Supporting Information for

Vibrational excitation induced and spontaneous conformational changes in solid *para*-H_2 – diminished matrix effects

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Table S1. Geometry of *trans*-FA in Cartesian coordinates (in Å) as optimized at the B3LYP/cc-pVTZ level of theory.

	Coordinates (angstroms)		
Atomic label	X	Y	Z
H	−0.653873	−1.341004	0.000000
O	−1.028176	−0.445958	0.000000
O	1.158081	0.117622	0.000000
C	0.000000	0.420204	0.000000
H	−0.385365	1.446471	0.000000

Table S2. Geometry of *cis*-FA in Cartesian coordinates (in Å) as optimized at the B3LYP/cc-pVTZ level of theory.

	Coordinates (angstroms)		
Atomic label	X	Y	Z
H	−1.774387	0.365731	0.001038
O	−1.056652	−0.279206	−0.000128
O	1.173407	−0.219111	0.000089
C	0.133552	0.360223	−0.000082
H	0.039031	1.459471	−0.000228

Table S3. Geometry of *trans*-AA in Cartesian coordinates (in Å) as optimized at the B3LYP/cc-pVTZ level of theory.

	Coordinates (angstroms)		
Atomic label	X	Y	Z
H	1.867442	0.355366	0.000000
O	1.243523	−0.385384	0.000000
O	−0.186783	1.344061	0.000000
C	0.000000	0.155508	0.000000
C	−1.062840	−0.905818	0.000000
H	−0.951127	−1.542045	0.877971
H	−2.042061	−0.438832	0.000000
H	−0.951127	−1.542045	−0.877971

Table S4. Geometry of *cis*-AA in Cartesian coordinates (in Å) as optimized at the B3LYP/cc-pVTZ level of theory.

	Coordinates (angstroms)		
Atomic label	X	Y	Z
H	1.413022	−1.117201	0.000000
O	1.317461	−0.158058	0.000000
O	−0.310033	1.347835	0.000000
C	0.000000	0.192609	0.000000
C	−0.973295	−0.965428	0.000000
H	−0.821869	−1.590139	0.882544
H	−1.988940	−0.583823	0.000000
H	−0.821869	−1.590139	−0.882544

Table S5. Geometry of glycine conformer **I** in Cartesian coordinates (in Angstrom units) as optimized at the B3LYP/cc-pVTZ level of theory.

	Coordinates (angstroms)		
Atomic label	X	Y	Z
N	0.411615	−1.927211	0.000000
C	−0.564547	−0.858984	0.000000
C	0.000000	0.553087	0.000000
O	1.168657	0.840010	0.000000
H	1.017779	−1.845176	0.807364
H	−1.219969	−0.950538	−0.869135
H	−1.219969	−0.950538	0.869135
O	−0.985122	1.480861	0.000000
H	1.017779	−1.845176	−0.807364
H	−0.557923	2.350320	0.000000

Table S6. Geometry of glycine conformer **III** in Cartesian coordinates (in Angstrom units) as optimized at the B3LYP/cc-pVTZ level of theory.

	Coordinates (angstroms)		
Atomic label	X	Y	Z
N	−0.633960	−0.098376	0.000111
C	−1.669036	−0.711691	−0.000073
C	−0.587135	1.255555	0.000000
O	−1.506535	1.561148	−0.000096
H	0.743893	−0.749902	0.000086
H	0.762436	−1.411804	−0.867953
H	0.762544	−1.411596	0.868284
O	1.927758	0.087724	−0.000078
H	1.938463	0.693379	−0.810731
H	1.938558	0.693555	0.810441

Table S7. Harmonic and anharmonic vibrational frequencies and their intensities of *trans*-FA as computed at the B3LYP/cc-pVTZ level of theory.

Mode (quanta)	ν_{harm} (cm^{-1})	ν_{anharm} (cm^{-1})	I_{harm} (km mol^{-1})	I_{anharm} (km mol^{-1})
1(1)	1055.0	1034.8	1.5	1.1
2(1)	685.9	618.1	138.9	135.7
3(1)	3723.8	3518.8	55.0	45.0
4(1)	3046.9	2886.8	47.7	46.8
5(1)	1826.2	1792.4	339.9	322.5
6(1)	1405.7	1374.9	2.6	2.4
7(1)	1306.9	1279.7	8.6	12.2
8(1)	1125.7	1093.1	249.9	246.3
9(1)	629.9	622.7	43.9	41.7
1(2)	2110.0	2064.0		0.1
2(2)	1371.9	1169.5		3.2
3(2)	7447.5	6857.0		3.7
4(2)	6093.9	5643.6		0.5
5(2)	3652.4	3565.6		3.7
6(2)	2811.3	2726.9		1.0
7(2)	2613.8	2513.4		1.1
8(2)	2251.3	2174.7		4.7
9(2)	1259.9	1246.6		0.2
2(1) 1(1)	1741.0	1651.4		0.3
3(1) 1(1)	4778.8	4552.1		0.0
3(1) 2(1)	4409.7	4123.7		0.8
4(1) 1(1)	4101.9	3903.3		0.0
4(1) 2(1)	3732.9	3502.0		0.0
4(1) 3(1)	6770.7	6401.9		0.1
5(1) 1(1)	2881.2	2821.6		0.2
5(1) 2(1)	2512.2	2409.5		0.0
5(1) 3(1)	5550.0	5310.4		0.5
5(1) 4(1)	4873.1	4668.8		1.2
6(1) 1(1)	2460.7	2408.6		0.0
6(1) 2(1)	2091.6	1985.9		0.0
6(1) 3(1)	5129.4	4885.5		0.4
6(1) 4(1)	4452.6	4238.4		0.0
6(1) 5(1)	3231.9	3162.6		1.0
7(1) 1(1)	2361.9	2296.8		0.0
7(1) 2(1)	1992.9	1867.8		0.0
7(1) 3(1)	5030.7	4761.4		1.1
7(1) 4(1)	4353.8	4146.2		0.4
7(1) 5(1)	3133.1	3055.7		3.6
7(1) 6(1)	2712.6	2627.5		0.1
8(1) 1(1)	2180.7	2124.3		0.0
8(1) 2(1)	1811.6	1703.2		0.1
8(1) 3(1)	4849.4	4610.9		0.1
8(1) 4(1)	4172.6	3977.6		0.4
8(1) 5(1)	2951.9	2881.1		1.7
8(1) 6(1)	2531.3	2458.1		0.2
8(1) 7(1)	2432.6	2342.6		2.6
9(1) 1(1)	1684.9	1657.2		0.0
9(1) 2(1)	1315.9	1240.5		0.0

9(1) 3(1)	4353.7	4137.2		0.2
9(1) 4(1)	3676.9	3509.9		0.2
9(1) 5(1)	2456.1	2408.7		0.0
9(1) 6(1)	2035.6	1993.6		0.1
9(1) 7(1)	1936.8	1883.5		2.3
9(1) 8(1)	1755.6	1712.8		1.0

Table S8. Harmonic and anharmonic vibrational frequencies and their intensities of *cis*-FA as computed at the B3LYP/cc-pVTZ level of theory.

Mode (quanta)	ν_{harm} (cm^{-1})	ν_{anharm} (cm^{-1})	I_{harm} (km mol^{-1})	I_{anharm} (km mol^{-1})
1(1)	3789.5	3587.8	54.1	43.9
2(1)	2953.9	2714.1	88.5	91.3
3(1)	1871.4	1836.5	280.4	264.2
4(1)	1420.5	1390.0	0.4	1.0
5(1)	1275.9	1225.9	308.9	305.7
6(1)	1111.5	1082.3	50.0	44.4
7(1)	1036.9	1018.4	0.1	0.0
8(1)	662.1	653.3	9.3	8.8
9(1)	534.4	443.0	84.1	80.6
1(2)	7579.1	6998.0		4.7
2(2)	5907.8	5417.8		0.4
3(2)	3742.9	3653.6		5.1
4(2)	2841.0	2847.4		1.5
5(2)	2551.8	2428.2		1.1
6(2)	2223.0	2150.7		3.3
7(2)	2073.7	2031.5		0.2
8(2)	1324.3	1306.8		0.2
9(2)	1068.7	818.2		4.7
2(1) 1(1)	6743.4	6367.5		0.1
3(1) 1(1)	5661.0	5421.1		0.0
3(1) 2(1)	4825.3	4613.5		1.4
4(1) 1(1)	5210.1	4976.0		0.0
4(1) 2(1)	4374.4	4112.3		0.1
4(1) 3(1)	3291.9	3223.5		0.8
5(1) 1(1)	5065.5	4802.2		1.2
5(1) 2(1)	4229.8	4005.0		0.5
5(1) 3(1)	3147.4	3057.6		0.3
5(1) 4(1)	2696.4	2614.3		0.4
6(1) 1(1)	4901.0	4661.6		0.1
6(1) 2(1)	4065.4	3857.7		0.9
6(1) 3(1)	2982.9	2911.4		0.4
6(1) 4(1)	2532.0	2466.7		0.4
6(1) 5(1)	2387.4	2294.1		5.7
7(1) 1(1)	4826.4	4605.9		0.0
7(1) 2(1)	3990.7	3780.4		0.3
7(1) 3(1)	2908.3	2848.6		0.3
7(1) 4(1)	2457.4	2410.2		0.0
7(1) 5(1)	2312.8	2240.7		0.0
7(1) 6(1)	2148.3	2094.8		0.1

8(1)	1(1)	4451.7	4238.5		0.4
8(1)	2(1)	3616.0	3431.8		0.1
8(1)	3(1)	2533.6	2484.9		0.0
8(1)	4(1)	2082.7	2043.3		0.0
8(1)	5(1)	1938.1	1876.7		0.4
8(1)	6(1)	1773.6	1728.5		6.6
8(1)	7(1)	1699.0	1671.2		0.0
9(1)	1(1)	4323.9	4006.7		0.4
9(1)	2(1)	3488.2	3223.3		0.0
9(1)	3(1)	2405.8	2277.0		0.0
9(1)	4(1)	1954.9	1830.2		0.0
9(1)	5(1)	1810.3	1651.5		0.4
9(1)	6(1)	1645.9	1516.0		0.0
9(1)	7(1)	1571.2	1463.8		1.5
9(1)	8(1)	1196.5	1094.4		0.0

Table S9. Harmonic and anharmonic vibrational frequencies and their intensities of *trans*-AA as computed at the B3LYP/cc-pVTZ level of theory.

