Electronic Supplementary Material (ESI) for Chemical Communications

Electronic Supplementary Information

for

The Conformational Locking of Asparagine

Carlos Cabezas, Marcelino Varela, Isabel Peña, José L. Alonso*, Santiago Mata, and Juan C. López

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Figure S1. (Top) Part of the rotational spectra of Asn, 2_{11}-1_{01} rotational transition, showing the nuclear quadrupole hyperfine components labelled with the quantum numbers I',F'- I'',F''. The coaxial arrangement of the adiabatic expansion and the resonator axis produces an instrumental Doppler doubling. The resonances frequencies are calculated as the average of the two Doppler components. Theoretical simulations of the nuclear quadrupole hyperfine structures for the 2_{11}-1_{01} rotational transition of conformers IIa (Middle) and Ib (Bottom).

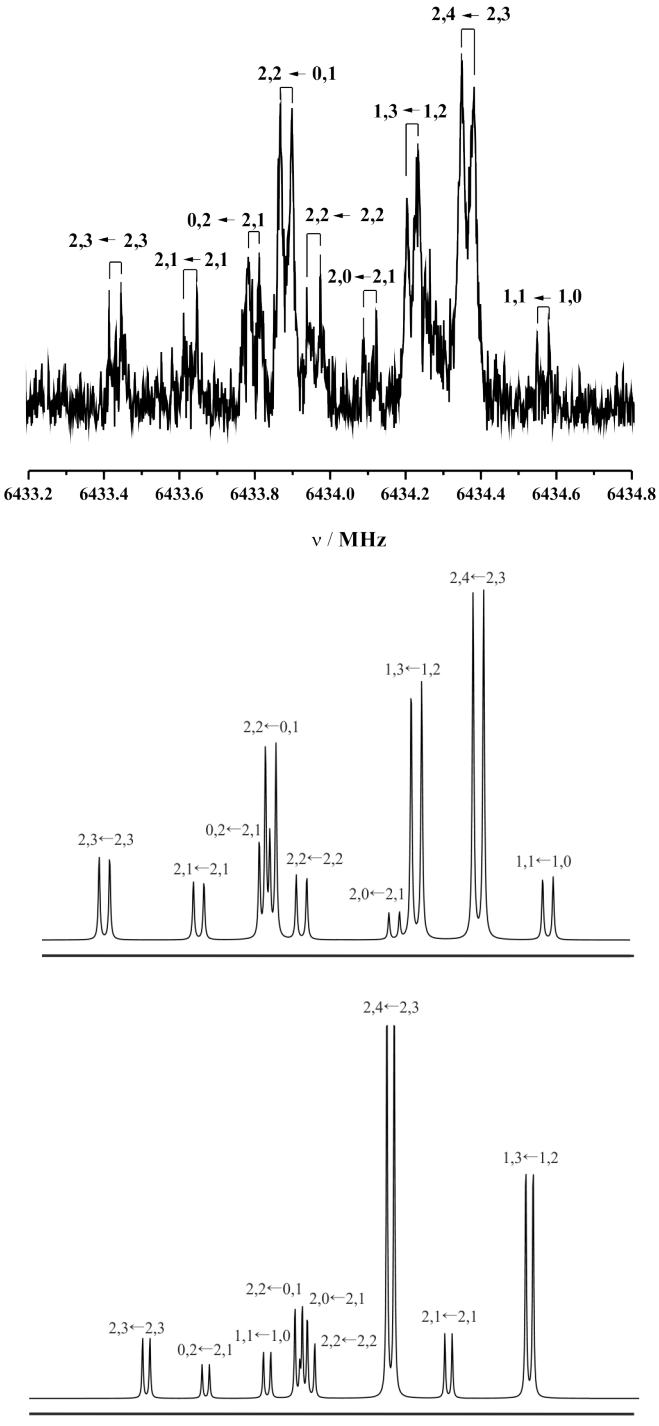

Table S1. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the conformer IIa of asparagine.

J′	K'_{-1}	K'_{+1}	J′′	K''_{-1}	K''_{+1}	I′	F′	I′′	F′′	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
1	1	0	0	0	0	2	3	2	2	3658.688	0.005
						2	2	2	2	3658.519	0.004
						2	1	2	2	3658.928	0.005
						1	2	1	1	3658.670	0.005
2	0	2	1	0	1	2	4	2	3	4922.254	-0.001
						2	3	2	3	4921.652	-0.003
						2	3	2	2	4922.452	0.001
						1	3	1	2	4922.218	-0.002
						1	2	1	1	4922.151	0.002
						0	2	2	1	4921.524	0.000
2	1	2	1	0	1	2	4	2	3	5578.523	-0.001
						2	3	2	2	5579.494	-0.003
						2	3	1	2	5578.950	-0.003
						2	2	0	1	5579.435	0.002
						1	3	1	2	5578.798	-0.002
						1	2	1	1	5578.266	-0.001
						1	1	1	0	5579.742	-0.002
						0	2	2	1	5577.431	-0.003
2	1	1	1	0	1	2	4	2	3	6434.365	0.001
						2	3	2	3	6433.433	0.001
						2	2	2	2	6433.962	0.002
						2	2	0	1	6433.882	0.002
						2	1	2	1	6433.633	0.001
						2	0	2	1	6434.104	0.000
						1	3	1	2	6434.219	-0.003
						1	1	1	0	6434.553	-0.004
						0	2	2	1	6433.799	0.004
3	0	3	2	0	2	2	5	2	4	7251.419	0.004
						2	4	2	3	7251.636	0.005
						1	4	1	3	7251.477	0.004
3	1	3	2	0	2	2	5	2	4	7666.299	0.002
						2	4	1	3	7666.516	0.000
						2	3	2	2	7667.058	0.002
						2	3	1	2	7666.112	-0.003
						1	4	2	3	7666.947	-0.003
						1	4	1	3	7666.637	0.001
						1	3	1	2	7666.191	0.000
						0	3	0	2	7666.027	-0.001
3	1	2	2	0	2	2	5	2	4	9369.960	0.000
						2	4	2	3	9369.508	-0.005
						2	3	2	2	9369.258	0.000
						1	4	1	3	9369.720	-0.002

Table S2: Cartesian coordinates for the ab initio predicted geometry (MP2/6-311++G(d,p) level of theory of the observed conformer of asparagine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.347100	-0.553690	0.013312
2	8	0	2.065837	-0.201711	-1.052526
3	8	0	1.223870	-1.698216	0.396394
4	1	0	1.913952	0.771264	-1.115897
5	6	0	0.689162	0.635482	0.740875
6	7	0	0.763917	1.825538	-0.112796
7	6	0	-0.730060	0.237555	1.184450
8	1	0	1.300007	0.802125	1.635755
9	1	0	-0.128860	1.974726	-0.583405
10	1	0	0.972234	2.656438	0.429358
11	1	0	-1.181503	1.070826	1.728775
12	6	0	-1.582256	-0.033910	-0.043383
13	1	0	-0.670141	-0.634535	1.838441
14	8	0	-2.010415	0.888099	-0.735780
15	7	0	-1.816647	-1.349235	-0.319022
16	1	0	-2.218108	-1.551396	-1.224552
17	1	0	-1.196483	-2.041565	0.078023

Rotational constants (GHZ): 2.2288787 1.4167071 1.1204599

Complete reference 19.

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