Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

The last link of the x-aminobutyric acid series: the five conformers of β-aminobutyric acid

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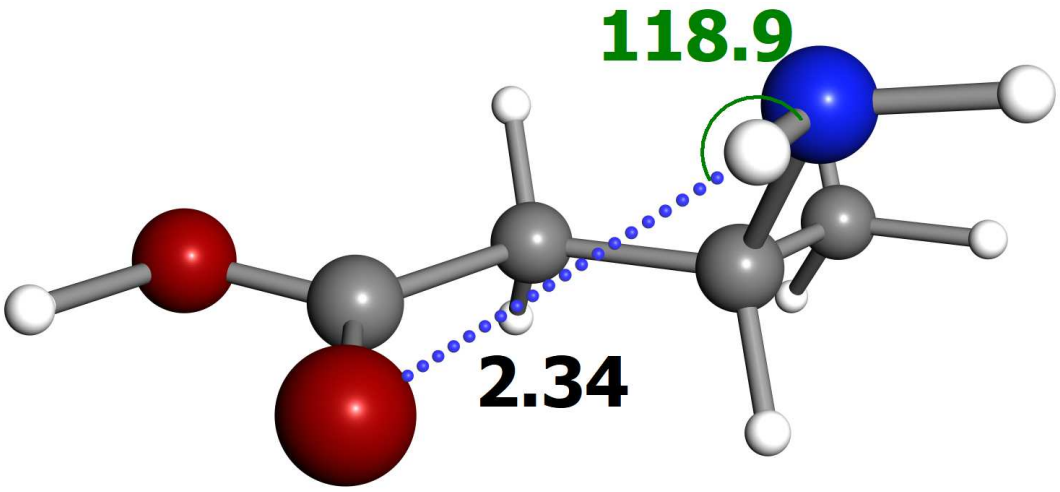
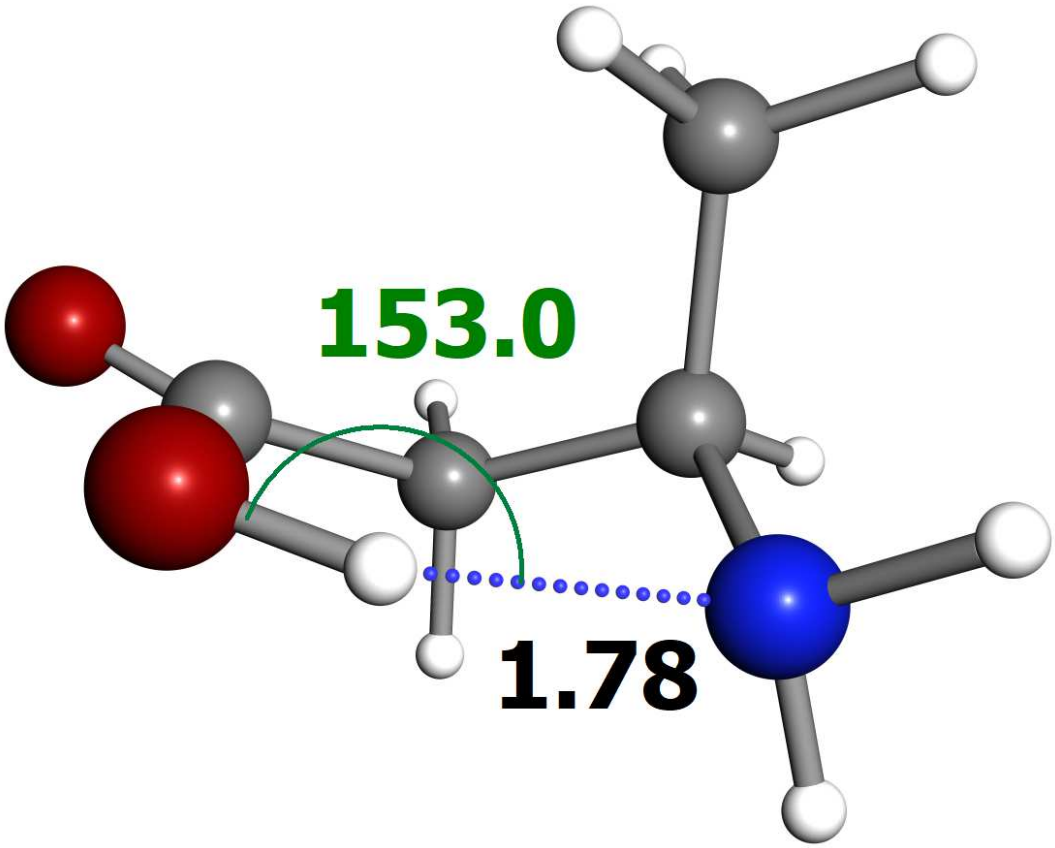
Fig. S01 N-H•••O=C angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 1l' of β-aminobutyric acid. The cartesian coordinates are also given.



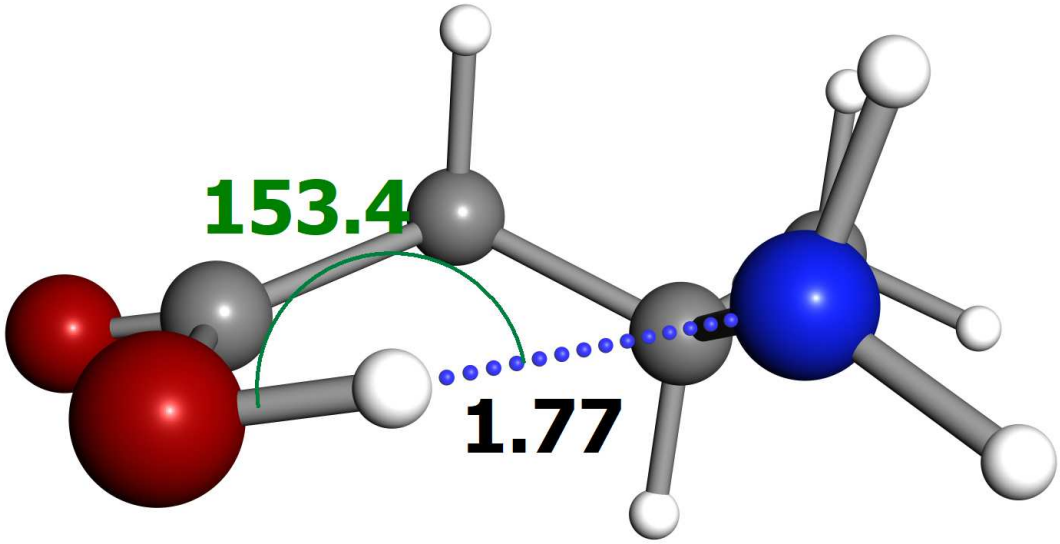
C	2.440196000000	-0.779844000000	0.160153000000
C	1.175045000000	0.060665000000	0.288890000000
N	1.261608000000	1.197437000000	-0.633420000000
C	-0.048160000000	-0.773273000000	-0.077737000000
C	-1.343753000000	-0.020159000000	0.085801000000
O	-2.400791000000	-0.756895000000	-0.336927000000
O	-1.465758000000	1.096405000000	0.544085000000
H	-3.184821000000	-0.207546000000	-0.189484000000
H	0.531158000000	1.868724000000	-0.412340000000
H	2.150434000000	1.673822000000	-0.507542000000
H	0.027490000000	-1.105092000000	-1.119359000000
H	-0.109916000000	-1.671481000000	0.548899000000
H	3.321996000000	-0.193725000000	0.439591000000
H	2.396054000000	-1.656681000000	0.813070000000
H	2.563399000000	-1.112426000000	-0.875345000000
H	1.065375000000	0.381934000000	1.336550000000

Fig. S02 C=O•••N-H angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 2II of β-aminobutyric acid. The cartesian coordinates are also given.