Mode (quanta)	v_{harm} (cm^{-1})	v_{anharm} (cm^{-1})	I_{harm} (km mol^{-1})	I_{anharm} (km mol^{-1})
1(1)	3744.4	3546.1	55.3	45.1
2(1)	3161.8	3007.1	5.1	4.1
3(1)	3053.3	2944.5	1.8	1.9
4(1)	1825.1	1791.3	313.3	278.3
5(1)	1473.1	1434.0	15.5	12.1
6(1)	1409.2	1374.8	53.2	32.9
7(1)	1342.6	1331.4	26.9	37.3
8(1)	1205.4	1165.3	210.7	190.9
9(1)	999.1	978.1	72.6	74.6
10(1)	860.2	842.7	3.4	3.2
11(1)	585.4	577.7	38.5	33.2
12(1)	423.0	424.3	4.3	4.5
13(1)	3110.0	2964.0	4.5	5.8
14(1)	1478.5	1426.3	8.4	6.9
15(1)	1070.3	1053.7	7.6	7.1
16(1)	670.6	655.3	90.6	69.8
17(1)	546.4	536.6	25.2	32.6
18(1)	73.2	64.9	0.3	0.1
1(2)	7488.8	6914.6		4.0
2(2)	6323.6	5924.6		0.4
3(2)	6106.7	5819.4		0.1
4(2)	3650.2	3563.5		3.0
5(2)	2946.2	2848.6		0.1
6(2)	2818.3	2734.4		0.1
7(2)	2685.1	2600.4		0.1
8(2)	2410.7	2320.6		0.6
9(2)	1998.2	1953.9		1.4
10(2)	1720.4	1679.2		5.0
11(2)	1170.8	1156.1		0.1
12(2)	845.9	849.8		0.2

13(2)		6220.0	5873.4	0.3
14(2)		2957.1	2860.0	0.3
15(2)		2140.7	2091.2	0.1
16(2)		1341.2	1273.2	18.9
17(2)		1092.8	1071.5	0.9
18(2)		146.3	120.7	0.1
2(1)	1(1)	6906.2	6553.1	0.0
3(1)	1(1)	6797.8	6476.7	0.0
3(1)	2(1)	6215.1	5895.2	0.1
4(1)	1(1)	5569.5	5335.9	0.7
4(1)	2(1)	4986.9	4796.7	0.2
4(1)	3(1)	4878.4	4720.5	0.1
5(1)	1(1)	5217.5	4980.2	0.0
5(1)	2(1)	4634.9	4429.6	0.5
5(1)	3(1)	4526.5	4343.4	0.0
5(1)	4(1)	3298.2	3224.4	0.1
6(1)	1(1)	5153.6	4917.5	0.2
6(1)	2(1)	4571.0	4377.4	0.2
6(1)	3(1)	4462.5	4316.4	0.0
6(1)	4(1)	3234.3	3164.7	0.1
6(1)	5(1)	2882.3	2805.2	0.3
7(1)	1(1)	5087.0	4836.2	0.5
7(1)	2(1)	4504.4	4306.4	0.1
7(1)	3(1)	4395.9	4233.8	0.2
7(1)	4(1)	3167.7	3093.4	0.7
7(1)	5(1)	2815.7	2736.5	0.0
7(1)	6(1)	2751.7	2671.8	0.4
8(1)	1(1)	4949.8	4704.3	0.4
8(1)	2(1)	4367.2	4168.9	0.1
8(1)	3(1)	4258.7	4095.2	0.2
8(1)	4(1)	3030.5	2951.9	1.0
8(1)	5(1)	2678.5	2597.2	0.1
8(1)	6(1)	2614.5	2535.9	0.2
8(1)	7(1)	2547.9	2458.7	1.6
9(1)	1(1)	4743.5	4522.8	0.1
9(1)	2(1)	4160.9	3980.4	0.1
9(1)	3(1)	4052.5	3905.5	0.1
9(1)	4(1)	2824.2	2766.9	0.0
9(1)	5(1)	2472.2	2410.3	0.1
9(1)	6(1)	2408.3	2349.5	0.5
9(1)	7(1)	2341.7	2278.6	0.5
9(1)	8(1)	2204.5	2139.2	2.2
10(1)	1(1)	4604.6	4386.0	0.1
10(1)	2(1)	4022.0	3850.2	0.0
10(1)	3(1)	3913.5	3773.4	0.0
10(1)	4(1)	2685.3	2636.4	0.4
10(1)	5(1)	2333.3	2276.1	0.0
10(1)	6(1)	2269.3	2208.3	0.8
10(1)	7(1)	2202.7	2142.4	0.0
10(1)	8(1)	2065.5	2003.7	1.6
10(1)	9(1)	1859.3	1818.2	1.3

11(1)	1(1)	4329.8	4121.5	0.1
11(1)	2(1)	3747.2	3585.0	0.0
11(1)	3(1)	3638.8	3508.2	0.0
11(1)	4(1)	2410.5	2363.3	0.1
11(1)	5(1)	2058.5	2011.5	0.0
11(1)	6(1)	1994.6	1947.5	0.2
11(1)	7(1)	1928.0	1880.1	2.1
11(1)	8(1)	1790.8	1740.7	1.8
11(1)	9(1)	1584.5	1555.7	0.1
11(1)	10(1)	1445.6	1423.6	10.9
12(1)	1(1)	4167.4	3969.2	0.1
12(1)	2(1)	3584.8	3431.4	0.1
12(1)	3(1)	3476.3	3354.9	0.0
12(1)	4(1)	2248.1	2213.8	0.2
12(1)	5(1)	1896.1	1860.6	0.0
12(1)	6(1)	1832.1	1798.8	13.1
12(1)	7(1)	1765.5	1727.5	0.7
12(1)	8(1)	1628.3	1588.4	0.6
12(1)	9(1)	1422.1	1399.7	1.9
12(1)	10(1)	1283.1	1265.0	0.1
12(1)	11(1)	1008.4	1002.8	0.2
13(1)	1(1)	6854.4	6515.3	0.0
13(1)	2(1)	6271.8	5955.2	0.2
13(1)	3(1)	6163.3	5800.0	0.2
13(1)	4(1)	4935.1	4758.9	0.0
13(1)	5(1)	4583.1	4386.4	0.1
13(1)	6(1)	4519.2	4338.5	0.1
13(1)	7(1)	4452.6	4270.1	0.4
13(1)	8(1)	4315.4	4134.0	0.2
13(1)	9(1)	4109.1	3942.3	0.0
13(1)	10(1)	3970.2	3812.8	0.0
13(1)	11(1)	3695.4	3546.8	0.0
13(1)	12(1)	3533.0	3393.3	0.0
14(1)	1(1)	5223.0	4982.2	0.0
14(1)	2(1)	4640.3	4425.2	0.2
14(1)	3(1)	4531.9	4365.9	0.2
14(1)	4(1)	3303.6	3226.7	0.0
14(1)	5(1)	2951.7	2864.7	0.0
14(1)	6(1)	2887.7	2806.4	0.2
14(1)	7(1)	2821.1	2739.7	0.0
14(1)	8(1)	2683.9	2599.8	0.0
14(1)	9(1)	2477.7	2406.8	0.1
14(1)	10(1)	2338.7	2278.2	0.0
14(1)	11(1)	2064.0	2013.8	0.0
14(1)	12(1)	1901.5	1860.7	0.0
14(1)	13(1)	4588.5	4396.5	0.2
15(1)	1(1)	4814.7	4592.8	0.0
15(1)	2(1)	4232.1	4050.4	0.0
15(1)	3(1)	4123.7	3970.9	0.3
15(1)	4(1)	2895.4	2835.3	0.0
15(1)	5(1)	2543.5	2475.4	0.0

15(1)	6(1)	2479.5	2418.0	0.2
15(1)	7(1)	2412.9	2349.4	0.1
15(1)	8(1)	2275.7	2210.9	0.0
15(1)	9(1)	2069.4	2024.4	0.0
15(1)	10(1)	1930.5	1887.7	0.0
15(1)	11(1)	1655.7	1624.4	0.0
15(1)	12(1)	1493.3	1475.4	0.0
15(1)	13(1)	4180.3	4008.5	0.1
15(1)	14(1)	2548.9	2478.1	0.1
16(1)	1(1)	4415.0	4199.4	0.5
16(1)	2(1)	3832.4	3661.7	0.0
16(1)	3(1)	3723.9	3584.8	0.0
16(1)	4(1)	2495.7	2445.2	0.0
16(1)	5(1)	2143.7	2088.7	0.0
16(1)	6(1)	2079.7	2034.4	0.0
16(1)	7(1)	2013.1	1955.2	0.0
16(1)	8(1)	1875.9	1810.3	0.0
16(1)	9(1)	1669.7	1633.0	0.0
16(1)	10(1)	1530.8	1496.5	0.0
16(1)	11(1)	1256.0	1235.2	0.0
16(1)	12(1)	1093.5	1080.1	0.0
16(1)	13(1)	3780.6	3623.1	0.1
16(1)	14(1)	2149.1	2090.1	0.0
16(1)	15(1)	1740.9	1702.3	0.2
17(1)	1(1)	4290.8	4079.7	0.5
17(1)	2(1)	3708.2	3542.9	0.0
17(1)	3(1)	3599.7	3467.0	0.0
17(1)	4(1)	2371.5	2326.5	0.1
17(1)	5(1)	2019.5	1968.8	0.0
17(1)	6(1)	1955.6	1911.5	0.0
17(1)	7(1)	1889.0	1841.3	0.0
17(1)	8(1)	1751.8	1701.3	0.1
17(1)	9(1)	1545.5	1518.4	0.7
17(1)	10(1)	1406.6	1377.9	0.0
17(1)	11(1)	1131.8	1113.4	0.0
17(1)	12(1)	969.4	962.3	0.0
17(1)	13(1)	3656.4	3505.7	0.1
17(1)	14(1)	2024.9	1968.8	0.1
17(1)	15(1)	1616.7	1584.9	0.3
17(1)	16(1)	1217.0	1184.4	3.1
18(1)	1(1)	3817.6	3608.4	0.0
18(1)	2(1)	3235.0	3058.8	0.1
18(1)	3(1)	3126.5	3000.4	0.0
18(1)	4(1)	1898.3	1854.8	0.0
18(1)	5(1)	1546.3	1497.6	0.9
18(1)	6(1)	1482.3	1446.5	0.1
18(1)	7(1)	1415.7	1370.1	0.0
18(1)	8(1)	1278.5	1228.5	0.1
18(1)	9(1)	1072.3	1039.3	0.1
18(1)	10(1)	933.4	908.3	0.1
18(1)	11(1)	658.6	638.3	11.6

18(1) 12(1)	496.1	492.4		0.3
18(1) 13(1)	3183.2	3043.8		2.7
18(1) 14(1)	1551.7	1501.7		0.4
18(1) 15(1)	1143.5	1106.7		1.3
18(1) 16(1)	743.7	733.5		0.1
18(1) 17(1)	619.6	600.0		3.3

Table S10. Harmonic and anharmonic vibrational frequencies and their intensities of *cis*-AA as computed at the B3LYP/cc-pVTZ level of theory.

