

Six Conformers of Neutral Aspartic Acid Identified in Gas Phase

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Table S1. Measured frequencies and residuals (in MHz) for the rotational transitions of conformer IIb-I of aspartic acid.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
2	1	1	1	0	1	3	2	6185.247	0.006
						2	1	6185.459	0.003
2	2	1	1	1	1	3	2	9027.502	-0.002
						2	1	9027.853	0.001
2	2	1	1	1	0	3	2	8893.736	-0.001
						2	1	8894.606	-0.004
						1	0	8893.503	-0.007
2	2	0	1	1	1	3	2	9036.504	0.001
						2	1	9036.821	-0.002
						1	0	9037.074	-0.004
2	2	0	1	1	0	3	2	8902.735	-0.002
3	0	3	2	0	2	4	3	6709.316	0.000
						3	2	6709.316	0.000
						2	1	6709.084	-0.002
3	1	3	2	1	2	4	3	6539.113	-0.001
						3	2	6538.813	-0.003
3	1	2	2	1	1	4	3	6939.785	0.001
						3	2	6939.467	0.001
3	1	3	2	0	2	4	3	7835.448	0.003
						3	2	7835.970	0.000
						2	1	7835.031	0.000
3	1	2	2	0	2	4	3	8637.280	0.006
						3	2	8637.222	0.004
						2	1	8637.068	0.004
4	0	4	3	0	3	5	4	8905.712	-0.001
						4	3	8905.743	-0.001
						3	2	8905.601	-0.001
4	1	4	3	1	3	5	4	8709.071	-0.001
						4	3	8708.949	-0.001
						3	2	8709.047	-0.001
4	1	3	3	1	2	5	4	9241.510	0.001
						4	3	9241.378	0.001
						3	2	9241.436	0.001
4	2	3	3	2	2	5	4	8986.405	0.002
						4	3	8985.926	0.000
						3	2	8986.528	0.001
4	2	2	3	2	1	5	4	9073.984	0.002
						4	3	9073.447	0.001
						3	2	9074.113	0.000
4	0	4	3	1	3	5	4	7779.580	-0.004
						4	3	7779.089	-0.003
						3	2	7779.653	-0.003
4	1	4	3	0	3	5	4	9835.205	0.004
						4	3	9835.603	0.001
						3	2	9834.994	0.000
5	0	5	4	0	4	6	5	11072.799	0.000
						5	4	11072.844	-0.001
						4	3	11072.728	-0.003
5	1	5	4	1	4	6	5	10871.815	0.000
						5	4	10871.759	0.000
						4	3	10871.789	0.000
5	1	4	4	1	3	6	5	11532.283	0.001
						5	4	11532.224	0.000
						4	3	11532.224	0.000
5	2	4	4	2	3	6	5	11221.632	0.003
						5	4	11221.389	0.003
						4	3	11221.656	0.003

Supplementary Material (ESI) for PCCP
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5	2	3	4	2	2	6	5	11390.278	0.002
						5	4	11389.968	0.001
						4	3	11390.306	0.001
5	0	5	4	1	4	6	5	10143.308	-0.003
						5	4	10142.982	-0.005
						4	3	10143.333	-0.006
5	1	5	4	0	4	6	5	11801.303	0.000
						5	4	11801.619	0.002
						4	3	11801.184	0.003
6	0	6	5	0	5	7	6	13211.826	-0.001
						6	5	13211.874	-0.004
						5	4	13211.784	0.003
6	1	6	5	1	5	7	6	13026.737	0.005
						6	5	13026.720	0.002
						5	4	13026.720	0.002
6	1	5	5	1	4	7	6	13807.929	0.000
						6	5	13807.910	0.001
						5	4	13807.885	0.000
6	0	6	5	1	5	7	6	12483.318	-0.003
						6	5	12483.106	-0.001
						5	4	12483.330	-0.001