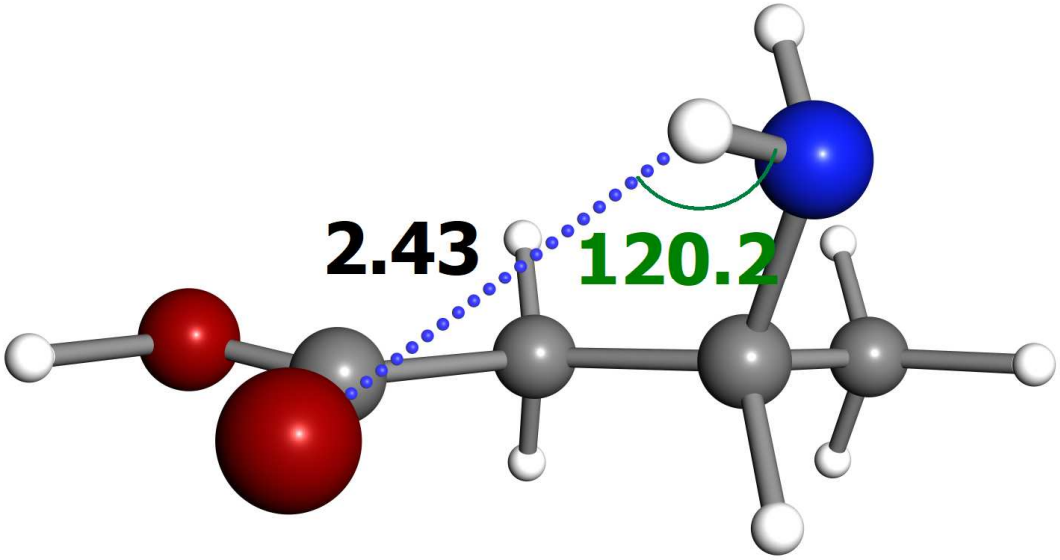
C	1.347120000000	-1.146332000000	-0.846225000000
C	1.230030000000	-0.320543000000	0.430669000000
N	1.552055000000	1.091493000000	0.127711000000
C	-0.186235000000	-0.375233000000	1.018669000000
C	-1.288484000000	0.047718000000	0.048347000000
O	-1.031832000000	1.162218000000	-0.661472000000
O	-2.332577000000	-0.553935000000	-0.060179000000
H	-0.092219000000	1.414523000000	-0.484030000000
H	1.754900000000	1.603654000000	0.983480000000
H	2.382161000000	1.150132000000	-0.456599000000
H	-0.418216000000	-1.388517000000	1.353799000000
H	-0.242224000000	0.285507000000	1.894152000000
H	2.378729000000	-1.146830000000	-1.213775000000
H	1.053519000000	-2.181995000000	-0.654993000000
H	0.700109000000	-0.742800000000	-1.631047000000
H	1.919544000000	-0.734046000000	1.179485000000

Fig. S03 C=O•••N-H angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 3II of β-aminobutyric acid. The cartesian coordinates are also given.



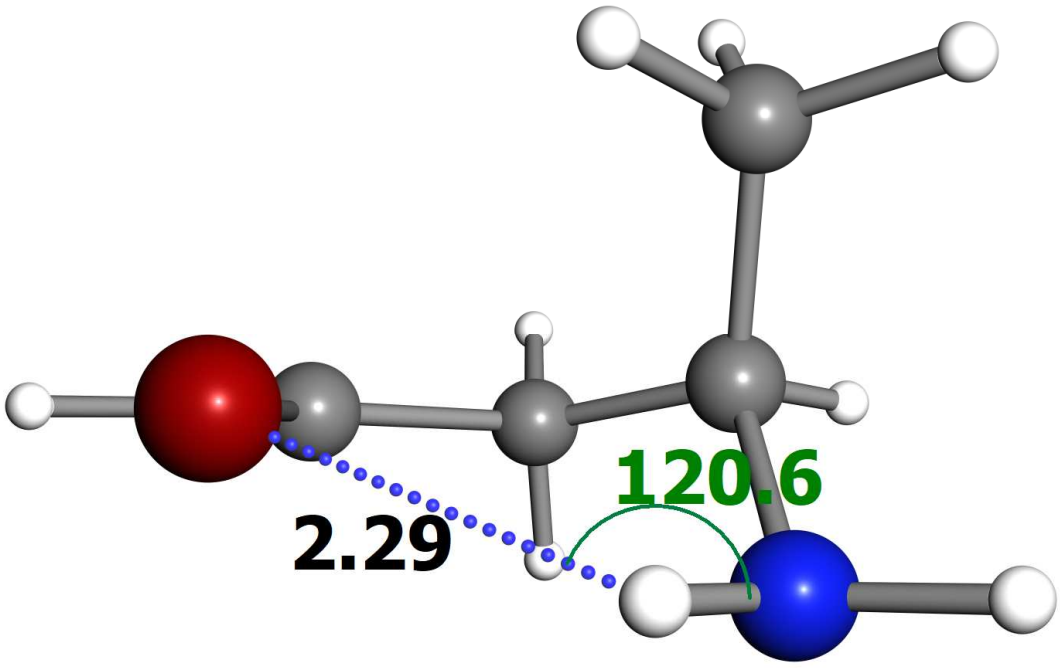
C	-2.394340000	-0.839898000	-0.093471000
C	-1.097671000	-0.066316000	-0.320185000
N	-1.162311000	1.337751000	0.136750000
C	0.084650000	-0.741652000	0.383506000
C	1.456275000	-0.170746000	0.025180000
O	1.515228000	1.167716000	-0.085455000
O	2.430054000	-0.872062000	-0.130349000
H	0.596887000	1.515003000	0.035371000
H	-1.794809000	1.877850000	-0.448447000
H	-1.536792000	1.374005000	1.083732000
H	-0.047824000	-0.644810000	1.470752000
H	0.111479000	-1.808207000	0.150493000
H	-3.234999000	-0.339767000	-0.584805000
H	-2.318181000	-1.856372000	-0.491688000
H	-2.611109000	-0.907447000	0.978997000
H	-0.884210000	-0.028073000	-1.395410000

Fig. S04 N-H•••O=C angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 4l’ of β-aminobutyric acid. The cartesian coordinates are also given.



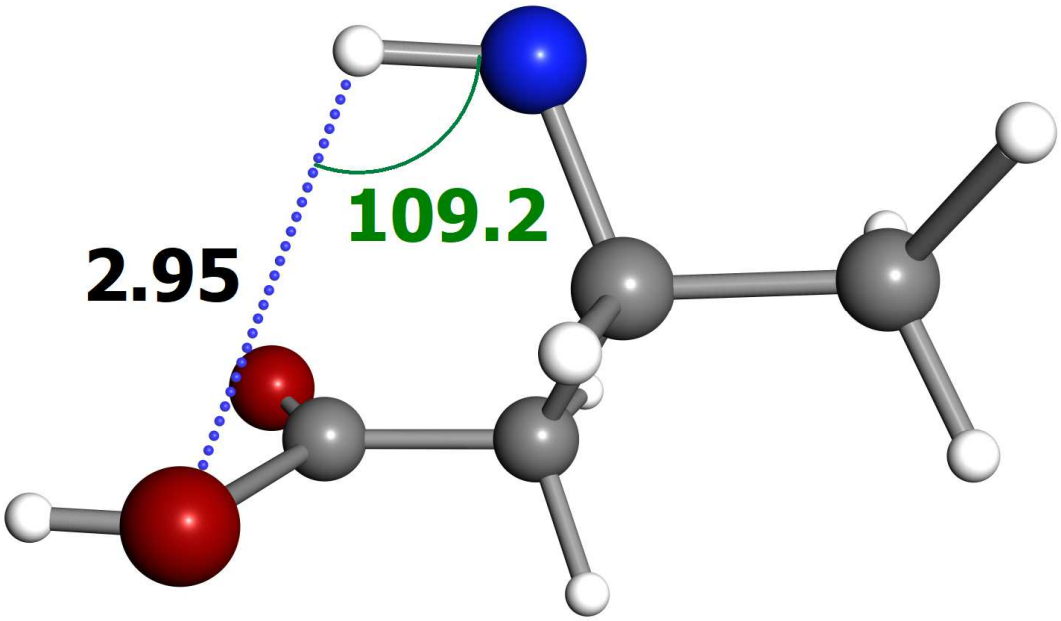
C	-2.452017000	-0.752400000	-0.192906000
C	-1.182668000	0.088663000	-0.282469000
N	-1.338440000	1.270929000	0.564079000
C	0.040852000	-0.772590000	0.055578000
C	1.344601000	-0.031627000	-0.102559000
O	2.385416000	-0.745999000	0.395462000
O	1.484042000	1.058029000	-0.615791000
H	3.177975000	-0.213888000	0.230287000
H	-1.437425000	0.994931000	1.538052000
H	-0.520352000	1.867819000	0.489076000
H	-0.022978000	-1.147300000	1.084738000
H	0.090479000	-1.655494000	-0.595355000
H	-3.319642000	-0.146583000	-0.463557000
H	-2.400041000	-1.620059000	-0.857667000
H	-2.594878000	-1.117126000	0.831536000
H	-1.064337000	0.452685000	-1.308891000

Fig. S05 N-H•••O=C angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 5l' of β-aminobutyric acid. The cartesian coordinates are also given.