Mode (quanta)	ν_{harm} (cm^{-1})	ν_{anharm} (cm^{-1})	I_{harm} (km mol^{-1})	I_{anharm} (km mol^{-1})
1(1)	3800.6	3607.8	42.7	34.1
2(1)	3156.1	3007.9	4.0	4.5
3(1)	3035.0	2935.5	4.7	5.9
4(1)	1860.1	1824.3	275.1	233.9
5(1)	1474.5	1433.3	6.2	6.9
6(1)	1395.8	1364.9	47.4	30.3
7(1)	1297.3	1247.8	383.7	389.7
8(1)	1204.8	1163.6	4.6	1.7
9(1)	987.7	972.0	11.6	10.8
10(1)	855.6	834.7	27.5	29.1
11(1)	598.9	591.5	6.3	5.2
12(1)	431.5	435.3	4.0	3.9
13(1)	3090.0	2948.8	7.8	9.3
14(1)	1487.8	1447.3	7.8	6.0
15(1)	1064.7	1038.8	4.9	4.7
16(1)	598.8	590.6	1.7	0.5
17(1)	474.1	457.6	97.1	93.2
18(1)	112.1	53.1	0.3	0.3
1(2)	7601.3	7043.4		3.9
2(2)	6312.3	5916.7		0.4
3(2)	6069.9	5763.0		0.1
4(2)	3720.2	3629.4		4.6
5(2)	2948.9	2840.6		0.0
6(2)	2791.6	2712.7		0.1
7(2)	2594.6	2481.7		0.4
8(2)	2409.7	2329.0		0.1
9(2)	1975.3	1930.0		2.9
10(2)	1711.1	1663.4		1.5
11(2)	1197.8	1182.6		0.8
12(2)	863.1	871.9		0.1
13(2)	6180.0	5832.5		0.3
14(2)	2975.7	2883.2		0.1
15(2)	2129.3	2074.8		0.1
16(2)	1197.7	1185.9		3.2
17(2)	948.3	906.4		6.9
18(2)	224.2	48.9		0.0
2(1) 1(1)	6956.8	6615.3		0.0
3(1) 1(1)	6835.6	6512.1		0.0
3(1) 2(1)	6191.1	5883.2		0.1

4(1)	1(1)	5660.7	5428.9	0.1
4(1)	2(1)	5016.2	4831.6	0.2
4(1)	3(1)	4895.0	4727.7	0.1
5(1)	1(1)	5275.1	5041.1	0.1
5(1)	2(1)	4630.6	4429.4	0.4
5(1)	3(1)	4509.4	4316.2	0.1
5(1)	4(1)	3334.5	3256.8	0.1
6(1)	1(1)	5196.4	4972.3	0.0
6(1)	2(1)	4551.9	4366.8	0.2
6(1)	3(1)	4430.7	4279.5	0.1
6(1)	4(1)	3255.9	3188.7	0.0
6(1)	5(1)	2870.2	2793.9	0.2
7(1)	1(1)	5097.9	4853.1	1.0
7(1)	2(1)	4453.4	4255.2	0.1
7(1)	3(1)	4332.2	4153.9	0.2
7(1)	4(1)	3157.4	3071.1	1.0
7(1)	5(1)	2771.7	2681.9	0.1
7(1)	6(1)	2693.1	2612.8	0.1
8(1)	1(1)	5005.5	4765.2	0.2
8(1)	2(1)	4361.0	4171.2	0.1
8(1)	3(1)	4239.8	4072.2	0.2
8(1)	4(1)	3064.9	2987.2	0.4
8(1)	5(1)	2679.3	2598.9	0.1
8(1)	6(1)	2600.6	2530.8	0.2
8(1)	7(1)	2502.1	2401.0	3.0
9(1)	1(1)	4788.3	4572.7	0.1
9(1)	2(1)	4143.8	3969.0	0.0
9(1)	3(1)	4022.6	3868.1	0.1
9(1)	4(1)	2847.7	2786.1	0.1
9(1)	5(1)	2462.1	2397.4	0.2
9(1)	6(1)	2383.4	2328.9	0.3
9(1)	7(1)	2284.9	2210.2	1.8
9(1)	8(1)	2192.5	2131.2	1.2
10(1)	1(1)	4656.2	4441.6	0.0
10(1)	2(1)	4011.7	3842.8	0.0
10(1)	3(1)	3890.5	3739.7	0.0
10(1)	4(1)	2715.6	2660.9	0.2
10(1)	5(1)	2330.0	2267.5	0.0
10(1)	6(1)	2251.3	2193.9	0.8
10(1)	7(1)	2152.8	2076.7	1.1
10(1)	8(1)	2060.4	1997.2	0.6
10(1)	9(1)	1843.2	1796.3	22.9
11(1)	1(1)	4399.5	4197.7	0.3
11(1)	2(1)	3755.0	3599.6	0.0
11(1)	3(1)	3633.8	3495.9	0.0
11(1)	4(1)	2459.0	2412.0	0.0
11(1)	5(1)	2073.3	2024.8	0.0
11(1)	6(1)	1994.7	1953.9	0.2
11(1)	7(1)	1896.2	1838.3	0.3
11(1)	8(1)	1803.7	1756.5	6.0
11(1)	9(1)	1586.5	1557.0	0.1

11(1)	10(1)	1454.4	1426.2	6.7
12(1)	1(1)	4232.2	4043.1	0.0
12(1)	2(1)	3587.7	3442.8	0.1
12(1)	3(1)	3466.5	3339.9	0.0
12(1)	4(1)	2291.6	2258.1	0.2
12(1)	5(1)	1906.0	1871.6	0.0
12(1)	6(1)	1827.3	1800.8	0.2
12(1)	7(1)	1728.8	1682.1	1.3
12(1)	8(1)	1636.4	1601.8	0.3
12(1)	9(1)	1419.2	1398.7	0.5
12(1)	10(1)	1287.1	1269.3	0.0
12(1)	11(1)	1030.4	1027.2	0.0
13(1)	1(1)	6890.6	6556.6	0.0
13(1)	2(1)	6246.1	5946.3	0.1
13(1)	3(1)	6124.9	5747.1	0.2
13(1)	4(1)	4950.1	4772.0	0.0
13(1)	5(1)	4564.4	4367.5	0.1
13(1)	6(1)	4485.8	4305.7	0.2
13(1)	7(1)	4387.3	4198.3	0.3
13(1)	8(1)	4294.8	4116.9	0.2
13(1)	9(1)	4077.6	3911.0	0.0
13(1)	10(1)	3945.5	3784.9	0.0
13(1)	11(1)	3688.9	3540.5	0.0
13(1)	12(1)	3521.5	3384.3	0.0
14(1)	1(1)	5288.5	5056.7	0.0
14(1)	2(1)	4644.0	4439.6	0.2
14(1)	3(1)	4522.8	4337.3	0.2
14(1)	4(1)	3347.9	3272.6	0.0
14(1)	5(1)	2962.3	2874.6	0.2
14(1)	6(1)	2883.6	2809.9	0.2
14(1)	7(1)	2785.1	2697.9	0.0
14(1)	8(1)	2692.7	2616.0	0.0
14(1)	9(1)	2475.5	2410.6	0.1
14(1)	10(1)	2343.4	2283.1	0.0
14(1)	11(1)	2086.7	2040.6	0.0
14(1)	12(1)	1919.4	1885.4	0.0
14(1)	13(1)	4577.8	4391.0	0.2
15(1)	1(1)	4865.3	4646.2	0.0
15(1)	2(1)	4220.8	4043.7	0.0
15(1)	3(1)	4099.6	3936.5	0.3
15(1)	4(1)	2924.8	2860.6	0.0
15(1)	5(1)	2539.1	2466.4	0.0
15(1)	6(1)	2460.4	2399.7	0.1
15(1)	7(1)	2362.0	2286.4	0.0
15(1)	8(1)	2269.5	2206.0	0.0
15(1)	9(1)	2052.3	2003.5	0.0
15(1)	10(1)	1920.2	1871.6	0.0
15(1)	11(1)	1663.6	1629.7	0.0
15(1)	12(1)	1496.2	1479.9	0.0
15(1)	13(1)	4154.6	3980.4	0.1
15(1)	14(1)	2552.5	2482.9	0.1

16(1)	1(1)	4399.5	4196.2	0.1
16(1)	2(1)	3755.0	3597.4	0.0
16(1)	3(1)	3633.8	3494.3	0.0
16(1)	4(1)	2458.9	2411.3	0.0
16(1)	5(1)	2073.3	2022.5	0.0
16(1)	6(1)	1994.6	1956.6	0.0
16(1)	7(1)	1896.1	1838.3	0.1
16(1)	8(1)	1803.7	1757.5	0.0
16(1)	9(1)	1586.5	1560.0	0.2
16(1)	10(1)	1454.4	1423.7	0.0
16(1)	11(1)	1197.7	1181.4	0.0
16(1)	12(1)	1030.4	1026.9	0.0
16(1)	13(1)	3688.8	3538.5	0.1
16(1)	14(1)	2086.7	2036.3	0.1
16(1)	15(1)	1663.5	1630.2	0.3
17(1)	1(1)	4274.8	4046.5	0.5
17(1)	2(1)	3630.3	3465.1	0.0
17(1)	3(1)	3509.1	3362.9	0.0
17(1)	4(1)	2334.2	2281.9	0.0
17(1)	5(1)	1948.6	1889.1	0.0
17(1)	6(1)	1869.9	1822.5	0.0
17(1)	7(1)	1771.4	1703.1	0.2
17(1)	8(1)	1679.0	1629.4	0.0
17(1)	9(1)	1461.8	1419.5	0.9
17(1)	10(1)	1329.7	1291.1	0.0
17(1)	11(1)	1073.0	1050.8	0.2
17(1)	12(1)	905.7	891.7	0.0
17(1)	13(1)	3564.1	3407.3	0.0
17(1)	14(1)	1962.0	1908.2	0.0
17(1)	15(1)	1538.8	1497.5	1.0
17(1)	16(1)	1073.0	1044.1	1.3
18(1)	1(1)	3912.7	3662.9	0.0
18(1)	2(1)	3268.2	3055.7	0.0
18(1)	3(1)	3147.0	2960.2	0.0
18(1)	4(1)	1972.2	1874.9	0.0
18(1)	5(1)	1586.5	1482.4	0.7
18(1)	6(1)	1507.9	1415.5	0.1
18(1)	7(1)	1409.4	1302.3	0.0
18(1)	8(1)	1316.9	1219.1	0.0
18(1)	9(1)	1099.7	1023.0	0.7
18(1)	10(1)	967.6	886.0	0.0
18(1)	11(1)	711.0	643.0	0.0
18(1)	12(1)	543.6	499.2	0.1
18(1)	13(1)	3202.1	3006.4	1.6
18(1)	14(1)	1599.9	1500.6	0.7
18(1)	15(1)	1176.7	1084.3	0.7
18(1)	16(1)	710.9	642.7	0.1
18(1)	17(1)	586.2	509.7	0.5

Table S11. Harmonic and anharmonic vibrational frequencies and their intensities of glycine conformer **I** as computed at the B3LYP/cc-pVTZ level of theory.

