
Observation of Two New Conformers of Neutral Proline

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Table S1. Observed frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the conformer Ia of proline.

J'	K' ₋₁	K' ₊₁	J''	K'' ₋₁	K'' ₊₁	F'	F''	V _{obs.}	V _{obs.} -V _{cal.}
1	1	1	0	0	0	2	1	5234.652	-0.003
						1	1	5235.198	-0.007
						0	1	5233.830	-0.003
1	1	0	0	0	0	2	1	5447.920	0.006
						1	1	5446.632	0.006
						0	1	5449.849	0.001
2	1	2	1	0	1	3	2	7989.551	-0.004
						2	1	7990.192	-0.005
						1	0	7989.896	-0.002
						2	2	7990.935	-0.001
						1	1	7988.045	-0.004
2	1	1	1	0	1	3	2	8628.853	0.003
						2	1	8627.528	0.005
						1	0	8630.291	0.003
						2	2	8628.265	0.002
						1	1	8628.441	0.003
3	1	3	2	0	2	4	3	10643.643	0.004
						3	2	10644.428	0.004
						2	1	10643.541	-0.003
						3	3	10645.306	0.003
						2	2	10642.180	0.002
3	1	2	2	0	2	4	3	11921.258	-0.003
						3	2	11920.005	-0.003
						2	1	11921.878	-0.003
3	0	3	2	1	2	4	3	6778.803	0.001
						3	2	6778.463	0.000
						2	1	6779.204	-0.001
4	0	4	3	1	3	5	4	9935.335	-0.001
						4	3	9934.907	0.001
						3	2	9935.600	-0.001

Table S2. Observed frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the conformer Ib of proline.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	F'	F''	V _{obs.}	V _{obs.} -V _{cal.}
1	1	1	0	0	0	2	1	5285.342	-0.001
						1	1	5286.035	-0.004
						0	1	5284.298	-0.001
1	1	0	0	0	0	2	1	5571.418	0.003
						1	1	5570.383	0.005
						0	1	5572.971	-0.000
2	1	2	1	0	1	3	2	7848.244	-0.001
						2	1	7849.014	-0.002
						1	0	7848.137	-0.002
						2	2	7849.355	-0.002
2	1	1	1	0	1	1	1	7847.286	-0.001
						3	2	8706.008	0.001
						2	1	8704.922	0.002
						1	0	8706.936	0.003
						2	2	8705.263	0.002
3	1	3	2	0	2	4	3	10277.722	0.006
						3	2	10278.529	0.001
						2	1	10277.524	-0.004
						3	3	10278.996	0.002
						2	2	10276.803	0.000
3	0	3	2	1	2	4	3	6277.914	-0.001
						3	2	6277.439	-0.000
						2	1	6278.311	0.001
3	1	2	2	0	2	4	3	11991.662	-0.001
						3	2	11990.551	-0.002
						2	1	11992.145	-0.002
4	0	4	3	1	3	5	4	9341.692	-0.002
						4	3	9341.256	-0.002
						3	2	9341.929	0.003

Table S3. Spectroscopic constants for the observed conformers of proline.

	<i>Ia</i>	<i>Ib</i>	<i>IIa</i> ^a	<i>IIb</i> ^a
A^b [MHz]	3857.2400(14) ^c	4003.9605(10)	3673.90038(148)	3923.5648(53)
B [MHz]	1590.45352(50)	1567.27215(37)	1688.42056(56)	1605.87630(62)
C [MHz]	1377.50091(53)	1281.48910(38)	1407.37716(55)	1279.79761(46)
Δ_J [kHz]	1.116(21)	1.110(15)	0.6341(89)	1.0198(105)
Δ_{JK} [kHz]	-5.32(17)	-7.14(12)	-2.402(47)	-4.645(85)
Δ_K [kHz]	-	-	5.118(311)	-0.0119(49)
δ_J [kHz]	-	-	0.1210(48)	0.2512(63)
δ_K [kHz]	-	-	0.581(214)	[0.0]
χ_{aa} [MHz]	2.4664(32)	1.1363(25)	0.8820(30)	0.0427(89)
χ_{bb} [MHz]	1.8300(56)	2.3208(32)	-0.5493(44)	-1.0822(116)
χ_{cc} [MHz]	-4.2964(56)	-3.4571(32)	-0.3327(44)	1.0394(116)
σ^d [kHz]	3.3	2.4	1.9	2.1
N^e	30	29	110	51

^aData for conformers *IIa* and *IIb* taken from reference 3 of the paper.

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

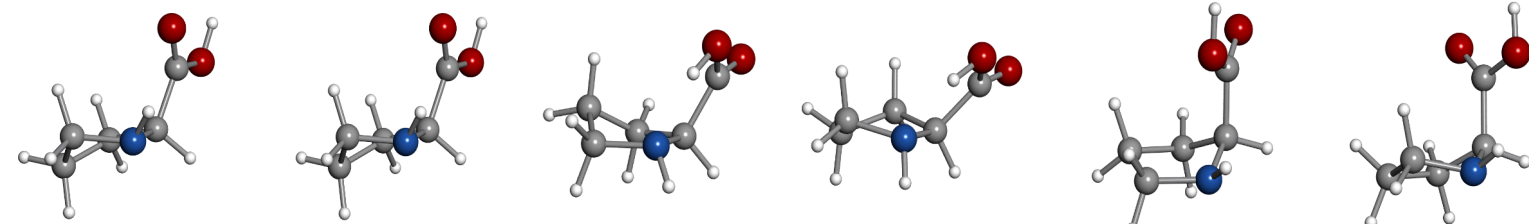
^cStandard error in parenthesis in the units of the last digit.

^drms deviation of the fit.

^eNumber of components fitted.

Table S4. Ab initio spectroscopic constants for the low-energy conformers of proline.

Theoretical ^a	Ia	Ib	IIa	IIb	IIIa	IIIb
A^b / MHz	3934.2	3948.9	3672.2	3976.9	3432.5	3409.7
B / MHz	1560.2	1589.2	1698.7	1594.3	1791.7	1803.6
C / MHz	1372.4	1306.5	1425.4	1276.7	1523.9	1502.2
χ_{aa} / MHz	3.02	0.83	0.90	0.09	3.94	-1.54
χ_{bb} / MHz	1.99	2.75	-0.80	-1.32	0.93	2.56
χ_{cc} / MHz	-5.01	-3.58	-0.10	1.23	-4.87	-1.02
$ \mu_a $ / D	0.0	0.1	5.4	5.6	0.9	0.1
$ \mu_b $ / D	1.7	1.4	0.7	0.8	1.3	1.2
$ \mu_c $ / D	0.8	0.7	1.8	1.4	0.9	0.2
$ \mu_{\text{total}} $ / D	1.9	1.5	5.7	5.8	1.9	1.2
ΔE^c / cm^{-1}	782	745	0	268	1299	1214



^a Optimized structures at the MP2/6-311++G(d,p) level of calculation.

^b A, B and C are the rotational constants; μ_a , μ_b and μ_c are the electric dipole moment components; χ_{aa} , χ_{bb} , and χ_{cc} are ^{14}N nuclear quadrupole coupling parameters.

^c Electronic energies relative to conformer Ia.