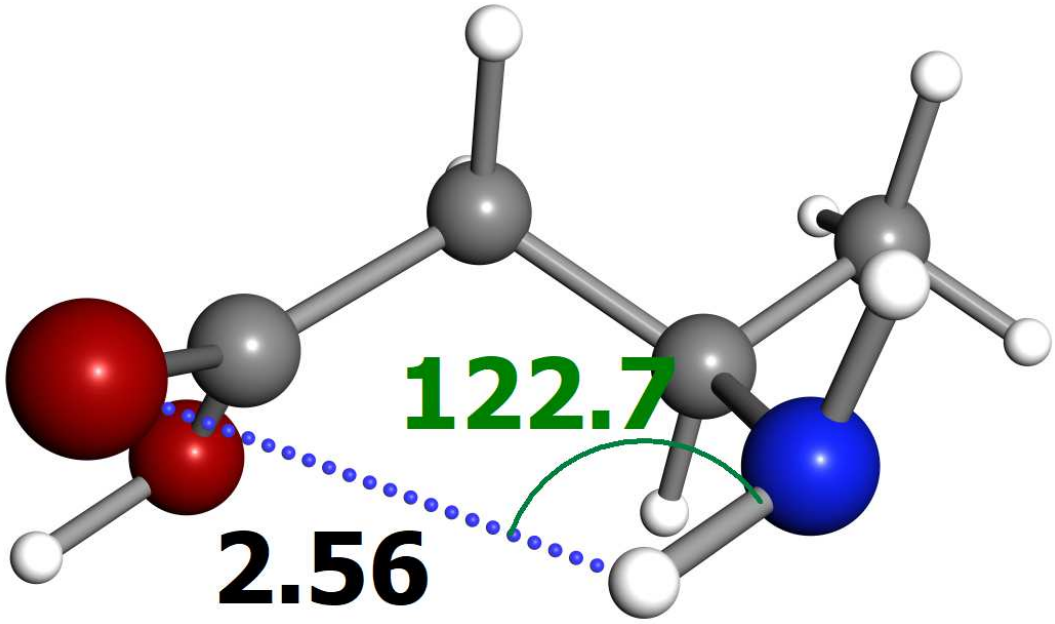
C	-1.617318000	-0.833944000	0.997804000
C	-1.289228000	-0.320321000	-0.409853000
N	-1.574527000	1.100312000	-0.631643000
C	0.161649000	-0.608519000	-0.801475000
C	1.187835000	0.101478000	0.046988000
O	2.431732000	-0.391191000	-0.181015000
O	0.981906000	1.007229000	0.827393000
H	3.030804000	0.139798000	0.364516000
H	-2.568086000	1.275215000	-0.511381000
H	-1.083631000	1.652487000	0.066712000
H	0.372994000	-1.682148000	-0.760022000
H	0.329158000	-0.285390000	-1.835421000
H	-2.680602000	-0.686673000	1.212535000
H	-1.399846000	-1.904788000	1.085570000
H	-1.038264000	-0.294354000	1.752202000
H	-1.907575000	-0.876805000	-1.125021000

Fig. S06 N-H•••O-H angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 6 of β-aminobutyric acid. The cartesian coordinates are also given.



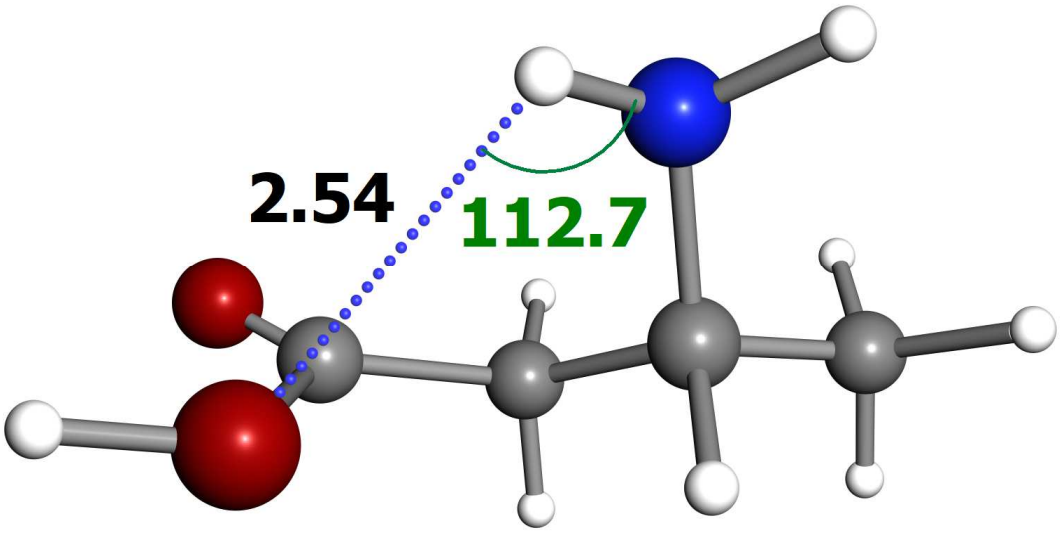
C	2.491879000000	-0.530768000000	-0.133578000000
C	1.121820000000	-0.036035000000	0.318312000000
N	1.103284000000	1.424960000000	0.260728000000
C	0.018543000000	-0.714709000000	-0.523649000000
C	-1.347848000000	-0.184842000000	-0.187341000000
O	-1.651745000000	-0.410398000000	1.120762000000
O	-2.096756000000	0.399110000000	-0.939254000000
H	-2.537052000000	-0.040787000000	1.255547000000
H	1.160444000000	1.741998000000	-0.704381000000
H	0.242365000000	1.800448000000	0.648310000000
H	0.191789000000	-0.530701000000	-1.587938000000
H	0.031314000000	-1.795820000000	-0.342205000000
H	3.272395000000	-0.091358000000	0.491564000000
H	2.554821000000	-1.621545000000	-0.073418000000
H	2.677005000000	-0.235079000000	-1.172996000000
H	0.965568000000	-0.313441000000	1.365898000000

Fig. S07 N-H•••O=C angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 7I' of β-aminobutyric acid. The cartesian coordinates are also given.



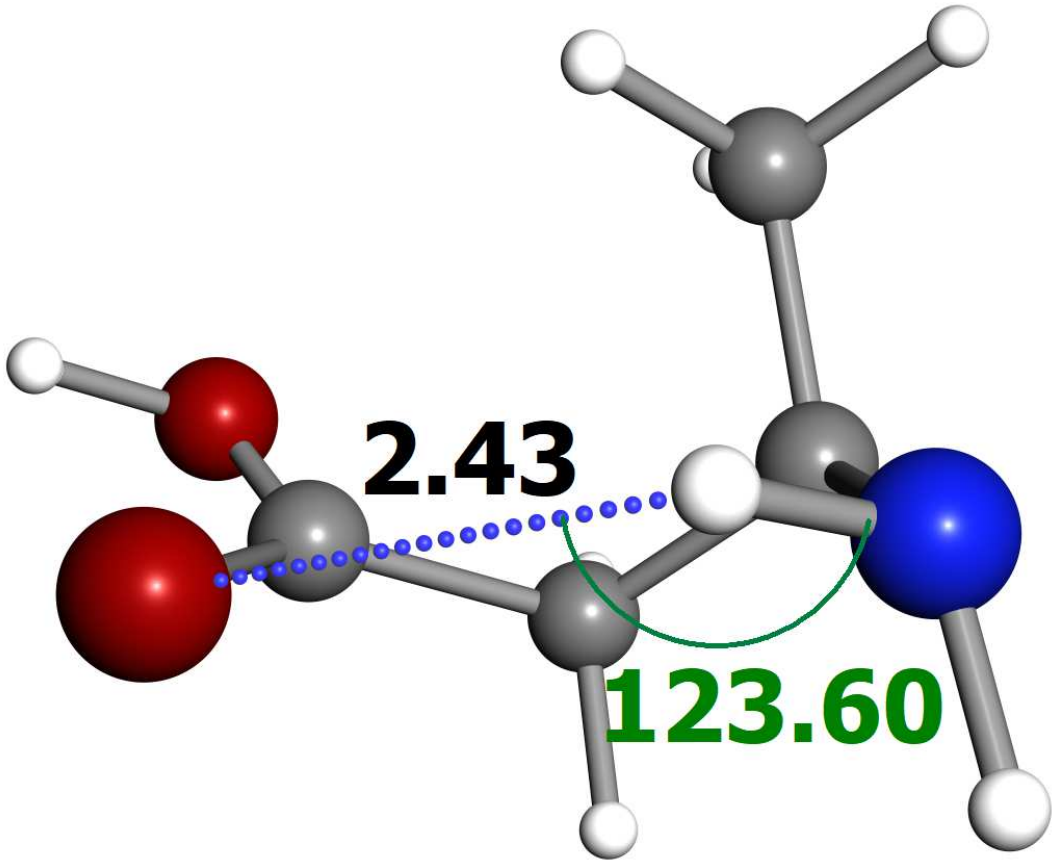
C	-2.436284000000	-0.687630000000	0.101485000000
C	-1.096505000000	-0.095358000000	-0.321607000000
N	-1.247927000000	1.349105000000	-0.473304000000
C	0.005289000000	-0.523225000000	0.683901000000
C	1.348704000000	-0.054919000000	0.204894000000
O	1.955390000000	-0.986856000000	-0.576477000000
O	1.831482000000	1.038874000000	0.413147000000
H	2.775261000000	-0.577115000000	-0.890716000000
H	-1.575391000000	1.749776000000	0.402834000000
H	-0.355020000000	1.792843000000	-0.671860000000
H	-0.198606000000	-0.058955000000	1.653209000000
H	0.009538000000	-1.611927000000	0.786058000000
H	-3.212959000000	-0.393552000000	-0.608431000000
H	-2.387695000000	-1.779207000000	0.147146000000
H	-2.717102000000	-0.315398000000	1.094071000000
H	-0.824739000000	-0.499547000000	-1.304577000000

Fig. S08 N-H•••O-H angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 8III of β-aminobutyric acid. The cartesian coordinates are also given.