Mode (quanta)	ν_{harm} (cm^{-1})	ν_{anharm} (cm^{-1})	I_{harm} (km mol^{-1})	I_{anharm} (km mol^{-1})
1(1)	3738.9	3533.4	53.4	40.5
2(1)	3499.7	3358.4	1.3	0.4
3(1)	3040.0	2924.2	17.9	18.5
4(1)	1820.2	1784.2	278.5	236.0
5(1)	1677.3	1654.6	18.5	19.5
6(1)	1458.8	1429.0	14.6	8.5
7(1)	1398.7	1360.9	15.5	12.3
8(1)	1311.3	1277.7	11.6	19.2
9(1)	1161.3	1115.5	111.8	57.2
10(1)	1123.7	1084.4	181.4	183.9
11(1)	922.0	841.6	137.7	55.7
12(1)	821.6	783.8	83.5	157.0
13(1)	637.6	628.9	6.7	3.4
14(1)	463.5	454.7	28.6	28.2
15(1)	259.6	248.9	9.6	10.0
16(1)	3568.3	3399.9	3.3	1.3
17(1)	3069.6	2917.0	7.6	10.2
18(1)	1387.0	1346.9	0.1	0.0
19(1)	1188.3	1156.1	1.2	0.2
20(1)	920.5	905.2	3.5	4.6
21(1)	658.1	603.9	89.0	64.4
22(1)	510.4	484.5	30.8	52.6
23(1)	215.5	17.9	42.1	5.0
24(1)	57.7	69.0	5.5	35.9
1(2)	7477.7	6885.2		5.0
2(2)	6999.4	6583.2		1.0
3(2)	6080.0	5732.5		0.2
4(2)	3640.5	3548.3		2.7
5(2)	3354.5	3218.5		0.0
6(2)	2917.7	2827.1		0.3
7(2)	2797.5	2701.9		0.5
8(2)	2622.6	2521.7		0.3
9(2)	2322.6	2225.0		0.4
10(2)	2247.4	2162.0		0.9
11(2)	1843.9	1658.7		1.4
12(2)	1643.1	1557.5		0.4
13(2)	1275.3	1257.8		0.1
14(2)	926.9	910.6		33.4
15(2)	519.2	497.7		0.2
16(2)	7136.7	6711.9		0.8
17(2)	6139.2	5777.1		0.4
18(2)	2774.0	2689.9		0.0
19(2)	2376.5	2309.9		0.1
20(2)	1841.0	1812.1		12.3
21(2)	1316.2	1168.7		7.8
22(2)	1020.9	970.0		1.0
23(2)	431.0	-91.7		0.2
24(2)	115.4	173.1		0.5

2(1)	1(1)	7238.5	6863.4	0.0
3(1)	1(1)	6778.8	6430.1	0.0
3(1)	2(1)	6539.7	6225.6	0.0
4(1)	1(1)	5559.1	5316.2	0.7
4(1)	2(1)	5319.9	5114.5	0.0
4(1)	3(1)	4860.2	4679.1	0.0
5(1)	1(1)	5416.1	5158.7	0.0
5(1)	2(1)	5176.9	4919.7	0.0
5(1)	3(1)	4717.2	4519.0	0.0
5(1)	4(1)	3497.5	3409.1	0.3
6(1)	1(1)	5197.7	4962.6	0.0
6(1)	2(1)	4958.5	4758.3	0.0
6(1)	3(1)	4498.8	4293.8	0.2
6(1)	4(1)	3279.1	3212.4	0.0
6(1)	5(1)	3136.1	3054.4	0.0
7(1)	1(1)	5137.6	4886.0	0.4
7(1)	2(1)	4898.4	4687.8	0.1
7(1)	3(1)	4438.7	4265.8	0.2
7(1)	4(1)	3219.0	3140.9	0.0
7(1)	5(1)	3076.0	2984.8	1.7
7(1)	6(1)	2857.6	2786.1	0.2
8(1)	1(1)	5050.1	4783.9	0.6
8(1)	2(1)	4811.0	4595.1	0.1
8(1)	3(1)	4351.3	4164.1	0.0
8(1)	4(1)	3131.5	3046.0	0.5
8(1)	5(1)	2988.5	2889.5	0.1
8(1)	6(1)	2770.1	2693.7	0.0
8(1)	7(1)	2710.0	2611.6	0.3
9(1)	1(1)	4900.1	4647.1	0.0
9(1)	2(1)	4661.0	4444.6	0.2
9(1)	3(1)	4201.3	4011.1	0.4
9(1)	4(1)	2981.5	2898.4	0.3
9(1)	5(1)	2838.5	2738.7	0.1
9(1)	6(1)	2620.1	2543.9	0.1
9(1)	7(1)	2560.0	2468.2	0.3
9(1)	8(1)	2472.6	2373.7	0.8
10(1)	1(1)	4862.6	4616.5	0.0
10(1)	2(1)	4623.4	4413.1	0.0
10(1)	3(1)	4163.7	3982.0	0.1
10(1)	4(1)	2943.9	2866.9	0.5
10(1)	5(1)	2801.0	2707.6	0.1
10(1)	6(1)	2582.6	2511.9	0.0
10(1)	7(1)	2522.5	2438.4	0.6
10(1)	8(1)	2435.0	2342.0	0.7
10(1)	9(1)	2285.0	2188.4	1.5
11(1)	1(1)	4660.8	4373.9	0.1
11(1)	2(1)	4421.7	4181.5	0.3
11(1)	3(1)	3962.0	3736.8	0.1
11(1)	4(1)	2742.2	2626.3	0.1
11(1)	5(1)	2599.2	2449.2	0.0
11(1)	6(1)	2380.8	2269.5	0.0

11(1)	7(1)	2320.7	2196.3	0.8
11(1)	8(1)	2233.3	2105.1	0.2
11(1)	9(1)	2083.3	1942.4	1.5
11(1)	10(1)	2045.7	1917.7	0.7
12(1)	1(1)	4560.4	4313.7	0.1
12(1)	2(1)	4321.3	4116.4	0.1
12(1)	3(1)	3861.6	3679.7	0.1
12(1)	4(1)	2641.8	2567.7	0.2
12(1)	5(1)	2498.8	2406.2	0.0
12(1)	6(1)	2280.4	2212.0	0.1
12(1)	7(1)	2220.3	2136.1	0.3
12(1)	8(1)	2132.9	2046.9	0.2
12(1)	9(1)	1982.9	1895.2	0.5
12(1)	10(1)	1945.3	1865.6	1.1
12(1)	11(1)	1743.5	1584.4	6.6
13(1)	1(1)	4376.5	4160.7	0.1
13(1)	2(1)	4137.3	3958.7	0.0
13(1)	3(1)	3677.6	3525.3	0.0
13(1)	4(1)	2457.9	2408.4	0.0
13(1)	5(1)	2314.9	2255.5	0.0
13(1)	6(1)	2096.5	2057.6	0.0
13(1)	7(1)	2036.4	1984.2	0.0
13(1)	8(1)	1948.9	1893.0	0.7
13(1)	9(1)	1798.9	1741.7	7.6
13(1)	10(1)	1761.3	1711.1	0.6
13(1)	11(1)	1559.6	1467.5	1.1
13(1)	12(1)	1459.2	1412.6	0.3
14(1)	1(1)	4202.3	3986.6	0.1
14(1)	2(1)	3963.2	3784.6	0.0
14(1)	3(1)	3503.4	3351.6	0.0
14(1)	4(1)	2283.7	2238.6	0.1
14(1)	5(1)	2140.7	2079.9	0.0
14(1)	6(1)	1922.3	1883.6	0.0
14(1)	7(1)	1862.2	1810.6	0.6
14(1)	8(1)	1774.8	1717.9	2.0
14(1)	9(1)	1624.8	1568.5	0.1
14(1)	10(1)	1587.2	1537.2	0.0
14(1)	11(1)	1385.4	1290.6	0.4
14(1)	12(1)	1285.0	1235.6	0.2
14(1)	13(1)	1101.1	1083.3	0.1
15(1)	1(1)	3998.5	3782.2	0.0
15(1)	2(1)	3759.3	3579.5	0.0
15(1)	3(1)	3299.6	3145.6	0.0
15(1)	4(1)	2079.8	2032.0	0.2
15(1)	5(1)	1936.9	1874.3	0.0
15(1)	6(1)	1718.5	1677.4	0.0
15(1)	7(1)	1658.4	1606.9	0.4
15(1)	8(1)	1570.9	1513.9	0.0
15(1)	9(1)	1420.9	1359.1	1.1
15(1)	10(1)	1383.3	1330.3	0.5
15(1)	11(1)	1181.6	1092.4	13.4