Table S2. Measured frequencies and residuals (in MHz) for the rotational transitions of conformer IIa-I of aspartic acid.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
2	1	1	1	0	1	3	2	6125.094	0.007
						2	1	6125.615	-0.003
3	1	3	2	0	2	4	3	7172.581	-0.003
						3	2	7172.757	-0.002
						2	1	7172.297	-0.003
3	1	2	2	0	2	4	3	8002.056	0.005
						3	2	8002.360	0.001
						2	1	8001.719	-0.002
4	0	4	3	0	3	5	4	6615.199	0.000
						4	3	6615.169	0.000
						3	2	6615.102	0.000
4	1	4	3	1	3	5	4	6382.942	-0.002
						4	3	6382.807	0.000
						3	2	6382.894	0.000
4	1	3	3	1	2	5	4	6935.199	0.000
						4	3	6935.066	0.001
						3	2	6935.161	0.000
4	2	3	3	2	2	5	4	6665.927	0.000
						4	3	6665.471	0.003
						3	2	6666.046	0.002
4	2	2	3	2	1	5	4	6720.882	-0.002
						4	3	6720.429	-0.001
						3	2	6720.999	-0.002
4	1	4	3	0	3	5	4	8575.017	-0.004
						4	3	8575.102	-0.002
						3	2	8574.896	0.001
4	1	3	3	0	3	5	4	9956.749	0.005
						4	3	9956.962	0.001
						3	2	9956.580	-0.003
5	0	5	4	0	4	6	5	8229.302	0.000
						5	4	8229.278	0.000
						4	3	8229.245	0.000
5	1	5	4	1	4	6	5	7969.148	-0.001
						5	4	7969.073	0.000
						4	3	7969.107	-0.001
5	1	4	4	1	3	6	5	8657.597	0.000
						5	4	8657.521	-0.002
						4	3	8657.567	0.003
5	2	4	4	2	3	6	5	8325.390	0.002
						5	4	8325.149	0.001
						4	3	8325.424	0.011
5	2	3	4	2	2	6	5	8433.739	-0.003
						5	4	8433.505	-0.002
						4	3	8433.763	-0.003
5	0	5	4	1	4	6	5	6269.480	0.000
						5	4	6269.343	0.000
						4	3	6269.450	-0.001
5	1	5	4	0	4	6	5	9928.970	-0.001
						5	4	9929.006	-0.003
						4	3	9928.900	-0.002
5	1	4	4	0	4	6	5	11999.149	0.007
						5	4	11999.318	0.002
						4	3	11999.041	-0.003
6	0	6	5	0	5	7	6	9820.132	0.000
						6	5	9820.112	0.000
						5	4	9820.094	0.001
6	1	6	5	1	5	7	6	9549.746	0.000

					6	5	9549.697	-0.001	
					5	4	9549.717	0.002	
6	1	5	5	1	4	7	6	10371.637	-0.001
					6	5	10371.591	-0.001	
					5	4	10371.610	-0.002	
6	2	5	5	2	4	7	6	9980.272	0.003
					5	4	9980.272	0.003	
					6	5	9980.130	0.003	
6	2	4	5	2	3	7	6	10165.224	-0.006
					5	4	10165.224	-0.006	
					6	5	10165.090	-0.004	
6	0	6	5	1	5	7	6	8120.463	0.001
					6	5	8120.382	0.000	
					5	4	8120.443	0.006	
6	1	6	5	0	5	7	6	11249.409	-0.006
					6	5	11249.431	0.002	
					5	4	11249.375	0.003	
7	0	7	6	0	6	8	7	11387.539	0.001
					7	6	11387.522	0.000	
					6	5	11387.511	-0.001	
7	1	7	6	1	6	8	7	11124.272	0.001
					7	6	11124.239	0.001	
					6	5	11124.249	0.002	
7	1	6	6	1	5	8	7	12074.865	-0.002
					7	6	12074.833	-0.002	
					6	5	12074.845	-0.002	
7	0	7	6	1	6	8	7	9958.256	0.001
					7	6	9958.205	0.001	
					6	5	9958.226	-0.007	
7	1	7	6	0	6	8	7	12553.555	0.000
					7	6	12553.555	0.000	
					6	5	12553.527	0.002	
8	0	8	7	0	7	9	8	12934.232	0.002
					8	7	12934.216	0.002	
					7	6	12934.210	0.000	
8	1	8	7	1	7	9	8	12692.557	0.003
					8	7	12692.532	0.002	
					7	6	12692.538	0.003	
8	1	7	7	1	6	9	8	13764.455	-0.004
					8	7	13764.430	-0.004	
					7	6	13764.438	-0.004	
8	0	8	7	1	7	9	8	11768.214	0.000
					8	7	11768.180	-0.001	
					7	6	11768.199	0.003	