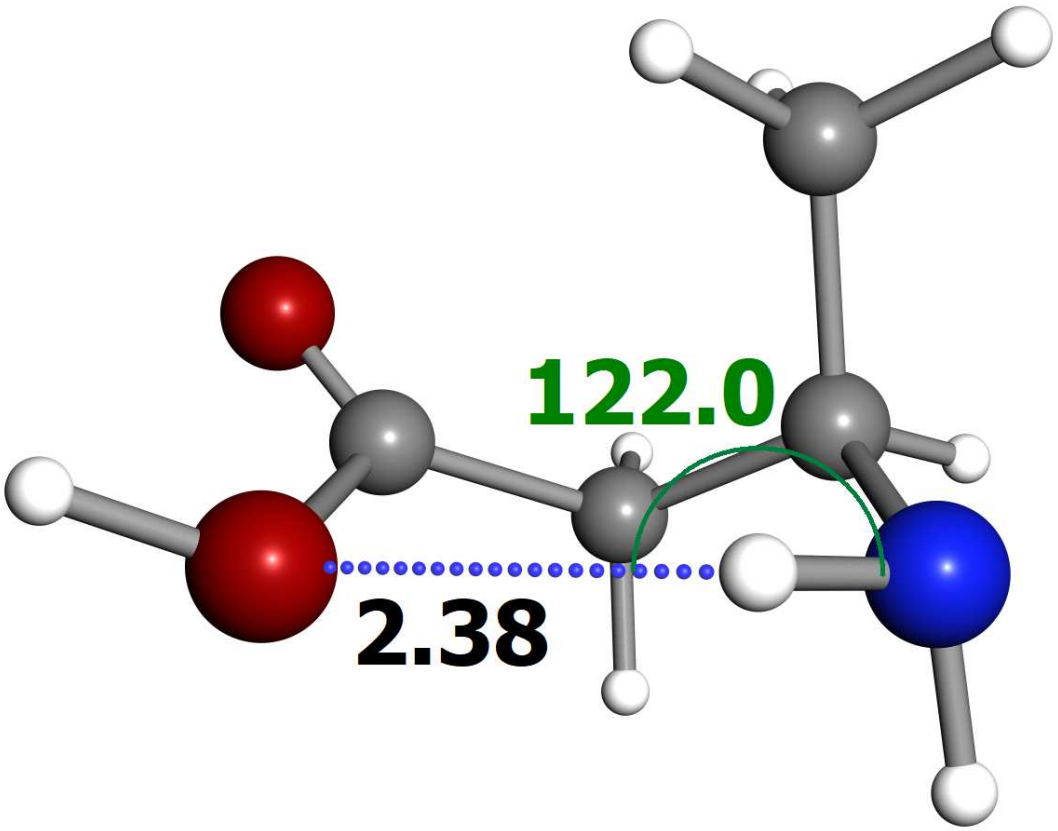
C	2.475288000000	-0.591375000000	0.198270000000
C	1.137650000000	0.136551000000	0.264488000000
N	1.080066000000	1.123099000000	-0.820728000000
C	-0.007441000000	-0.861672000000	0.081853000000
C	-1.379684000000	-0.240553000000	0.005043000000
O	-1.496338000000	0.832980000000	0.840258000000
O	-2.297954000000	-0.632308000000	-0.677130000000
H	-2.411715000000	1.136726000000	0.747072000000
H	0.326312000000	1.783810000000	-0.651432000000
H	1.939640000000	1.665181000000	-0.838132000000
H	0.136245000000	-1.436247000000	-0.836788000000
H	-0.022185000000	-1.560566000000	0.928285000000
H	3.303378000000	0.105146000000	0.366907000000
H	2.530722000000	-1.374637000000	0.959992000000
H	2.602814000000	-1.046233000000	-0.789084000000
H	1.033778000000	0.602045000000	1.255335000000

Fig. S09 N-H•••O=C angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 9I' of β-aminobutyric acid. The cartesian coordinates are also given.



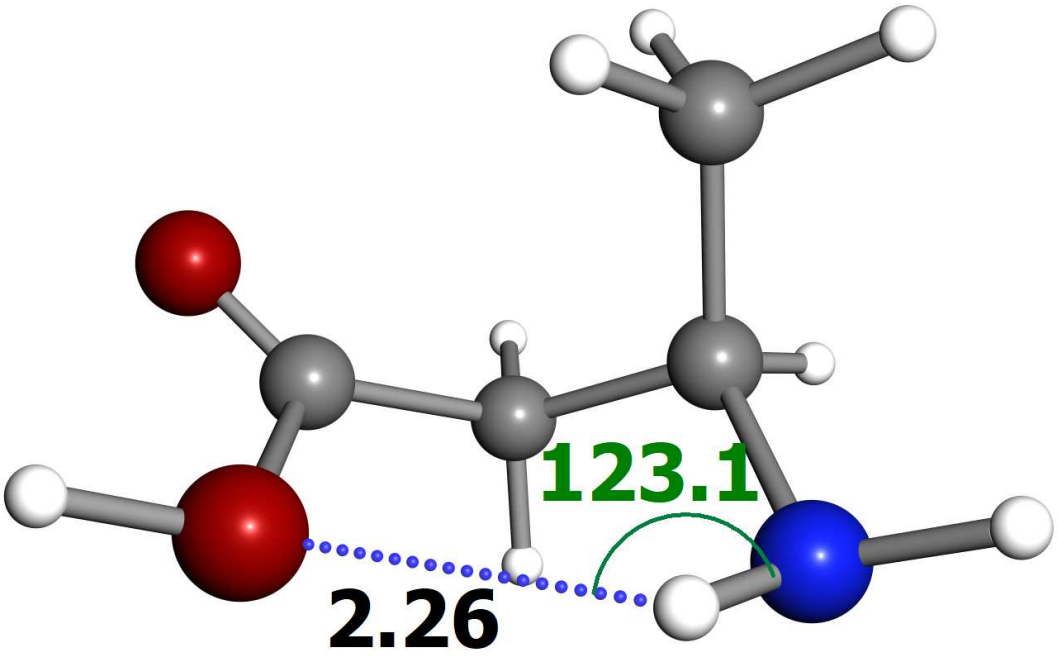
C	-1.224249000	1.320604000	-0.655303000
C	-1.296184000	0.211429000	0.390596000
N	-1.836177000	-0.994980000	-0.230362000
C	0.073042000	0.022592000	1.099730000
C	1.161993000	-0.246884000	0.097073000
O	2.047367000	0.777904000	0.009223000
O	1.241774000	-1.238268000	-0.599672000
H	2.680878000	0.521283000	-0.678236000
H	-1.165071000	-1.363814000	-0.900326000
H	-1.966059000	-1.721748000	0.468462000
H	0.319967000	0.912558000	1.684204000
H	0.008703000	-0.840569000	1.769489000
H	-2.221362000	1.512015000	-1.057889000
H	-0.824465000	2.244235000	-0.225971000
H	-0.576968000	1.023593000	-1.488504000
H	-2.003124000	0.513779000	1.172317000

Fig. S10 N-H•••O-H angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 10III of β-aminobutyric acid. The cartesian coordinates are also given.