15(1)	12(1)	1081.2	1029.2	0.5
15(1)	13(1)	897.2	877.4	0.7
15(1)	14(1)	723.1	703.2	0.1
16(1)	1(1)	7307.2	6933.3	0.0
16(1)	2(1)	7068.0	6580.9	1.7
16(1)	3(1)	6608.3	6295.7	0.0
16(1)	4(1)	5388.6	5183.8	0.0
16(1)	5(1)	5245.6	5005.4	1.5
16(1)	6(1)	5027.2	4828.3	0.1
16(1)	7(1)	4967.1	4757.9	0.1
16(1)	8(1)	4879.6	4665.1	0.1
16(1)	9(1)	4729.6	4515.1	0.1
16(1)	10(1)	4692.0	4483.5	0.0
16(1)	11(1)	4490.3	4251.6	0.5
16(1)	12(1)	4389.9	4186.1	0.1
16(1)	13(1)	4206.0	4028.6	0.0
16(1)	14(1)	4031.8	3854.6	0.0
16(1)	15(1)	3827.9	3649.8	0.0
17(1)	1(1)	6808.5	6456.2	0.0
17(1)	2(1)	6569.3	6251.5	0.0
17(1)	3(1)	6109.6	5689.3	0.5
17(1)	4(1)	4889.8	4705.0	0.0
17(1)	5(1)	4746.9	4546.7	0.0
17(1)	6(1)	4528.5	4330.6	0.2
17(1)	7(1)	4468.4	4280.0	0.1
17(1)	8(1)	4380.9	4184.5	0.0
17(1)	9(1)	4230.9	4036.9	0.2
17(1)	10(1)	4193.3	4008.1	0.0
17(1)	11(1)	3991.6	3763.2	0.0
17(1)	12(1)	3891.2	3706.3	0.0
17(1)	13(1)	3707.2	3551.3	0.0
17(1)	14(1)	3533.1	3377.7	0.0
17(1)	15(1)	3329.2	3171.5	0.0
17(1)	16(1)	6637.9	6321.3	0.0
18(1)	1(1)	5125.8	4881.1	0.0
18(1)	2(1)	4886.7	4674.3	0.2
18(1)	3(1)	4427.0	4239.4	0.0
18(1)	4(1)	3207.2	3131.5	0.0
18(1)	5(1)	3064.2	2964.0	0.3
18(1)	6(1)	2845.8	2773.1	0.0
18(1)	7(1)	2785.7	2696.9	0.0
18(1)	8(1)	2698.3	2609.8	0.0
18(1)	9(1)	2548.3	2460.1	0.0
18(1)	10(1)	2510.7	2428.7	0.0
18(1)	11(1)	2309.0	2182.9	0.1
18(1)	12(1)	2208.6	2129.0	0.0
18(1)	13(1)	2024.6	1976.1	0.0
18(1)	14(1)	1850.5	1802.2	0.0
18(1)	15(1)	1646.6	1595.6	0.0
18(1)	16(1)	4955.3	4746.8	0.5
18(1)	17(1)	4456.6	4268.2	0.0

19(1)	1(1)	4927.1	4689.4	0.0
19(1)	2(1)	4687.9	4483.5	0.0
19(1)	3(1)	4228.2	4046.0	0.2
19(1)	4(1)	3008.5	2938.9	0.1
19(1)	5(1)	2865.5	2777.6	0.2
19(1)	6(1)	2647.1	2583.5	0.0
19(1)	7(1)	2587.0	2506.8	0.0
19(1)	8(1)	2499.6	2418.1	0.0
19(1)	9(1)	2349.5	2264.2	0.0
19(1)	10(1)	2312.0	2238.3	0.0
19(1)	11(1)	2110.2	1993.8	0.1
19(1)	12(1)	2009.8	1937.5	0.0
19(1)	13(1)	1825.9	1784.8	0.0
19(1)	14(1)	1651.7	1610.6	0.0
19(1)	15(1)	1447.9	1406.2	0.0
19(1)	16(1)	4756.6	4554.4	0.1
19(1)	17(1)	4257.9	4074.4	0.1
19(1)	18(1)	2575.3	2498.3	0.1
20(1)	1(1)	4659.4	4438.3	0.0
20(1)	2(1)	4420.2	4233.8	0.0
20(1)	3(1)	3960.5	3797.6	0.1
20(1)	4(1)	2740.7	2685.7	0.0
20(1)	5(1)	2597.8	2529.1	0.2
20(1)	6(1)	2379.4	2331.1	0.2
20(1)	7(1)	2319.3	2260.9	0.0
20(1)	8(1)	2231.8	2168.9	0.0
20(1)	9(1)	2081.8	2020.7	0.0
20(1)	10(1)	2044.2	1987.5	0.0
20(1)	11(1)	1842.5	1743.2	0.1
20(1)	12(1)	1742.1	1686.3	0.1
20(1)	13(1)	1558.1	1534.0	0.0
20(1)	14(1)	1384.0	1360.2	0.0
20(1)	15(1)	1180.1	1153.3	0.0
20(1)	16(1)	4488.8	4304.6	0.0
20(1)	17(1)	3990.1	3823.9	0.0
20(1)	18(1)	2307.5	2250.0	0.0
20(1)	19(1)	2108.8	2060.9	0.0
21(1)	1(1)	4396.9	4129.6	0.6
21(1)	2(1)	4157.8	3934.0	0.0
21(1)	3(1)	3698.1	3498.9	0.0
21(1)	4(1)	2478.3	2386.8	0.0
21(1)	5(1)	2335.3	2229.2	0.0
21(1)	6(1)	2116.9	2031.4	0.1
21(1)	7(1)	2056.8	1965.2	0.0
21(1)	8(1)	1969.4	1859.5	0.0
21(1)	9(1)	1819.4	1713.1	0.0
21(1)	10(1)	1781.8	1681.9	0.0
21(1)	11(1)	1580.0	1444.9	0.0
21(1)	12(1)	1479.6	1387.2	0.0
21(1)	13(1)	1295.7	1229.7	0.1
21(1)	14(1)	1121.5	1057.3	0.0

21(1)	15(1)	917.7	851.7	0.0
21(1)	16(1)	4226.4	4004.0	0.0
21(1)	17(1)	3727.7	3524.7	0.1
21(1)	18(1)	2045.1	1951.0	0.0
21(1)	19(1)	1846.3	1759.9	0.0
21(1)	20(1)	1578.6	1509.6	0.1
22(1)	1(1)	4249.3	4014.4	0.4
22(1)	2(1)	4010.1	3817.5	0.0
22(1)	3(1)	3550.4	3382.0	0.0
22(1)	4(1)	2330.7	2269.7	0.0
22(1)	5(1)	2187.7	2112.3	0.0
22(1)	6(1)	1969.3	1917.7	0.2
22(1)	7(1)	1909.2	1843.0	0.0
22(1)	8(1)	1821.7	1749.6	0.0
22(1)	9(1)	1671.7	1600.0	0.1
22(1)	10(1)	1634.1	1568.4	0.0
22(1)	11(1)	1432.4	1326.1	0.0
22(1)	12(1)	1332.0	1268.7	0.0
22(1)	13(1)	1148.1	1118.0	0.0
22(1)	14(1)	973.9	939.9	0.0
22(1)	15(1)	770.0	735.1	0.0
22(1)	16(1)	4078.8	3887.5	0.0
22(1)	17(1)	3580.0	3408.1	0.3
22(1)	18(1)	1897.4	1833.9	0.1
22(1)	19(1)	1698.7	1643.3	1.0
22(1)	20(1)	1430.9	1390.2	4.4
22(1)	21(1)	1168.5	1072.3	10.0
23(1)	1(1)	3954.4	3551.7	0.0
23(1)	2(1)	3715.2	3347.4	0.0
23(1)	3(1)	3255.5	2913.0	0.0
23(1)	4(1)	2035.7	1800.3	0.0
23(1)	5(1)	1892.8	1639.4	0.4
23(1)	6(1)	1674.4	1450.5	0.0
23(1)	7(1)	1614.3	1376.6	0.0
23(1)	8(1)	1526.8	1283.2	0.0
23(1)	9(1)	1376.8	1133.7	0.0
23(1)	10(1)	1339.2	1101.2	0.3
23(1)	11(1)	1137.5	827.2	0.7
23(1)	12(1)	1037.1	789.9	0.3
23(1)	13(1)	853.1	644.0	0.0
23(1)	14(1)	679.0	474.5	0.1
23(1)	15(1)	475.1	259.5	0.0
23(1)	16(1)	3783.8	3418.5	0.4
23(1)	17(1)	3285.1	2937.0	0.2
23(1)	18(1)	1602.5	1354.2	0.1
23(1)	19(1)	1403.8	1166.2	0.2
23(1)	20(1)	1136.0	920.5	15.1
23(1)	21(1)	873.6	620.5	0.1
23(1)	22(1)	725.9	501.2	0.1
24(1)	1(1)	3796.5	3599.8	0.0
24(1)	2(1)	3557.4	3397.9	0.0

24(1) 3(1)	3097.7	2970.7		0.2
24(1) 4(1)	1877.9	1850.5		0.2
24(1) 5(1)	1734.9	1698.9		0.7
24(1) 6(1)	1516.5	1506.1		0.0
24(1) 7(1)	1456.4	1427.5		0.2
24(1) 8(1)	1369.0	1335.9		0.0
24(1) 9(1)	1219.0	1184.7		1.6
24(1) 10(1)	1181.4	1153.5		0.0
24(1) 11(1)	979.7	899.8		0.0
24(1) 12(1)	879.3	849.7		0.0
24(1) 13(1)	695.3	702.6		1.6
24(1) 14(1)	521.2	523.5		0.1
24(1) 15(1)	317.3	315.3		0.1
24(1) 16(1)	3626.0	3468.9		0.3
24(1) 17(1)	3127.3	2996.6		0.8
24(1) 18(1)	1444.7	1418.4		2.1
24(1) 19(1)	1245.9	1224.2		2.3
24(1) 20(1)	978.2	975.6		1.1
24(1) 21(1)	715.8	677.3		0.4
24(1) 22(1)	568.1	557.7		1.0
24(1) 23(1)	273.2	31.1		0.3

Table S12. Harmonic and anharmonic vibrational frequencies and their intensities of glycine conformer **III** as computed at the B3LYP/cc-pVTZ level of theory.

