

Supporting Information

for

The Alanine model dipeptide Ac-Ala-NH₂ exists as a mixture of C₇^{eq} and C₅ conformers

Carlos Cabezas,^a Marcelino Varela,^a Vanessa Cortijo,^a Ana I. Jiménez,^b Isabel Peña,^a Adam M. Daly,^a Juan C. López,^a Carlos Cativiela,^b José L. Alonso^{*a}

Contents

Table S1: Transition frequencies of the C₇^{eq} conformer of Ac-Ala-NH₂.

Table S2: Transition frequencies of the C₅ conformer of Ac-Ala-NH₂.

Table S1. Frequencies^a (in MHz) of the observed rotational transitions and residuals for the C₇^{eq} conformer of Ac-Ala-NH₂.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'	F'	I''	F''	v _{obs.}	v _{obs.} -v _{cal.}
2	1	2	1	0	1	2	4	2	3	5342.1287	-0.0022
						2	3	1	2	5342.8426	-0.0012
						1	3	2	2	5341.8165	0.0021
						1	2	2	1	5342.7670	0.0006
3	0	3	2	0	2	2	5	2	4	6037.4223	-0.0005
						2	4	2	3	6037.4381	-0.0001
						1	4	1	3	6037.5506	0.0006
						1	3	1	2	6037.3922	0.0001
3	1	3	2	1	2	0	3	0	2	6037.5179	-0.0036
						2	5	2	4	5791.1037	0.0006
						2	4	2	3	5791.1715	-0.0003
						2	3	2	2	5791.3168	-0.0010
3	1	2	2	1	1	1	4	1	3	5791.2338	0.0011
						1	3	1	2	5791.0862	0.0030
						2	5	2	4	6423.4684	-0.0009
						2	4	2	3	6423.4808	0.0021
3	1	3	2	0	2	1	4	1	3	6423.6154	0.0001
						1	3	1	2	6423.3286	-0.0013
						2	5	2	4	7074.0064	0.0024
						2	4	1	3	7074.6980	-0.0029
4	0	4	3	0	3	2	3	2	2	7074.4771	-0.0020
						2	2	1	1	7073.4983	-0.0027
						1	4	2	3	7073.7805	-0.0051
						1	3	0	2	7074.1750	-0.0017
4	1	4	3	1	3	2	6	2	5	7961.1026	0.0001
						2	3	2	2	7961.2726	-0.0023
						1	5	1	4	7961.2347	0.0002
						2	6	2	5	7699.7596	0.0008
4	1	3	3	1	2	2	5	2	4	7699.8110	-0.0026
						2	4	2	3	7699.8897	-0.0009
						1	5	1	4	7699.8248	0.0036
						2	6	2	5	8536.7335	0.0011
4	1	4	3	0	3	2	4	2	3	8536.8499	0.0034
						1	5	1	4	8536.7962	0.0010
						1	4	1	3	8536.6569	0.0005
						2	6	2	5	8736.3430	0.0030
4	0	4	3	1	3	2	5	1	4	8736.9667	0.0022
						2	4	2	3	8736.7986	0.0014
						1	5	2	4	8736.1706	0.0020
						1	4	0	3	8736.4221	0.0018
5	0	5	4	1	4	1	3	2	2	8737.1035	0.0004
						2	6	2	5	6924.5240	0.0027
						2	5	2	4	6924.2749	0.0005
						2	4	2	3	6924.3661	-0.0014
5	0	5	4	1	4	2	7	2	6	9054.8660	0.0000
						2	6	2	5	9054.6670	-0.0009
						2	5	2	4	9054.7506	-0.0014
						2	4	2	3	9055.0247	-0.0021
5	0	5	4	1	4	1	6	1	5	9054.9386	-0.0019

^a Observed: obs.; observed–calculated: obs.–cal.

Table S2. Frequencies^a (in MHz) of the observed rotational transitions and residuals for the C₅ conformer of Ac-Ala-NH₂.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'	F'	I''	F''	v _{obs.}	v _{obs.} -v _{cal.}
2	0	2	1	0	1	2	4	2	3	3528.7716	0.0025
						1	3	1	2	3528.9183	0.0013
						1	2	1	1	3528.8425	0.0049
3	0	3	2	0	2	2	5	2	4	5276.1991	0.0028
						2	4	2	3	5276.2601	0.0038
						2	3	2	2	5276.4390	0.0045
						1	4	1	3	5276.3160	0.0022
						1	3	1	2	5276.2310	0.0017
3	1	3	2	1	2	2	5	2	4	5085.6957	0.0007
						2	4	2	3	5085.8853	0.0029
						1	4	1	3	5085.9275	0.0016
3	1	2	2	1	1	2	5	2	4	5512.6793	0.0003
						2	4	2	3	5512.9105	0.0008
						2	3	2	2	5512.9468	-0.0009
						1	4	1	3	5512.7697	0.0001
4	0	4	3	0	3	2	6	2	5	7003.7764	0.0034
						2	5	2	4	7003.8665	0.0033
						2	4	2	3	7004.0038	0.0021
						2	3	2	2	7003.9844	0.0019
						1	5	1	4	7003.8881	0.0007
4	1	4	3	1	3	1	4	1	3	7003.7927	0.0024
						2	6	2	5	6773.5084	-0.0028
						2	5	2	4	6773.5922	-0.0008
						2	4	2	3	6773.7732	-0.0025
						1	5	1	4	6773.6505	-0.0027
4	1	3	3	1	2	1	4	1	3	6773.5440	-0.0042
						2	6	2	5	7341.7875	-0.0042
						2	4	2	3	7341.9432	-0.0033
						0	4	0	3	7341.7480	-0.0020
5	0	5	4	0	4	2	7	2	6	8706.7173	-0.0020
						2	6	2	5	8706.8261	-0.0048
						2	5	2	4	8706.9601	-0.0019
						1	6	1	5	8706.8384	0.0003
						1	5	1	4	8706.7283	-0.0004

^a Observed: obs.; observed–calculated: obs.–cal.