	3624.3	0.28
3348.3	0.76	3533.8	0.46	3349.2	0.74	3539.4	0.76
3101.0	0.38	3235.4	1.55	3096.1	0.28	3234.5	1.70
3083.4	1.00	3225.0	0.66	3083.8	1.00	3225.3	0.60
3071.8	0.63	3212.5	0.53	3071.4	0.51	3212.5	0.53
3058.4	0.50	3191.8	0.40	3058.9	0.50	3194.9	0.39
3039.2	0.34	3124.8	0.35	3043.0	0.27	3125.7	0.02
3029.2	0.25	3106.1	0.99	3028.0	0.27	3102.1	0.67
2964.9	0.57	3070.9	1.45	2960.7	0.25	3073.7	0.11
2943.1	0.86	3063.9	0.74	2937.7	0.73	3061.6	1.42
2882.9	0.66	1689.9	0.56	2909.4	0.52	1690.9	0.66
2872.1	0.40	1668.1	0.02	2884.7	0.37	1663.6	0.09
1626.7	0.39	1659.7	0.17	2866.1	0.43	1661.0	0.14
1458.1	0.20	1542.5	0.05	1626.1	0.51	1542.8	0.06
1450.3	0.15	1501.6	0.02	1585.7	0.31	1503.7	0.01
1365.5	0.25	1495.7	0.13	1498.2	0.27	1500.3	0.05
1329.2	0.29	1489.3	0.16	1445.3	0.28	1483.4	0.33
1307.1	0.23	1395.1	0.25	1361.3	0.33	1399.4	0.36
1285.2	0.29	1390.1	0.05	1325.4	0.24	1388.4	0.23
1241.2	0.43	1357.2	0.21	1292.6	0.30	1347.1	0.07
1236.3	0.62	1333.9	0.12	1281.8	0.25	1320.5	0.25
1219.0	0.31	1308.2	0.11	1238.2	0.59	1309.0	0.04
1214.4	0.20	1279.3	0.79	1130.6	0.19	1291.5	0.08
1185.9	0.16	1246.4	0.14	1083.9	0.38	1278.1	0.76
1152.8	0.16	1212.2	0.12	1082.5	0.38	1217.2	0.09
1138.7	0.15	1173.7	0.15	1032.6	0.90	1174.6	0.13
1104.2	0.17	1163.2	0.08	1017.0	0.55	1153.9	0.10
1074.3	0.16	1138.2	0.15	1007.6	0.30	1123.4	0.14
1034.9	0.81	1102.3	0.06	993.6	0.24	1101.1	0.02
1033.4	0.79	1064.6	0.80	950.0	0.31	1064.4	0.96
984.5	0.74	1011.6	0.01	934.4	0.27	1048.5	0.63
940.5	0.19	1006.5	0.34	867.5	0.24	1004.0	0.00
918.4	0.23	977.8	0.01	781.7	0.81	972.1	0.02
847.6	0.19	936.4	0.08	753.8	0.28	968.2	0.05

830.3	0.20	892.2	0.04	722.5	0.30	887.8	0.08
824.0	0.25	871.3	0.11	568.4	0.21	869.5	0.07
795.8	0.54	866.3	0.06	551.4	0.36	835.9	0.11
739.1	0.43	828.4	0.30			797.2	0.56
718.7	0.67	783.6	0.01			779.4	0.06
588.1	0.20	755.6	0.47			759.6	0.07
559.6	0.15	742.2	0.54			741.5	0.32
550.1	0.12	598.3	0.17			615.4	0.16
520.2	0.12	569.3	0.41			563.8	0.42
438.5	0.11	531.3	0.22			545.2	0.23
		503.1	0.07			480.2	0.13
		443.9	0.04			456.1	0.03
		422.1	0.06			332.7	0.41
		332.7	0.11			319.8	0.17
		305.4	0.27			299.0	0.06
		277.5	0.10			278.1	0.08
		206.4	0.33			211.3	0.31
		142.3	0.34			103.0	0.85
		88.4	1.56			93.7	0.75
		56.1	5.29			60.7	0.94

^a The frequencies of the calculated Raman spectra should be scaled with the factors 0.953 and 0.974, in the high ($>2750\text{ cm}^{-1}$) and low ($<1700\text{ cm}^{-1}$) frequency ranges, respectively.

Table S2. Intramolecular distances (\AA) between different atoms, between the N-H and the center of the π system, between the nitrogen carrying the lone pair and the hydrogen atom, and the nitrogen and fluorine atoms in the different conformers of 2-(2-fluoro-phenyl)-ethylamine.

	G1h	G1f	G2h	G2f	G3h	G3f	A2	A1f	A1h
N-H(19)... π	4.80	3.27	3.38	4.27	4.62	4.71	5.51	5.81	5.44
N-H(20)... π	3.29	4.78	4.38	3.37	4.71	4.17	5.49	5.47	5.80
N...F	4.29	3.49	4.23	3.23	4.41	3.00	5.16	4.31	4.33
N... π	3.91	3.92	4.01	3.98	4.02	3.85	5.16	5.13	5.13
N-H(19)...F	4.95	3.20	4.04	2.81	5.15	3.92	5.04	4.84	4.18
N-H(20)...F	4.07	4.46	4.95	2.96	4.92	2.60	4.22	5.05	4.98
C-H(9)... π	4.77	3.82	4.77	3.82	4.77	3.81	3.74	3.80	3.72
C-H(10)... π	3.80	4.78	3.79	4.78	3.69	4.78	3.77	3.73	3.80
C-H(14)...N	3.20	4.02	3.46	4.32	3.17	4.31	4.72	4.67	4.65
C-H(12)...N	2.67	3.39	2.80	3.45	2.65	3.39	2.79	2.68	2.66
C-H(13)...N	3.39	2.68	3.45	2.82	3.39	2.73	2.77	2.66	2.67
C-H(9)...N	2.08	2.15	2.08	2.07	2.15	2.07	2.08	2.08	2.15
C-H(10)...N	2.15	2.08	2.07	2.08	2.08	2.15	2.08	2.16	2.08
C-H(9)...F	4.06	4.52	3.99	4.29	3.96	4.21	2.69	2.65	2.69
C-H(10)...F	2.75	4.48	2.67	4.28	2.81	4.25	3.92	3.84	3.96
C-H(12)...F	3.83	3.69	3.83	3.78	3.80	3.79	3.83	3.83	3.83
C-H(13)...F	2.54	2.40	2.57	2.46	2.50	2.47	2.55	2.59	2.56
C-H(12)... π	3.46	3.46	3.46	3.46	3.46	3.46	3.47	3.46	3.47
C-H(13)... π (F side)	3.45	3.46	3.46	3.46	3.45	3.45	3.46	3.47	3.45