Mode (quanta)	ν_{harm} (cm^{-1})	ν_{anharm} (cm^{-1})	I_{harm} (km mol^{-1})	I_{anharm} (km mol^{-1})
1(1)	3739.3	3548.0	60.8	47.8
2(1)	3581.4	3406.6	3.3	0.9
3(1)	3508.5	3357.2	1.5	0.4
4(1)	3077.6	2948.9	6.0	5.6
5(1)	3047.5	2913.9	16.2	16.0
6(1)	1816.7	1781.4	280.2	250.5
7(1)	1675.7	1584.6	24.5	19.9
8(1)	1458.3	1418.0	2.7	2.3
9(1)	1387.1	1337.3	0.0	0.1
10(1)	1361.5	1317.0	15.5	8.3
11(1)	1350.3	1340.5	37.9	33.0
12(1)	1193.8	1176.0	1.1	1.5
13(1)	1164.9	1122.5	224.1	131.7
14(1)	1131.1	1092.0	30.5	17.4
15(1)	911.5	897.6	3.7	2.6
16(1)	892.7	858.7	156.7	147.6
17(1)	798.8	784.6	77.5	75.9
18(1)	684.8	658.9	98.4	82.1
19(1)	596.2	600.5	48.8	49.3
20(1)	517.5	496.7	24.8	30.0
21(1)	498.3	486.1	12.2	9.0
22(1)	262.1	271.8	2.2	1.7
23(1)	239.5	379.0	42.4	27.1
24(1)	32.2	38.1	0.0	3.3

1(2)		7478.6	6923.2	4.1
2(2)		7162.9	6724.4	0.9
3(2)		7016.9	6587.0	1.0
4(2)		6155.1	5796.6	0.4
5(2)		6095.0	5736.9	0.2
6(2)		3633.5	3545.6	3.0
7(2)		3351.4	3200.9	0.0
8(2)		2916.6	2811.5	0.2
9(2)		2774.2	2677.0	0.0
10(2)		2723.1	2618.8	0.1
11(2)		2700.5	2597.8	0.9
12(2)		2387.6	2323.1	0.1
13(2)		2329.8	2232.9	1.7
14(2)		2262.2	2173.4	0.1
15(2)		1823.1	1798.0	0.1
16(2)		1785.4	1699.2	5.2
17(2)		1597.6	1562.1	4.1
18(2)		1369.6	1269.3	5.4
19(2)		1192.4	1179.6	3.6
20(2)		1035.0	1016.8	0.8
21(2)		996.7	971.2	0.2
22(2)		524.1	545.5	0.3
23(2)		479.0	824.3	1.3
24(2)		64.4	67.3	0.1
2(1)	1(1)	7320.7	6954.6	0.0
3(1)	1(1)	7247.7	6880.5	0.0
3(1)	2(1)	7089.9	6588.0	1.8
4(1)	1(1)	6816.9	6479.9	0.0
4(1)	2(1)	6659.0	6337.3	0.0
4(1)	3(1)	6586.0	6263.3	0.0
5(1)	1(1)	6786.8	6446.2	0.0
5(1)	2(1)	6628.9	6304.1	0.0
5(1)	3(1)	6556.0	6229.9	0.0
5(1)	4(1)	6125.1	5699.4	0.5
6(1)	1(1)	5556.0	5329.3	0.7
6(1)	2(1)	5398.2	5189.5	0.0
6(1)	3(1)	5325.2	5115.3	0.0
6(1)	4(1)	4894.3	4714.6	0.2
6(1)	5(1)	4864.3	4680.1	0.3
7(1)	1(1)	5415.0	5163.3	0.0
7(1)	2(1)	5257.1	5001.5	1.6
7(1)	3(1)	5184.1	4911.3	0.0
7(1)	4(1)	4753.2	4549.3	0.0
7(1)	5(1)	4723.2	4512.5	0.0
7(1)	6(1)	3492.4	3398.0	0.0
8(1)	1(1)	5197.6	4965.9	0.0
8(1)	2(1)	5039.7	4824.2	0.0
8(1)	3(1)	4966.8	4749.9	0.0
8(1)	4(1)	4535.9	4327.6	0.2
8(1)	5(1)	4505.8	4285.1	0.2
8(1)	6(1)	3275.1	3200.1	0.1

8(1)	7(1)	3134.0	3033.5	0.0
9(1)	1(1)	5126.4	4889.4	0.0
9(1)	2(1)	4968.6	4746.7	0.5
9(1)	3(1)	4895.6	4670.5	0.2
9(1)	4(1)	4464.7	4273.0	0.0
9(1)	5(1)	4434.6	4234.1	0.0
9(1)	6(1)	3203.9	3123.7	0.0
9(1)	7(1)	3062.8	2943.8	2.6
9(1)	8(1)	2845.4	2755.2	0.0
10(1)	1(1)	5100.8	4864.6	0.0
10(1)	2(1)	4943.0	4722.6	0.3
10(1)	3(1)	4870.0	4648.5	0.2
10(1)	4(1)	4439.1	4241.3	0.0
10(1)	5(1)	4409.0	4223.1	0.0
10(1)	6(1)	3178.3	3098.4	0.5
10(1)	7(1)	3037.2	2936.5	0.1
10(1)	8(1)	2819.8	2733.4	0.1
10(1)	9(1)	2748.7	2647.2	0.0
11(1)	1(1)	5089.6	4835.1	0.9
11(1)	2(1)	4931.7	4711.6	0.0
11(1)	3(1)	4858.7	4637.7	0.0
11(1)	4(1)	4427.8	4236.8	0.0
11(1)	5(1)	4397.8	4203.6	0.0
11(1)	6(1)	3167.0	3083.6	0.4
11(1)	7(1)	3026.0	2920.5	0.1
11(1)	8(1)	2808.6	2721.8	0.1
11(1)	9(1)	2737.4	2646.0	0.0
11(1)	10(1)	2711.8	2620.0	0.0
12(1)	1(1)	4933.1	4710.9	0.0
12(1)	2(1)	4775.2	4567.4	0.0
12(1)	3(1)	4702.2	4492.4	0.0
12(1)	4(1)	4271.4	4091.1	0.1
12(1)	5(1)	4241.3	4055.3	0.1
12(1)	6(1)	3010.5	2944.3	0.0
12(1)	7(1)	2869.5	2773.4	0.2
12(1)	8(1)	2652.1	2579.8	0.0
12(1)	9(1)	2580.9	2497.5	0.1
12(1)	10(1)	2555.3	2468.9	0.0
12(1)	11(1)	2544.1	2466.7	0.0
13(1)	1(1)	4904.2	4663.0	0.2
13(1)	2(1)	4746.3	4529.3	0.0
13(1)	3(1)	4673.4	4455.3	0.0
13(1)	4(1)	4242.5	4053.7	0.0
13(1)	5(1)	4212.4	4020.1	0.1
13(1)	6(1)	2981.7	2901.7	0.8
13(1)	7(1)	2840.6	2737.8	0.0
13(1)	8(1)	2623.2	2539.3	0.3
13(1)	9(1)	2552.0	2463.3	0.0
13(1)	10(1)	2526.4	2437.8	0.1
13(1)	11(1)	2515.2	2411.2	1.7
13(1)	12(1)	2358.7	2279.5	0.0

14(1)	1(1)	4870.4	4638.7	0.0
14(1)	2(1)	4712.5	4496.8	0.1
14(1)	3(1)	4639.6	4421.9	0.1
14(1)	4(1)	4208.7	4025.3	0.1
14(1)	5(1)	4178.6	3991.1	0.3
14(1)	6(1)	2947.9	2873.8	0.0
14(1)	7(1)	2806.8	2703.6	0.2
14(1)	8(1)	2589.4	2508.7	0.0
14(1)	9(1)	2518.2	2427.8	0.0
14(1)	10(1)	2492.6	2404.5	0.1
14(1)	11(1)	2481.4	2396.4	0.1
14(1)	12(1)	2324.9	2251.0	0.0
14(1)	13(1)	2296.0	2213.7	0.4
15(1)	1(1)	4650.8	4445.4	0.0
15(1)	2(1)	4493.0	4302.9	0.0
15(1)	3(1)	4420.0	4228.3	0.0
15(1)	4(1)	3989.1	3825.5	0.0
15(1)	5(1)	3959.0	3791.6	0.1
15(1)	6(1)	2728.3	2678.5	0.0
15(1)	7(1)	2587.2	2510.7	0.2
15(1)	8(1)	2369.8	2311.7	0.2
15(1)	9(1)	2298.7	2235.3	0.0
15(1)	10(1)	2273.1	2214.5	0.0
15(1)	11(1)	2261.8	2199.5	0.0
15(1)	12(1)	2105.3	2060.0	0.1
15(1)	13(1)	2076.4	2018.4	0.0
15(1)	14(1)	2042.6	1986.3	0.0
16(1)	1(1)	4632.0	4406.2	0.0
16(1)	2(1)	4474.1	4274.9	0.6
16(1)	3(1)	4401.1	4200.0	0.3
16(1)	4(1)	3970.2	3789.4	0.0
16(1)	5(1)	3940.2	3755.4	0.1
16(1)	6(1)	2709.4	2642.7	0.2
16(1)	7(1)	2568.4	2446.5	0.0
16(1)	8(1)	2351.0	2275.2	0.0
16(1)	9(1)	2279.8	2195.1	0.1
16(1)	10(1)	2254.2	2171.6	0.4
16(1)	11(1)	2243.0	2159.8	0.3
16(1)	12(1)	2086.5	2020.3	0.1
16(1)	13(1)	2057.6	1979.2	1.1
16(1)	14(1)	2023.8	1934.1	2.0
16(1)	15(1)	1804.2	1753.3	0.1
17(1)	1(1)	4538.1	4330.5	0.1
17(1)	2(1)	4380.2	4193.7	0.1
17(1)	3(1)	4307.3	4119.7	0.1
17(1)	4(1)	3876.4	3716.1	0.0
17(1)	5(1)	3846.3	3682.0	0.0
17(1)	6(1)	2615.6	2567.6	0.1
17(1)	7(1)	2474.5	2403.7	0.0
17(1)	8(1)	2257.1	2201.4	0.1
17(1)	9(1)	2185.9	2123.7	0.0