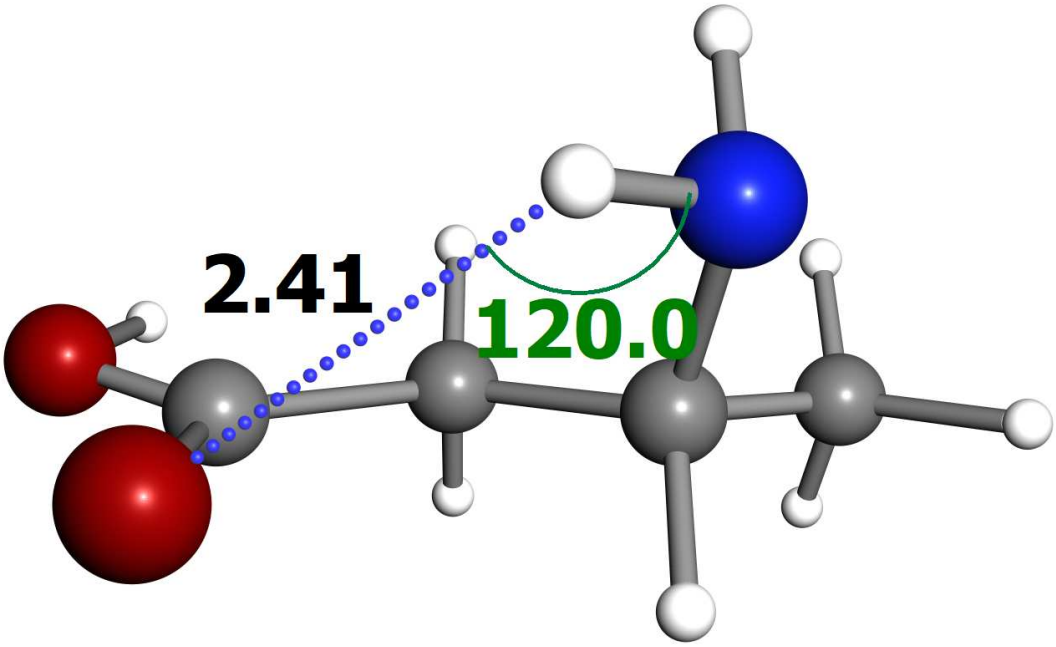
C	1.258905000000	-1.254814000000	-0.729322000000
C	1.291515000000	-0.207235000000	0.379766000000
N	1.794452000000	1.051733000000	-0.165332000000
C	-0.079645000000	-0.120450000000	1.104988000000
C	-1.236393000000	0.010833000000	0.150931000000
O	-1.228131000000	1.214463000000	-0.493277000000
O	-2.076330000000	-0.832569000000	-0.070871000000
H	-1.992106000000	1.195547000000	-1.089694000000
H	1.120376000000	1.435254000000	-0.822268000000
H	1.898315000000	1.740666000000	0.574687000000
H	-0.248767000000	-1.031173000000	1.685126000000
H	-0.071953000000	0.739168000000	1.783499000000
H	2.261771000000	-1.387489000000	-1.140936000000
H	0.890465000000	-2.215038000000	-0.355916000000
H	0.598976000000	-0.934606000000	-1.543833000000
H	2.011154000000	-0.529618000000	1.141668000000

Fig. S11 N-H•••O-H angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 11III of β-aminobutyric acid. The cartesian coordinates are also given.



C	1.260006000000	-1.209700000000	-0.798340000000
C	1.277934000000	-0.242053000000	0.390298000000
N	1.724621000000	1.116011000000	0.069178000000
C	-0.093137000000	-0.189727000000	1.090488000000
C	-1.243957000000	0.013902000000	0.138927000000
O	-1.162623000000	1.213889000000	-0.506236000000
O	-2.143295000000	-0.769182000000	-0.069716000000
H	-1.934912000000	1.250903000000	-1.090612000000
H	2.631410000000	1.079235000000	-0.388486000000
H	1.076130000000	1.549575000000	-0.582384000000
H	-0.281725000000	-1.131125000000	1.610274000000
H	-0.078257000000	0.630366000000	1.815170000000
H	2.264572000000	-1.306147000000	-1.222360000000
H	0.916968000000	-2.205567000000	-0.496515000000
H	0.595533000000	-0.841845000000	-1.588085000000
H	1.980202000000	-0.629662000000	1.138132000000

Fig. S12 N-H•••O=C angle (in green) and hydrogen bond distance in Amstrongs (in black) for conformer 12I' of β-aminobutyric acid. The cartesian coordinates are also given.



C	-2.433662000000	-0.768891000000	-0.206034000000
C	-1.175871000000	0.090726000000	-0.279496000000
N	-1.341931000000	1.249225000000	0.593145000000
C	0.062496000000	-0.762555000000	0.033328000000
C	1.362765000000	0.008691000000	-0.113064000000
O	2.477480000000	-0.635109000000	0.335255000000
O	1.456992000000	1.106832000000	-0.602466000000
H	2.216832000000	-1.483901000000	0.710398000000
H	-1.446567000000	0.953863000000	1.560624000000
H	-0.531244000000	1.857689000000	0.532618000000
H	-0.013420000000	-1.158008000000	1.056493000000
H	0.111926000000	-1.627213000000	-0.643840000000
H	-3.308853000000	-0.168353000000	-0.463417000000
H	-2.372731000000	-1.621792000000	-0.888984000000
H	-2.572101000000	-1.155751000000	0.811011000000
H	-1.060461000000	0.477277000000	-1.297640000000

Table S01. Experimental and calculated spectroscopic parameters for the twelve calculated conformers of β-aminobutyric acid. Ab initio energies are included for the predicted species. All the calculations were done at MP2 using the 6-311++G(d,p) basis set. A, B, and C represent the rotational constants (in MHz); μ_a, μ_b, and μ_c are the electric dipole moment components (in D); Δ_J, Δ_{JK}, and δ_J represent the centrifugal distortion constants (in kHz); χ_{aa}, χ_{bb}, and χ_{cc}, are the diagonal elements of the ^{14}N nuclear quadrupole coupling tensor (in MHz); ΔE is the relative energy (in cm^{-1}) with respect to the global minimum. ΔE_{ZPE} is the relative energy (in cm^{-1}) with respect to the global minimum, taking into account the zero-point energy(ZPE). [a]The values in parenthesis represent the standard error. [b]rms deviation of the fit; [c]Number of quadrupole hyperfine components.

	Experimental					Calculated											
	Rotamer 1	**Rotamer 2**	**Rotamer 3**	**Rotamer 4**	**Rotamer 5**	**1I'**	**2II**	**3II**	**4I'**	**5I'**	**6**	**7I'**	**8III**	**9I'**	**10III**	**11III**	**12I'**
A	5225.68290(79)[a]	4217.8797(26)	5005.35189(72)	5153.4375(15)	4530.9679(16)	5228.8	4195.2	4993.9	5139.6	4505.2	4807.4	4719.2	5038.4	4011.0	3989.3	4042.7	5100.5
B	1588.98441(15)	1911.9396(51)	1687.32715(32)	1574.45638(42)	1698.28098(66)	1595.4	1938.7	1695.3	1574.7	1717.8	1559.8	1657.6	1585.3	1974.9	1978.0	1962.6	1575.8
C	1337.16163(18)	1698.81743(71)	1332.26858(26)	1335.74345(43)	1648.12292(78)	1346.1	1715.8	1338.4	1347.9	1649.6	1523.2	1409.4	1455.2	1676.6	1681.2	1686.4	1346.6
Δ_J	0.1584(51)	0.430(20)	0.1247(50)	0.1510(93)	0.297(18)												
Δ_{JK}	1.451(76)	-	0.205(36)	-	4.41(32)												
δ_J	-	-	0.0237(45)	-	-												
μ_a						-0.3	6.2	6.7	-0.9	-0.1	0.1	0.0	1.5	0.9	0.1	1.2	-1.0
μ_b	…			…	…	0.8	-0.0	-0.5	1.9	1.3	-1.2	-1.5	1.3	1.1	1.1	0.1	-4.1
μ_c	…			…	…	-0.8	-1.9	-0.6	0.7	-0.5	0.2	0.5	2.0	1.3	0.8	-1.0	1.5
χ_{aa}	1.6358(31)	-1.6909(27)	-3.047(30)	-2.703(12)	1.4530(17)	1.83	-1.85	-3.25	-2.82	1.57	-2.35	-1.18	1.80	-3.16	-3.25	2.01	-2.84
χ_{bb}	1.6543(20)	1.2239(68)	1.2185(21)	0.834(18)	2.5729(18)	1.63	1.20	1.31	0.75	2.60	2.42	2.72	0.52	2.49	2.54	0.78	0.75
χ_{cc}	-3.2901(20)	0.4671(68)	1.8285(21)	1.869(18)	-4.0259(18)	-3.40	0.65	1.94	2.07	-4.17	-0.07	-1.54	-2.33	0.67	0.71	-2.78	2.09
σ[b]	2.1	2.8	2.5	3.4	3.2												
N[c]	48	37	49	29	20												
ΔE						231	0	139	594	670	754	769	788	784	939	951	2503
ΔE_{ZPE}						0	12	98	324	467	509	538	566	612	755	774	2171
ΔG_{ZPE}						0	248	278	289	472	373	319	521	606	762	815	2163

Table S02. Experimental and calculated spectroscopic parameters for the detected conformers of β-aminobutyric acid. Ab initio energies are included for the predicted species. All the calculations were done at MP2 using the 6-311++G(d,p) basis set. *A*, *B*, and *C* represent the rotational constants (in MHz); μ_a, μ_b, and μ_c are the electric dipole moment components (in D); Δ_J, Δ_{JK}, and δ_J represent the centrifugal distortion constants (in kHz); χ_{aa}, χ_{bb}, and χ_{cc}, are the diagonal elements of the ^{14}N nuclear quadrupole coupling tensor (in MHz); ΔE is the relative energy (in cm^{-1}) with respect to the global minimum. ΔE_{ZPE} is the relative energy (in cm^{-1}) with respect to the global minimum, taking into account the zero-point energy (ZPE). [a]The values in parenthesis represent the standard error. [b]rms deviation of the fit; [c]Number of quadrupole hyperfine components.