Table S3. Measured frequencies and residuals (in MHz) for the rotational transitions of conformer Ia-II of aspartic acid.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
3	0	3	2	0	2	4	3	5148.432	0.002
						3	2	5148.405	0.000
						2	1	5148.175	-0.002
3	1	3	2	1	2	4	3	4931.483	0.001
						3	2	4931.134	-0.002
						2	1	4931.501	-0.005
3	1	2	2	1	1	4	3	5423.503	0.003
						3	2	5423.143	0.001
4	0	4	3	0	3	5	4	6825.407	0.001
						4	3	6825.407	0.001
						3	2	6825.287	0.001
4	1	4	3	1	3	5	4	6565.782	-0.006
						4	3	6565.639	0.000
						3	2	6565.752	0.003
4	1	3	3	1	2	5	4	7220.478	0.002
						4	3	7220.323	0.002
						3	2	7220.408	0.002
5	0	5	4	0	4	6	5	8471.967	-0.003
						5	4	8471.985	0.001
						4	3	8471.897	0.000
5	1	5	4	1	4	6	5	8192.833	-0.002
						5	4	8192.757	-0.001
5	1	4	4	1	3	6	5	9007.374	0.001
						5	4	9007.295	0.000
						4	3	9007.318	0.000
6	0	6	5	0	5	7	6	10086.433	0.000
						6	5	10086.456	0.000
						5	4	10086.387	0.002
6	1	6	5	1	5	7	6	9811.738	0.001
						6	5	9811.698	0.003
						5	4	9811.711	0.004
6	1	5	5	1	4	7	6	10780.560	-0.005
						6	5	10780.520	-0.003
						5	4	10780.520	-0.003

Table S4. Measured frequencies and residuals (in MHz) for the rotational transitions of conformer Ib-I of aspartic acid.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
2	1	2	1	0	1	3	2	5761.296	-0.002
2	1	1	1	0	1	3	2	6169.062	0.000
						2	1	6169.231	0.002
						1	0	6168.892	0.003
3	0	3	2	0	2	4	3	6783.928	0.000
						3	2	6783.907	0.000
3	1	3	2	1	2	4	3	6612.855	-0.002
						3	2	6612.821	-0.002
3	1	2	2	1	1	4	3	7020.221	0.001
3	1	3	2	0	2	4	3	7835.463	-0.002
						3	2	7835.361	0.002
						2	1	7835.481	-0.001
3	1	2	2	0	2	4	3	8650.592	0.000
						3	2	8650.756	0.001
						2	1	8650.513	-0.002
4	0	4	3	0	3	5	4	9002.089	0.002
						4	3	9002.061	0.001
						3	2	9002.080	-0.001
4	1	4	3	1	3	5	4	8806.694	0.000
						4	3	8806.674	-0.000
						3	2	8806.680	0.001
4	1	3	3	1	2	5	4	9347.795	-0.002
						4	3	9347.780	-0.002
						3	2	9347.807	0.001
4	1	4	3	0	3	5	4	9858.228	-0.002
						4	3	9858.126	0.000
						3	2	9858.247	0.003
4	1	3	3	0	3	5	4	11214.459	0.000
						4	3	11214.629	0.000
						3	2	11214.404	-0.001
4	0	4	3	1	3	5	4	7950.549	-0.001
						4	3	7950.606	-0.001
						3	2	7950.520	0.003
5	0	5	4	0	4	6	5	11189.277	-0.002
						4	3	11189.277	-0.002
						5	4	11189.251	0.000
5	1	5	4	1	4	6	5	10992.809	0.000
						5	4	10992.794	0.000
						4	3	10992.801	0.001
5	1	4	4	1	3	6	5	11663.318	-0.001
						5	4	11663.305	-0.001
						4	3	11663.327	0.002
5	1	5	4	0	4	6	5	11848.951	-0.001
						5	4	11848.861	0.001
						4	3	11848.966	0.003
5	1	4	4	0	4	6	5	13875.692	-0.001
						5	4	13875.874	0.000
5	0	5	4	1	4	6	5	10333.136	0.000
						5	4	10333.185	0.001
						4	3	10333.115	0.001
6	0	6	5	0	5	7	6	13347.830	-0.001
						5	4	13347.830	-0.001
						6	5	13347.801	-0.002
6	1	6	5	1	5	7	6	13170.651	0.003
						5	4	13170.651	0.003
						6	5	13170.636	-0.002
6	1	5	5	1	4	7	6	13962.153	0.002
						5	4	13962.153	0.002
						6	5	13962.133	-0.001