17(1)	10(1)	2160.3	2099.3	0.1
17(1)	11(1)	2149.1	2088.6	0.1
17(1)	12(1)	1992.6	1945.7	0.0
17(1)	13(1)	1963.7	1901.3	2.5
17(1)	14(1)	1929.9	1872.8	0.3
17(1)	15(1)	1710.4	1680.8	0.1
17(1)	16(1)	1691.5	1658.9	0.0
18(1)	1(1)	4424.1	4207.5	0.7
18(1)	2(1)	4266.3	4065.3	0.0
18(1)	3(1)	4193.3	3991.4	0.0
18(1)	4(1)	3762.4	3589.6	0.0
18(1)	5(1)	3732.3	3556.1	0.0
18(1)	6(1)	2501.6	2440.8	0.0
18(1)	7(1)	2360.5	2274.5	0.0
18(1)	8(1)	2143.1	2075.5	0.0
18(1)	9(1)	2071.9	2000.2	0.0
18(1)	10(1)	2046.4	1975.1	0.0
18(1)	11(1)	2035.1	1958.3	0.0
18(1)	12(1)	1878.6	1821.6	0.0
18(1)	13(1)	1849.7	1775.0	0.0
18(1)	14(1)	1815.9	1751.1	0.0
18(1)	15(1)	1596.4	1556.9	0.2
18(1)	16(1)	1577.5	1516.1	0.1
18(1)	17(1)	1483.6	1441.6	0.0
19(1)	1(1)	4335.5	4131.4	0.2
19(1)	2(1)	4177.6	3995.5	0.0
19(1)	3(1)	4104.6	3921.6	0.0
19(1)	4(1)	3673.7	3521.0	0.0
19(1)	5(1)	3643.7	3487.3	0.0
19(1)	6(1)	2412.9	2369.3	0.0
19(1)	7(1)	2271.9	2205.6	0.0
19(1)	8(1)	2054.5	2007.0	0.0
19(1)	9(1)	1983.3	1930.7	0.0
19(1)	10(1)	1957.7	1905.3	0.1
19(1)	11(1)	1946.4	1890.7	1.4
19(1)	12(1)	1790.0	1752.4	0.0
19(1)	13(1)	1761.1	1708.3	0.6
19(1)	14(1)	1727.3	1681.0	0.3
19(1)	15(1)	1507.7	1486.7	0.0
19(1)	16(1)	1488.9	1447.1	0.5
19(1)	17(1)	1395.0	1374.1	1.5
19(1)	18(1)	1281.0	1251.2	0.0
20(1)	1(1)	4256.8	4055.6	0.4
20(1)	2(1)	4098.9	3915.7	0.0
20(1)	3(1)	4025.9	3841.7	0.0
20(1)	4(1)	3595.0	3439.1	0.3
20(1)	5(1)	3565.0	3405.4	0.0
20(1)	6(1)	2334.2	2289.9	0.0
20(1)	7(1)	2193.2	2124.2	0.0
20(1)	8(1)	1975.8	1927.2	0.2
20(1)	9(1)	1904.6	1849.2	0.0

20(1)	10(1)	1879.0	1825.2	0.0
20(1)	11(1)	1867.8	1812.1	0.0
20(1)	12(1)	1711.3	1671.7	1.1
20(1)	13(1)	1682.4	1630.4	0.0
20(1)	14(1)	1648.6	1601.1	0.0
20(1)	15(1)	1429.0	1405.8	1.0
20(1)	16(1)	1410.2	1365.3	0.0
20(1)	17(1)	1316.3	1292.1	0.0
20(1)	18(1)	1202.3	1161.2	2.9
20(1)	19(1)	1113.7	1094.0	0.0
21(1)	1(1)	4237.6	4033.3	0.0
21(1)	2(1)	4079.8	3892.4	0.0
21(1)	3(1)	4006.8	3818.3	0.0
21(1)	4(1)	3575.9	3418.6	0.0
21(1)	5(1)	3545.8	3384.8	0.0
21(1)	6(1)	2315.1	2265.0	0.1
21(1)	7(1)	2174.0	2101.6	0.0
21(1)	8(1)	1956.6	1903.9	0.1
21(1)	9(1)	1885.5	1827.0	0.0
21(1)	10(1)	1859.9	1800.3	0.1
21(1)	11(1)	1848.6	1791.5	3.5
21(1)	12(1)	1692.1	1649.0	0.0
21(1)	13(1)	1663.2	1606.8	0.1
21(1)	14(1)	1629.4	1576.8	0.1
21(1)	15(1)	1409.9	1383.9	0.0
21(1)	16(1)	1391.0	1348.6	7.0
21(1)	17(1)	1297.2	1266.6	0.1
21(1)	18(1)	1183.2	1145.1	0.0
21(1)	19(1)	1094.5	1075.1	0.7
21(1)	20(1)	1015.8	990.1	0.0
22(1)	1(1)	4001.4	3819.0	0.1
22(1)	2(1)	3843.5	3679.1	0.0
22(1)	3(1)	3770.5	3605.1	0.0
22(1)	4(1)	3339.6	3203.8	0.0
22(1)	5(1)	3309.6	3170.1	0.0
22(1)	6(1)	2078.8	2053.6	0.3
22(1)	7(1)	1937.7	1887.5	0.0
22(1)	8(1)	1720.4	1689.0	0.1
22(1)	9(1)	1649.2	1612.7	0.0
22(1)	10(1)	1623.6	1588.9	0.2
22(1)	11(1)	1612.3	1576.4	0.1
22(1)	12(1)	1455.9	1436.2	0.0
22(1)	13(1)	1427.0	1395.9	0.7
22(1)	14(1)	1393.2	1359.1	0.1
22(1)	15(1)	1173.6	1169.2	0.0
22(1)	16(1)	1154.7	1134.1	73.5
22(1)	17(1)	1060.9	1056.8	0.5
22(1)	18(1)	946.9	931.0	0.0
22(1)	19(1)	858.2	862.4	0.4
22(1)	20(1)	779.5	780.5	0.0
22(1)	21(1)	760.4	757.5	0.7

23(1)	1(1)	3978.8	3927.7	0.0
23(1)	2(1)	3820.9	3787.8	0.4
23(1)	3(1)	3747.9	3712.9	0.1
23(1)	4(1)	3317.0	3306.8	0.2
23(1)	5(1)	3287.0	3274.8	0.0
23(1)	6(1)	2056.2	2161.6	0.0
23(1)	7(1)	1915.2	1996.3	0.5
23(1)	8(1)	1697.8	1799.9	0.0
23(1)	9(1)	1626.6	1716.9	0.1
23(1)	10(1)	1601.0	1693.7	0.0
23(1)	11(1)	1589.8	1684.4	0.0
23(1)	12(1)	1433.3	1547.3	1.8
23(1)	13(1)	1404.4	1501.9	0.1
23(1)	14(1)	1370.6	1472.0	0.4
23(1)	15(1)	1151.0	1287.2	22.5
23(1)	16(1)	1132.2	1260.1	1.1
23(1)	17(1)	1038.3	1180.3	0.6
23(1)	18(1)	924.3	1036.6	3.1
23(1)	19(1)	835.7	973.7	0.1
23(1)	20(1)	757.0	884.0	0.0
23(1)	21(1)	737.8	866.3	0.0
23(1)	22(1)	501.5	666.4	0.0
24(1)	1(1)	3771.5	3588.2	0.0
24(1)	2(1)	3613.6	3440.0	0.3
24(1)	3(1)	3540.7	3364.5	0.0
24(1)	4(1)	3109.8	2976.9	1.9
24(1)	5(1)	3079.7	2913.1	0.3
24(1)	6(1)	1848.9	1818.3	1.9
24(1)	7(1)	1707.9	1645.0	0.6
24(1)	8(1)	1490.5	1454.9	0.2
24(1)	9(1)	1419.3	1370.8	0.5
24(1)	10(1)	1393.7	1346.9	0.0
24(1)	11(1)	1382.5	1345.2	0.0
24(1)	12(1)	1226.0	1197.3	8.3
24(1)	13(1)	1197.1	1145.1	0.4
24(1)	14(1)	1163.3	1126.1	0.3
24(1)	15(1)	943.7	931.4	0.4
24(1)	16(1)	924.9	903.2	0.4
24(1)	17(1)	831.0	826.3	0.2
24(1)	18(1)	717.0	696.3	0.5
24(1)	19(1)	628.4	626.7	8.8
24(1)	20(1)	549.7	541.2	1.1
24(1)	21(1)	530.5	527.6	0.1
24(1)	22(1)	294.3	308.9	0.3
24(1)	23(1)	271.7	493.9	1.9

Table S13. Vibrational band positions ($\tilde{\nu}$, in cm^{-1}) used to determine the column densities ($N_t(\mathbf{X})$ for species **X** in cm^{-2}).

Species	Experiment	$\tilde{\nu}$			
trans-FA	Ar (6929.9 cm^{-1})	1768.1	1106.4, 1104.3	–	–
	Ar (6934.7 cm^{-1})	1768.1	1104.3	–	–
	n-H_2	1765.4	1108.8	–	–
	p-H_2	1768.1	1106.3	–	–
cis-FA	Ar	1808.0	1243.5	–	–
	n-H_2	1804.8	1250.1	–	–
	p-H_2	1807.7	1247.8	–	–
trans-AA	Ar	1379.6	1259.3	1180.2, 1150.5	985.8
cis-AA	Ar	1807.3	1285.3, 1271.7	–	–
glycine **I**	Ar	1781.1	–	–	–
	n-H_2	1781.0	–	–	–
	p-H_2	1784.7	–	–	–
glycine **III**	Ar	1774.9, 1769.0	–	–	–
	n-H_2	1770.6	–	–	–
	p-H_2	1779.0	–	–	–