	Experimental					Calculated				
	Rotamer 1	Rotamer 2	Rotamer 3	Rotamer 4	Rotamer 5	1I'	2II	3II	4I'	5I'
A	5225.68290(79)[a]	4217.8797(26)	5005.35189(72)	5153.4375(15)	4530.9679(16)	5228.8	4195.2	4993.9	5139.6	**4505.2**
B	1588.98441(15)	1911.9396(51)	1687.32715(32)	1574.45638(42)	1698.28098(66)	1595.4	1938.7	1695.3	1574.7	**1717.8**
C	1337.16163(18)	1698.81743(71)	1332.26858(26)	1335.74345(43)	1648.12292(78)	1346.1	1715.8	1338.4	1347.9	**1649.6**
Δ_J	0.1584(51)	0.430(20)	0.1247(50)	0.1510(93)	0.297(18)					
Δ_{JK}	1.451(76)	-	0.205(36)	-	4.41(32)					
δ_J	-	-	0.0237(45)	-	-					
$\lvert\mu_a\rvert$						0.3	6.2	6.7	0.9	**0.1**
$\lvert\mu_b\rvert$	...			...	...	0.8	0.0	0.5	1.9	**1.3**
$\lvert\mu_c\rvert$	...			...	...	0.8	1.9	0.6	0.7	**0.5**
χ_{aa}	1.6358(31)	-1.6909(27)	-3.047(30)	-2.703(12)	1.4530(17)	1.83	-1.85	-3.25	-2.82	**1.57**
χ_{bb}	1.6543(20)	1.2239(68)	1.2185(21)	0.834(18)	2.5729(18)	1.63	1.20	1.31	0.75	**2.60**
χ_{cc}	-3.2901(20)	0.4671(68)	1.8285(21)	1.869(18)	-4.0259(18)	-3.40	0.65	1.94	2.07	**-4.17**
σ[b]	2.1	2.8	2.5	3.4	3.2					
N[c]	48	37	49	29	20					
ΔE						231	0	139	594	**670**
ΔE_{ZPE}						0	12	98	324	**467**
ΔG_{ZPE}						0	248	278	289	**472**

Table S03. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of conformer 1I′ of β-aminobutyric acid.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
3	1	3	2	1	2	4	3	8392.897	0.001
3	1	3	2	1	2	2	1	8393.042	-0.004
3	1	3	2	1	2	3	2	8393.088	-0.000
3	0	3	2	0	2	4	3	8728.070	-0.000
3	0	3	2	0	2	2	1	8728.151	-0.002
3	0	3	2	0	2	3	2	8728.174	0.002
3	1	2	2	1	1	4	3	9148.027	0.001
3	1	2	2	1	1	3	2	9148.160	-0.001
3	1	2	2	1	1	2	1	9147.870	-0.001
4	1	4	3	1	3	5	4	11176.726	0.001
4	1	4	3	1	3	3	2	11176.812	-0.001
4	1	4	3	1	3	4	3	11176.834	0.001
4	0	4	3	0	3	5	4	11580.073	0.001
4	0	4	3	0	3	3	2	11580.103	-0.000
4	0	4	3	0	3	4	3	11580.193	-0.001
4	1	3	3	1	2	3	2	12181.622	0.001
4	1	3	3	1	2	5	4	12181.677	0.000
4	1	3	3	1	2	4	3	12181.754	0.002
5	1	5	4	1	4	6	5	13949.795	0.000
5	1	5	4	1	4	4	3	13949.851	-0.001
5	1	5	4	1	4	5	4	13949.874	-0.000
1	1	1	0	0	0	0	1	6562.011	-0.003
1	1	1	0	0	0	2	1	6562.757	-0.001
1	1	1	0	0	0	1	1	6563.253	-0.002
2	1	2	1	0	1	3	2	9237.001	0.000
2	1	2	1	0	1	1	0	9237.150	0.000
2	1	2	1	0	1	2	1	9237.565	-0.003
3	1	3	2	0	2	2	1	11790.170	0.000
3	1	3	2	0	2	4	3	11790.288	0.002
3	1	3	2	0	2	3	2	11790.956	-0.001
4	1	4	3	0	3	3	2	14238.831	0.002
4	1	4	3	0	3	5	4	14238.941	0.001
4	1	4	3	0	3	4	3	14239.619	0.000
5	1	5	4	0	4	4	3	16608.572	-0.005
5	1	5	4	0	4	6	5	16608.667	0.004
5	1	5	4	0	4	5	4	16609.300	0.001
1	1	0	0	0	0	1	1	6813.847	0.006
1	1	0	0	0	0	2	1	6814.824	-0.004
1	1	0	0	0	0	0	1	6816.313	0.004
2	1	1	1	0	1	2	1	9991.804	0.004
2	1	1	1	0	1	3	2	9992.820	-0.002
2	1	1	1	0	1	1	0	9993.855	0.001
3	1	2	2	0	2	3	2	13300.263	0.000
3	1	2	2	0	2	4	3	13301.238	-0.000
3	1	2	2	0	2	2	1	13301.697	-0.001

4	1	3	3	0	3	4	3	16753.841	-0.002
4	1	3	3	0	3	5	4	16754.842	-0.003
4	1	3	3	0	3	3	2	16755.168	0.002

Table S04. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of conformer 2II of β-aminobutyric acid.

J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
2	1	2	1	1	1	2	1	7007.954	-0.001
2	1	2	1	1	1	3	2	7008.471	-0.002
2	1	2	1	1	1	1	0	7009.107	-0.000
2	0	2	1	0	1	3	2	7207.435	0.002
2	0	2	1	0	1	1	0	7206.969	-0.000
2	0	2	1	0	1	2	1	7207.405	-0.005
2	0	2	1	0	1	2	2	7206.906	0.003
2	0	2	1	0	1	1	1	7208.242	0.005
2	1	1	1	1	0	2	1	7434.205	0.005
2	1	1	1	1	0	3	2	7434.737	0.004
2	1	1	1	1	0	1	0	7435.166	0.004
3	1	3	2	1	2	3	2	10503.899	-0.001
3	1	3	2	1	2	4	3	10504.041	-0.001
3	1	3	2	1	2	2	1	10504.062	0.001
3	0	3	2	0	2	2	1	10776.138	-0.001
3	0	3	2	0	2	3	2	10776.246	-0.001
3	0	3	2	0	2	4	3	10776.246	-0.000
3	2	2	2	2	1	3	2	10831.800	-0.002
3	2	2	2	2	1	4	3	10832.345	0.000
3	2	2	2	2	1	2	1	10832.642	-0.005
3	2	1	2	2	0	3	2	10887.778	0.003
3	2	1	2	2	0	4	3	10888.342	0.002
3	2	1	2	2	0	2	1	10888.644	-0.006
3	1	2	2	1	1	3	2	11142.684	0.001
3	1	2	2	1	1	2	1	11142.802	-0.003
3	1	2	2	1	1	4	3	11142.835	-0.001
4	1	4	3	1	3	4	3	13990.112	0.004
4	1	4	3	1	3	3	2	13990.153	-0.001
4	1	4	3	1	3	5	4	13990.168	0.002
4	0	4	3	0	3	3	2	14305.446	0.002
4	0	4	3	0	3	5	4	14305.494	-0.002
4	0	4	3	0	3	4	3	14305.507	-0.001
1	1	0	0	0	0	2	1	6129.793	-0.001
1	1	0	0	0	0	1	1	6129.930	-0.004
2	1	1	1	0	1	3	2	9953.691	0.004
2	1	1	1	0	1	2	1	9953.802	0.001
3	1	2	2	0	2	4	3	13889.087	-0.000