Table S5. Measured frequencies and residuals (in MHz) for the rotational transitions of conformer III_β-I of aspartic acid.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
3	0	3	2	0	2	4	3	6683.414	0.000
						3	2	6683.389	-0.000
3	1	3	2	1	2	4	3	6517.814	0.001
						3	2	6517.773	-0.004
						2	1	6517.783	0.000
3	1	2	2	1	1	4	3	6903.072	0.005
						3	2	6903.047	0.006
4	0	4	3	0	3	5	4	8875.080	0.001
						4	3	8875.049	-0.001
4	1	4	3	1	3	5	4	8681.662	-0.005
						4	3	8681.645	-0.003
						3	2	8681.645	-0.003
4	1	3	3	1	2	5	4	9193.869	0.000
						4	3	9193.853	-0.001
						3	2	9193.880	-0.001
5	0	5	4	0	4	6	5	11039.742	0.001
						4	3	11039.742	0.001
						5	4	11039.710	0.000
5	1	5	4	1	4	6	5	10838.928	0.002
						5	4	10838.910	0.001
						4	3	10838.919	0.004
5	1	4	4	1	3	6	5	11474.936	-0.005

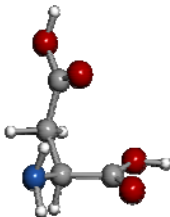
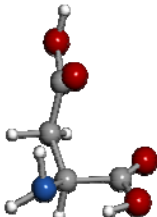
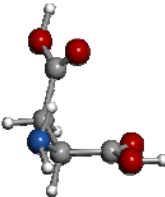
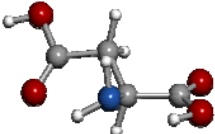
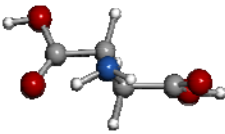
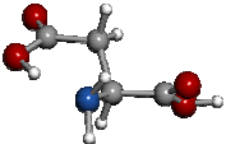
Table S6. Measured frequencies and residuals (in MHz) for the rotational transitions of conformer Ia-I of aspartic acid.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
2	1	1	1	0	1	3	2	6100.568	0.000
						4	3	7216.346	0.001
						3	2	7217.310	-0.001
						2	1	7216.080	-0.001
3	1	2	2	0	2	4	3	7980.755	0.000
						3	2	7979.581	-0.002
						2	1	7981.238	-0.001
4	0	4	3	0	3	5	4	6702.063	0.000
						4	3	6702.180	0.000
						3	2	6702.075	0.001
4	1	4	3	1	3	5	4	6485.680	0.000
						4	3	6485.767	0.000
						3	2	6485.779	-0.001
4	1	3	3	1	2	5	4	6994.375	0.000
						4	3	6994.416	-0.001
						3	2	6994.288	-0.001
4	1	4	3	0	3	5	4	8658.953	0.001
						4	3	8659.914	0.002
						3	2	8658.748	0.001
4	1	3	3	0	3	5	4	9932.059	0.001
						4	3	9930.835	0.000
						3	2	9932.413	-0.001
5	0	5	4	0	4	6	5	8343.095	0.000
						4	3	8343.095	0.000
						5	4	8343.234	0.000
5	1	5	4	1	4	6	5	8098.863	0.000
						5	4	8098.931	0.000
						4	3	8098.923	-0.001
5	1	4	4	1	3	6	5	8733.185	0.000
						5	4	8733.227	0.000
						4	3	8733.136	0.000
5	0	5	4	1	4	6	5	6386.206	0.001
						5	4	6385.502	0.001
						4	3	6386.425	0.001
5	1	5	4	0	4	6	5	10055.752	0.000
						5	4	10056.664	0.000
						4	3	10055.597	0.000
5	1	4	4	0	4	6	5	11963.181	0.001
6	0	6	5	0	5	7	6	9963.593	0.000
						5	4	9963.593	0.000
						6	5	9963.750	-0.001
6	1	6	5	1	5	7	6	9707.119	0.000
						6	5	9707.181	0.000
						5	4	9707.161	0.001
6	1	5	5	1	4	7	6	10464.841	0.000
						6	5	10464.890	-0.001
						5	4	10464.808	0.000
6	0	6	5	1	5	7	6	8250.937	0.000
						6	5	8250.320	-0.001
						5	4	8251.092	0.000
6	1	6	5	0	5	7	6	11419.777	0.000
						6	5	11420.611	0.000
						5	4	11419.661	0.001
7	0	7	6	0	6	8	7	11563.019	0.000
						6	5	11563.019	0.000
						7	6	11563.187	0.000
7	1	7	6	1	6	8	7	11310.011	-0.001