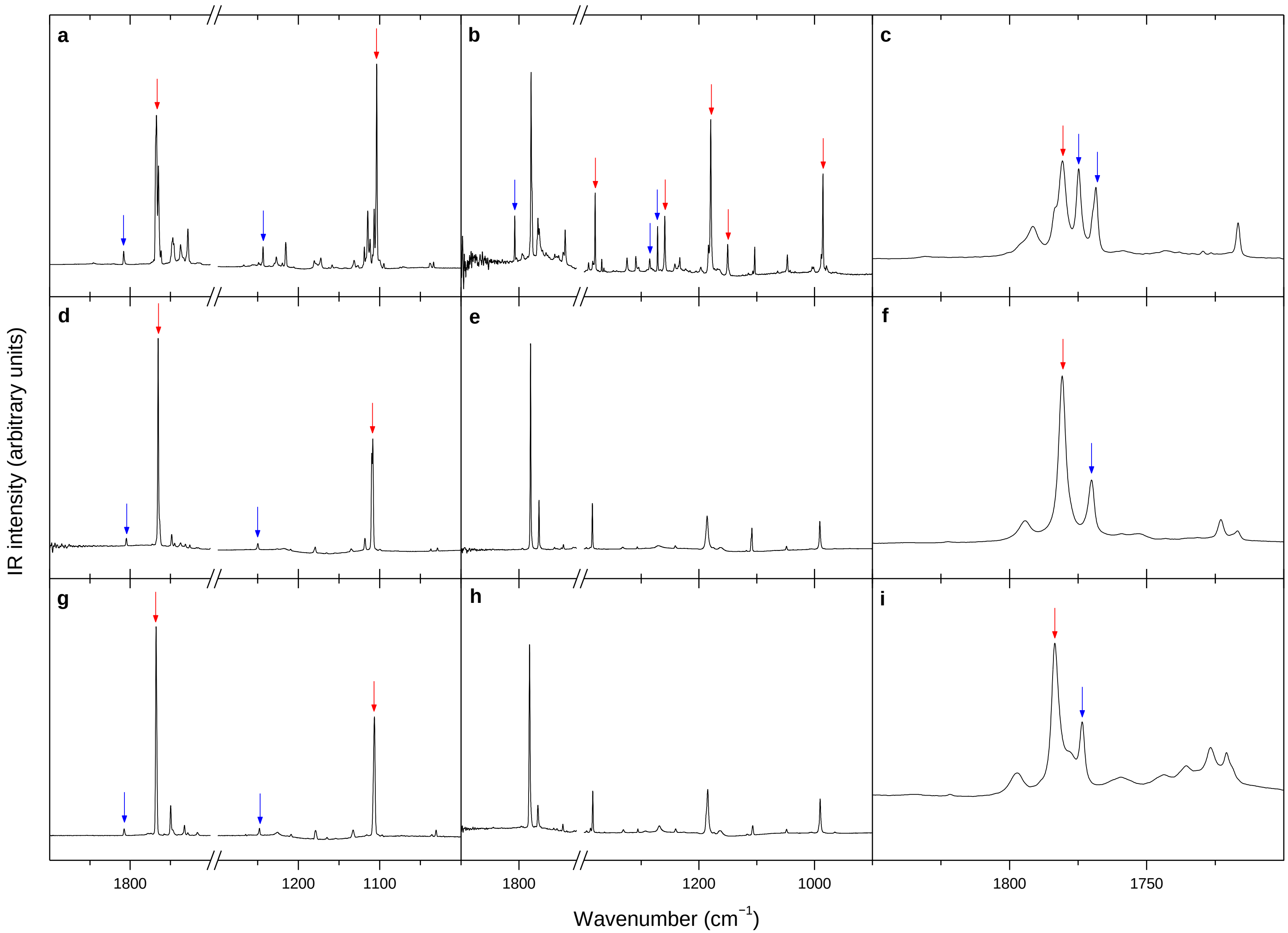

Figure S1. MIR spectra taken after excitations showing the bands used to determine the column density values in the case of the FA (**a**), AA (**b**), and glycine (**c**) isolated in Ar as well as the same species in *n*-H_2 (**d**–**f**), and *p*-H_2 (**g**–**i**) matrices as marked by arrows. Red arrows denote the *cis* carboxylic acids and glycine **I** conformers, whereas the blue ones represent the *trans* form of carboxylic acids and the glycine **III** conformer.

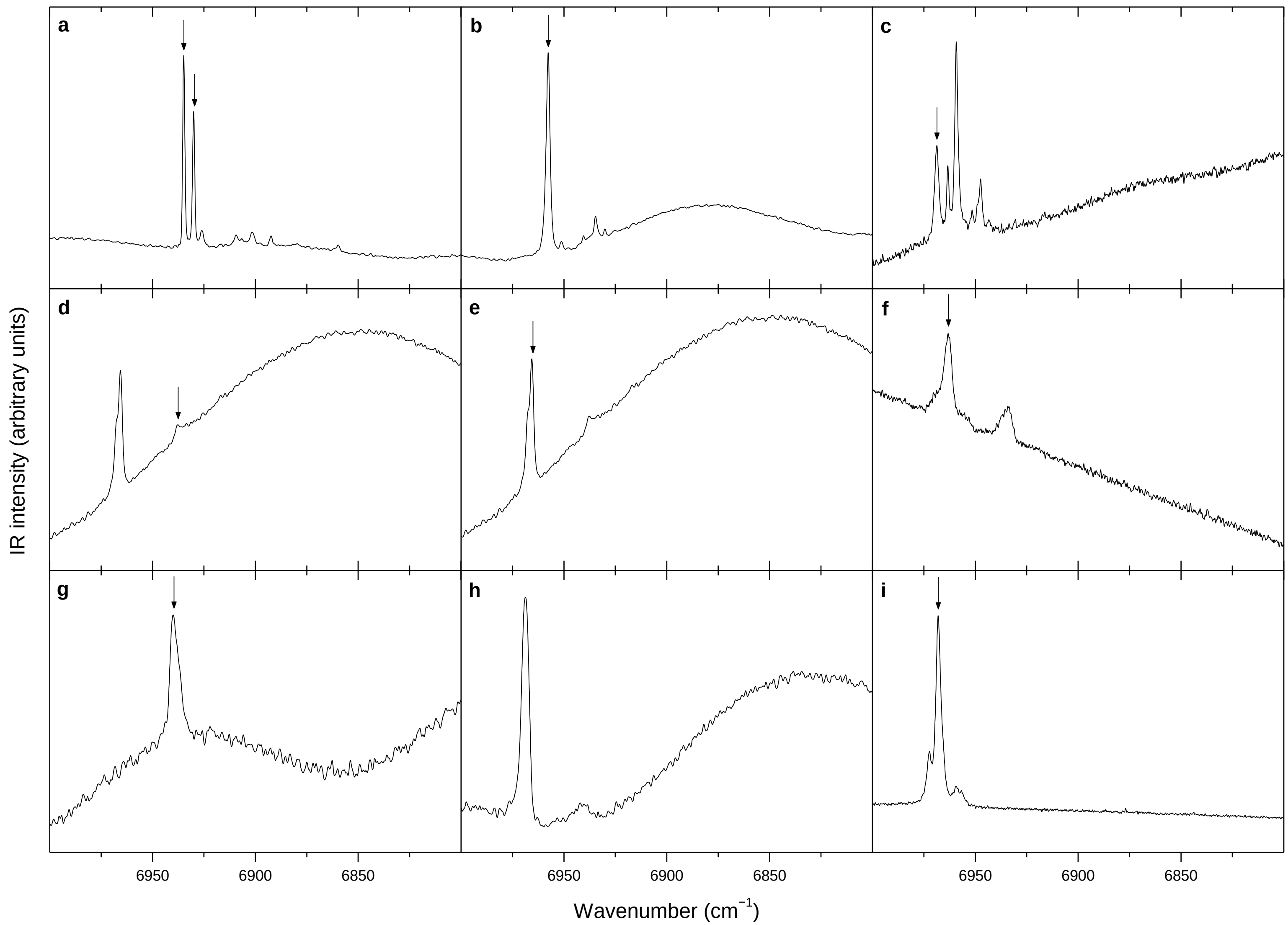

Figure S2. Bands used for the NIR excitations in the case of the FA (**a**), AA (**b**), and glycine (**c**) isolated in Ar as well as the same species in *n*-H_2 (**d**–**f**), and *p*-H_2 (**g**–**i**) matrices as marked by arrows.

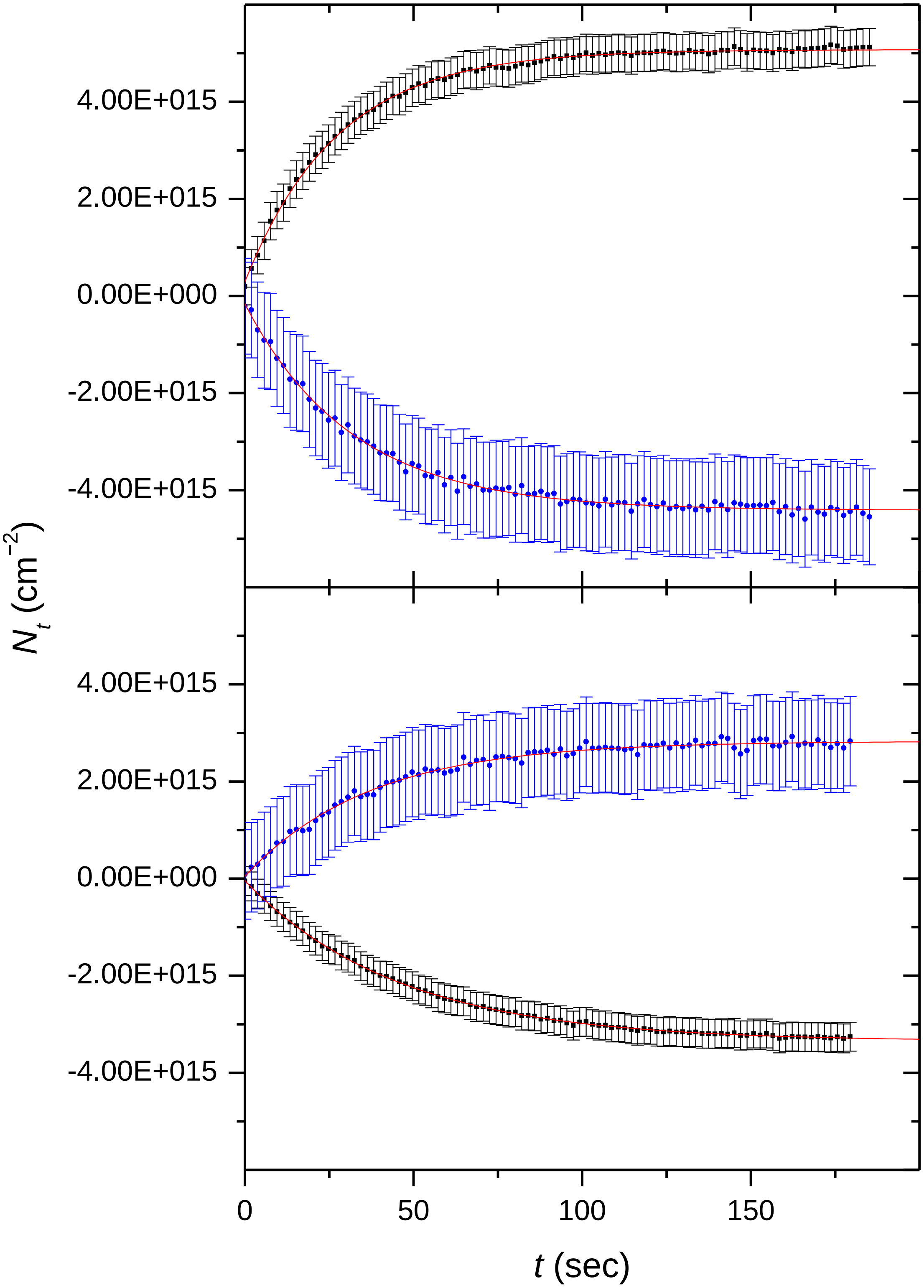

Figure S3. Kinetic plots of the AA–Ar system during (**a**) and after (**b**) the NIR laser excitation of 6957.9 cm^{-1}. Blue symbols show the column densities of the *trans*, the black ones display those of the *cis* isomers, whereas the red traces display the kinetic fit.