Table S05. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of conformer 3II of β-aminobutyric acid.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
2	0	2	1	0	1	3	2	6012.258	0.000
2	0	2	1	0	1	2	1	6012.181	-0.005
2	0	2	1	0	1	1	0	6011.435	0.001
2	0	2	1	0	1	2	2	6011.271	-0.001
2	1	1	1	1	0	3	2	6394.423	-0.000
2	1	1	1	1	0	2	1	6393.485	0.002
2	1	1	1	1	0	1	0	6395.465	0.001
3	1	3	2	1	2	4	3	8509.996	-0.001
3	1	3	2	1	2	3	2	8509.718	-0.001
3	1	3	2	1	2	2	1	8509.977	0.004
3	0	3	2	0	2	4	3	8951.849	-0.001
3	0	3	2	0	2	3	2	8951.808	0.004
3	0	3	2	0	2	2	1	8951.662	-0.001
3	2	2	2	2	1	4	3	9058.984	-0.002
3	2	2	2	2	1	3	2	9058.008	0.002
3	2	1	2	2	0	4	3	9165.944	-0.003
3	2	1	2	2	0	3	2	9164.976	-0.000
3	2	1	2	2	0	2	1	9166.490	0.001
3	1	2	2	1	1	4	3	9573.872	-0.001
3	1	2	2	1	1	3	2	9573.602	-0.001
3	1	2	2	1	1	2	1	9573.887	-0.000
4	1	4	3	1	3	5	4	11317.948	-0.000
4	1	4	3	1	3	4	3	11317.820	-0.001
4	1	4	3	1	3	3	2	11317.900	0.000
4	0	4	3	0	3	5	4	11817.327	-0.001
4	0	4	3	0	3	4	3	11817.292	0.000
4	0	4	3	0	3	3	2	11817.244	0.003
4	2	3	3	2	2	4	3	12057.011	0.000
4	2	3	3	2	2	5	4	12057.430	0.001
4	2	3	3	2	2	3	2	12057.536	-0.000
4	1	3	3	1	2	4	3	12730.348	-0.000
4	1	3	3	1	2	3	2	12730.449	0.000
4	1	3	3	1	2	5	4	12730.478	0.000
5	1	5	4	1	4	5	4	14104.851	-0.001
5	1	5	4	1	4	4	3	14104.886	0.001
5	1	5	4	1	4	6	5	14104.925	0.002
5	0	5	4	0	4	6	5	14599.517	-0.000
5	0	5	4	0	4	5	4	14599.486	-0.001
5	0	5	4	0	4	4	3	14599.465	-0.001
1	1	1	0	0	0	2	1	6337.558	-0.001
1	1	1	0	0	0	1	1	6337.927	0.002
2	1	2	1	0	1	3	2	9002.129	-0.002
2	1	2	1	0	1	2	1	9002.460	0.001
1	1	0	0	0	0	2	1	6692.590	0.003
1	1	0	0	0	0	1	1	6693.136	0.001

1	1	0	0	0	0	0	1	6691.760	-0.005
2	1	1	1	0	1	3	2	10067.266	0.004
2	1	1	1	0	1	2	1	10067.779	-0.006
2	1	1	1	0	1	1	0	10066.109	0.001

Table S06. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of conformer 4I of β-aminobutyric acid.

J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
2	0	2	1	0	1	3	2	5808.907	-0.000
2	1	1	1	1	0	3	2	6059.259	-0.001
3	1	3	2	1	2	3	2	8365.296	0.004
3	1	3	2	1	2	2	1	8365.511	0.004
3	1	3	2	1	2	4	3	8365.538	-0.004
3	0	3	2	0	2	2	1	8684.453	0.007
3	0	3	2	0	2	3	2	8684.569	0.005
3	0	3	2	0	2	4	3	8684.612	0.002
3	1	2	2	1	1	3	2	9081.079	-0.002
3	1	2	2	1	1	4	3	9081.312	-0.008
3	1	2	2	1	1	2	1	9081.346	-0.002
4	1	4	3	1	3	4	3	11141.180	-0.003
4	1	4	3	1	3	3	2	11141.250	0.000
4	1	4	3	1	3	5	4	11141.300	0.000
4	0	4	3	0	3	4	3	11526.871	-0.000
4	0	4	3	0	3	5	4	11526.913	0.001
4	0	4	3	0	3	3	2	11526.840	0.004
5	0	5	4	0	4	5	4	14327.718	0.001
5	0	5	4	0	4	6	5	14327.753	-0.002
1	1	1	0	0	0	0	1	6488.769	0.005
1	1	1	0	0	0	2	1	6489.142	0.003
1	1	1	0	0	0	1	1	6489.388	-0.001
2	1	2	1	0	1	3	2	9160.662	0.001
2	1	2	1	0	1	2	1	9160.872	0.001
2	1	2	1	0	1	1	0	9159.774	-0.005
3	1	3	2	0	2	4	3	11717.292	-0.004
3	1	3	2	0	2	2	1	11717.102	-0.004
3	1	3	2	0	2	3	2	11717.324	0.000
1	1	0	0	0	0	2	1	6727.803	0.003

Table S07. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of conformer 5I of β-aminobutyric acid.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
1	1	1	0	0	0	0	1	6177.791	-0.004
1	1	1	0	0	0	2	1	6178.950	-0.002
1	1	1	0	0	0	1	1	6179.721	-0.003
3	0	3	2	1	2	4	3	7253.533	0.001
3	0	3	2	1	2	3	2	7252.764	-0.006
3	0	3	2	1	2	2	1	7254.065	0.001
2	1	2	1	0	1	1	0	9475.025	0.005
2	1	2	1	0	1	3	2	9475.087	0.001
2	1	2	1	0	1	2	1	9475.949	0.005
4	0	4	3	1	3	4	3	10668.145	0.004
4	0	4	3	1	3	5	4	10669.028	0.002
4	0	4	3	1	3	3	2	10669.386	-0.004
3	1	3	2	0	2	2	1	12746.162	-0.003
3	1	3	2	0	2	4	3	12746.411	0.002
3	1	3	2	0	2	3	2	12747.391	-0.001
4	1	4	3	0	3	4	3	15994.754	-0.005
4	1	4	3	0	3	5	4	15993.731	0.001
4	1	4	3	0	3	3	2	15993.518	0.003
1	1	0	0	0	0	2	1	6229.440	-0.000
2	1	1	1	0	1	3	2	9626.031	0.000

Fig. S13 Calculated relaxed potential energy surface varying the C-C-C=O dihedral angle of structures 1I' and 8III. As can be seen, structure 8III experiences conformer interconversion into structure 1I' and it is "missing" during the expansion. The calculation was done using the MP2 theory and Pople´s 6-311++G (d,p) basis set.

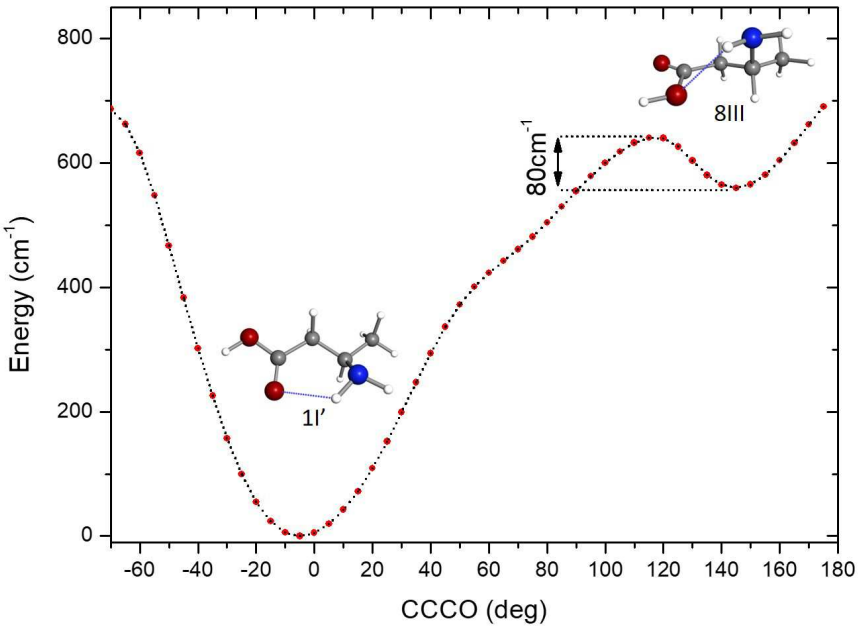


Fig. S14 Calculated relaxed potential energy surface varying the C-C-C=O dihedral angle of structures 5I' and 11III. The calculation was done using the MP2 theory and Pople´s 6-311++G (d,p) basis set. The barrier decreases to 390 cm^{-1} when the B3LYP method is used (see Figure S05), indicating that structure 11III could experience conformer interconversion into structure 5I'.