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						7	6	11310.069	-0.001
						6	5	11310.040	-0.001
7	1	6	6	1	5	8	7	12187.280	0.000
						7	6	12187.341	0.001
						6	5	12187.254	0.000
7	0	7	6	1	6	8	7	10106.836	-0.001
						7	6	10106.326	0.000
						6	5	10106.950	0.000
8	0	8	7	1	7	9	8	11940.054	0.001
						8	7	11939.649	0.001
						7	6	11940.133	0.000

Table S7. Rotational parameters for the observed conformers of aspartic acid.

Parameter	Ib-I	IIb-I	III _β b-I	IIa-I	Ia-I	Ia-II
						
A (MHz) ^a	2553.85523(70)	2612.20878(26)	2651.953(31)	3416.43489(66)	3378.20873(26)	3198.861(19)
B (MHz)	1205.08478(10)	1191.01132(17)	1183.51697(30)	902.904474(79)	907.373507(28)	945.84803(17)
C (MHz)	1069.14318(10)	1057.33169(16)	1054.98929(34)	764.631177(96)	780.042139(32)	781.75139(18)
Δ _J (kHz)	0.2852(17)	0.3663(21)	0.3043(72)	0.03471(83)	0.04293(33)	0.0456(27)
Δ _{JK} (kHz)	0.732(41)	-	-	0.358(18)	0.441(10)	-
δ _J (kHz)	0.0540(11)	0.0492(16)	-	-	-	-
χ _{aa} (MHz)	-0.2774(35)	-3.5601(63)	-0.295(27)	-3.3602(87)	0.9560(35)	-3.995(19)
χ _{bb} (MHz)	-0.2640(35)	2.6538(54)	-0.350(45)	1.4823(73)	2.7296(23)	2.524(32)
χ _{cc} (MHz)	0.5414(35)	0.9064(54)	0.645(45)	1.8778(73)	-3.6856(23)	1.470(32)
σ ^c (kHz)	1.5	2.5	2.8	2.8	0.7	2.3
N ^d	59	78	22	101	68	34

^a A, B and C represent the rotational constants; Δ_J, Δ_{JK} and δ_J are the quartic centrifugal distortion constants; and χ_{aa}, χ_{bb}, and χ_{cc} are elements of the ¹⁴N nuclear quadrupole coupling tensor.

^b Standard error in parentheses in units of the last digit.

^c rms deviation of the fit.

^d Number of transitions.

Figure S1. Rotational transition $4_{0,4} \leftarrow 3_{0,3}$ for all the observed conformers of aspartic acid, showing the ^{14}N quadrupole hyperfine structure. Because the molecular beam and the microwave radiation travel parallel to each other in our setup, each rotational transition appears as a doublet (\square) due to the Doppler effect.

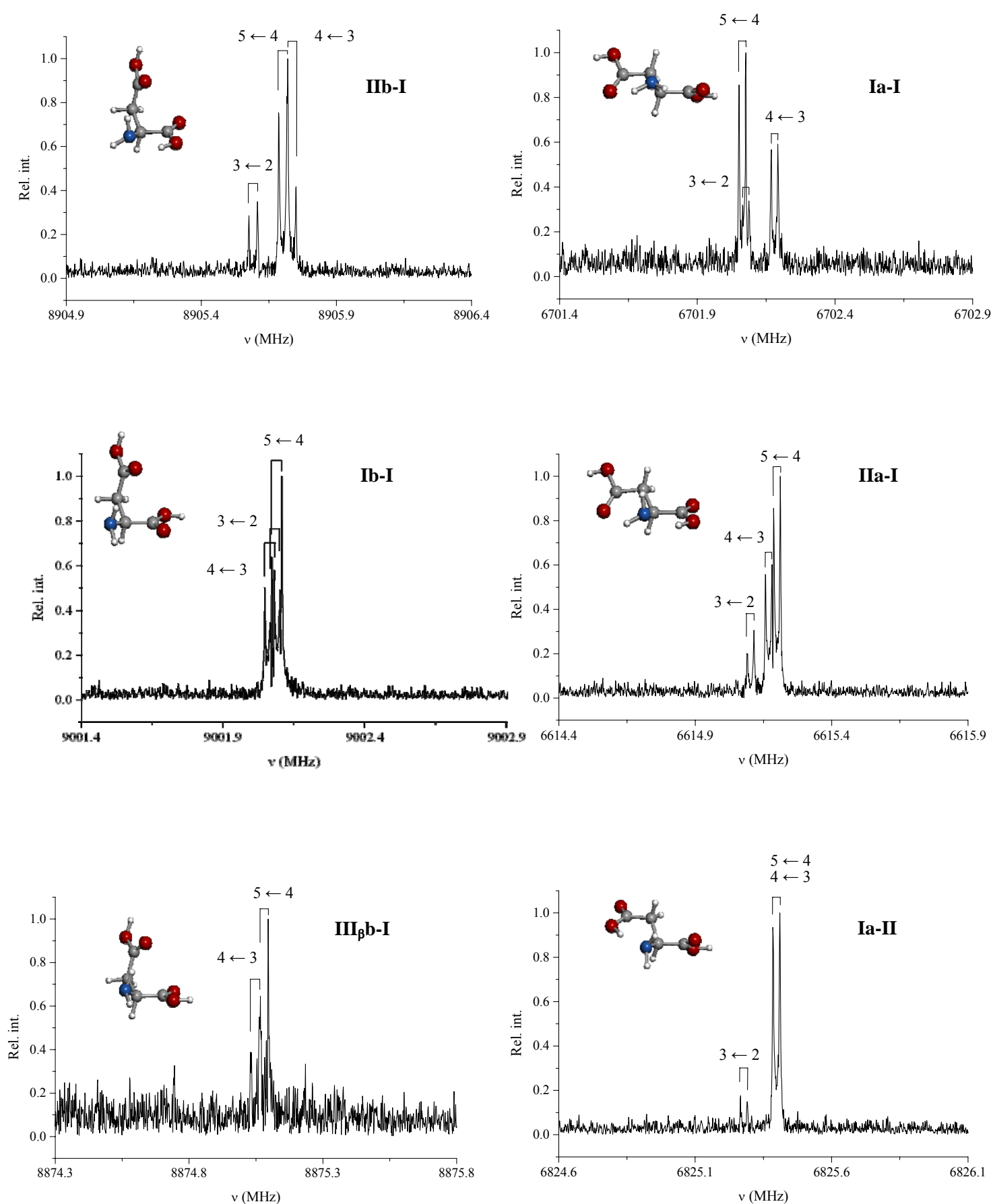


Figure S2. Interconversion barrier between conformers Ib-I \leftrightarrow III $_{\beta}$ b-I of aspartic acid calculated at the B3LYP/6-311++G(d,p) level of theory.