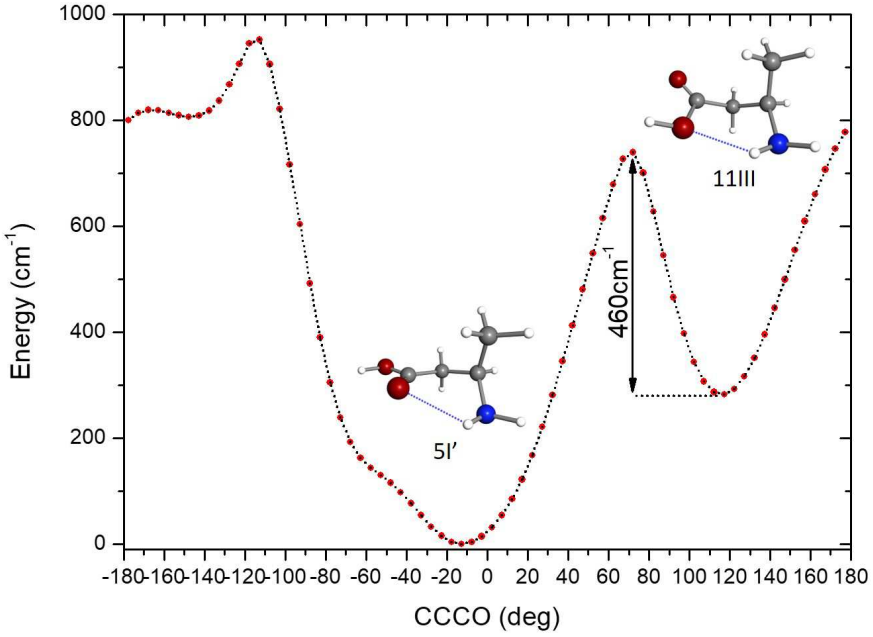


Fig. S15 Calculated relaxed potential energy surface varying the C-C-C=O dihedral angle of structures 9I' and 10III. As can be seen, structure 10III experiences conformer interconversion into structure 9I' and it is "missing" during the expansion. The calculation was done using the MP2 theory and Pople´s 6-311++G (d,p) basis set.

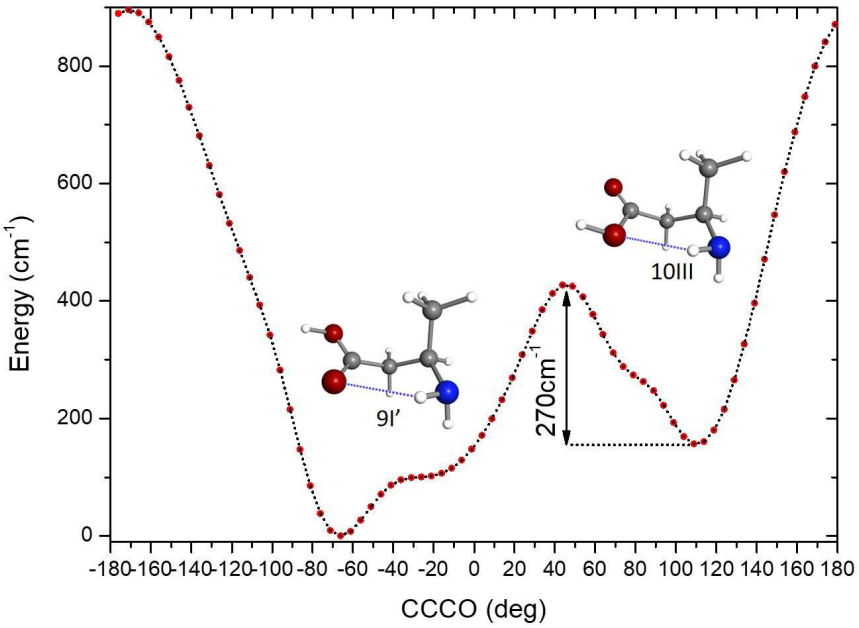


Fig. S16 Calculated relaxed potential energy surface varying the C-C-C=O dihedral angle of structures 1I' and 8III. As can be seen, structure 8III experiences conformer interconversion into structure 1I' and it is "missing" during the expansion. The calculation was done using the B3LYP density functional with the Grimme D3 dispersion interactions and Pople´s 6-311++G (d,p) basis set.

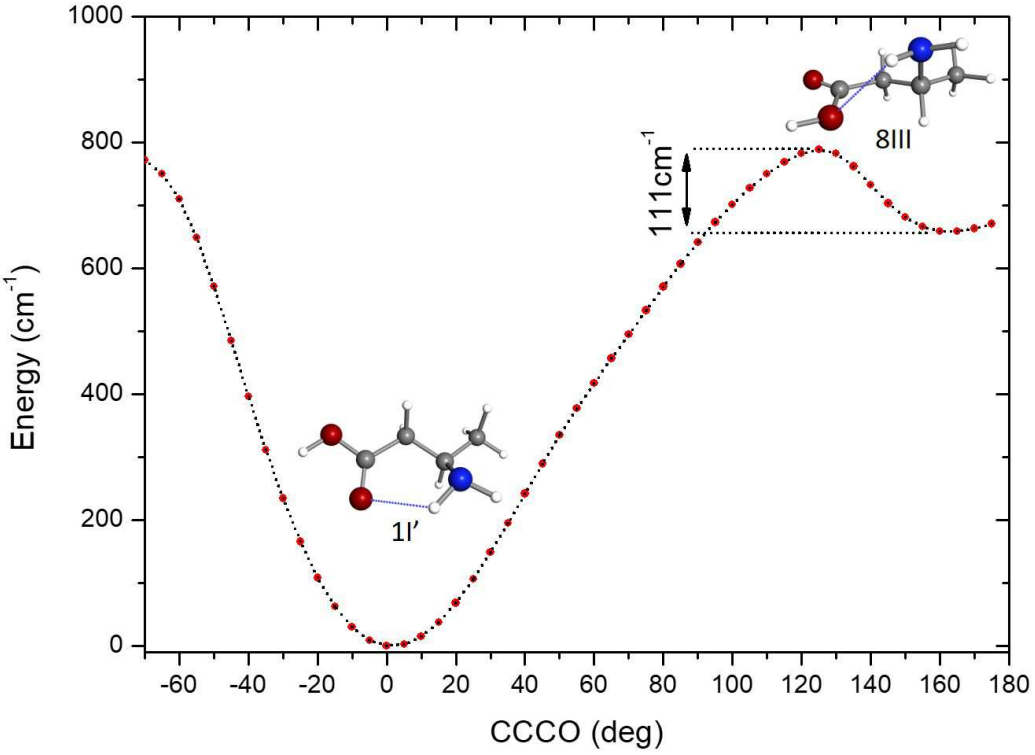


Fig. S17 Calculated relaxed potential energy surface varying the C-C-C=O dihedral angle of structures 5I' and 11III. As can be seen, structure 11III experiences conformer interconversion into structure 5I' and it is "missing" during the expansion. The calculation was done using the B3LYP density functional with the Grimme D3 dispersion interactions and Pople´s 6-311++G (d,p) basis set.

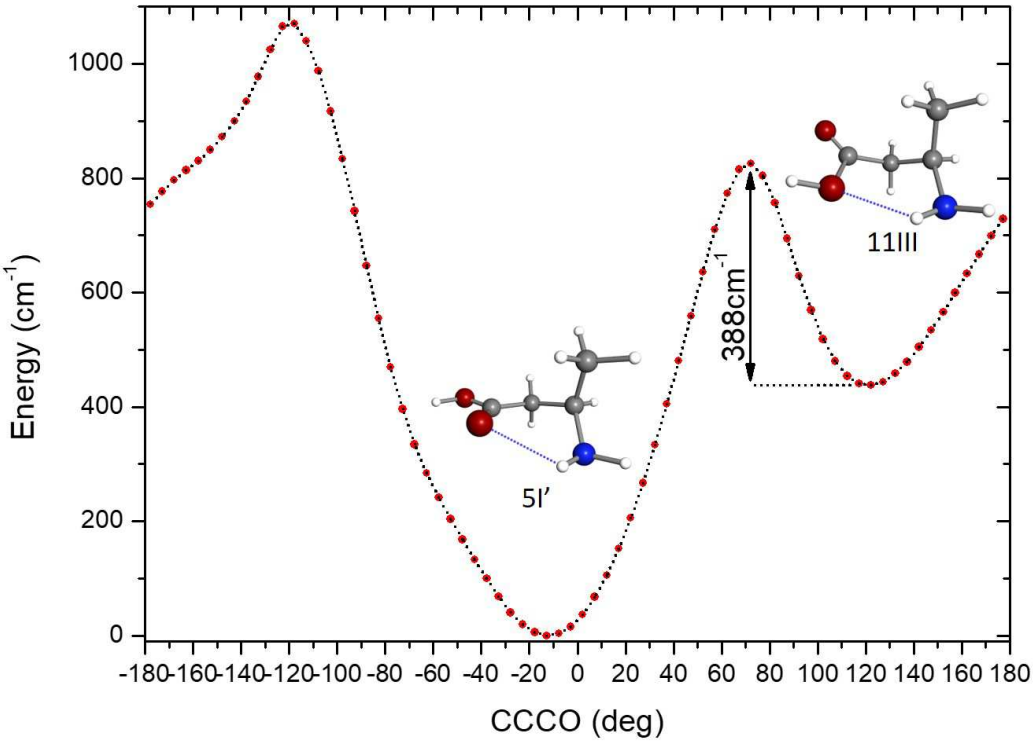


Fig. S18 Calculated relaxed potential energy surface varying the C-C-C=O dihedral angle of structures 9I' and 10III. As can be seen, structure 10III experiences conformer interconversion into structure 9I' and it is "missing" during the expansion. The calculation was done using the B3LYP density functional with the Grimme D3 dispersion interactions and Pople´s 6-311++G (d,p) basis set.