SUPPORTING INFORMATION

Conformational impact of the aliphatic side chain in local anaesthetics: benzocaine, butamben and isobutamben

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1. Studied Systems

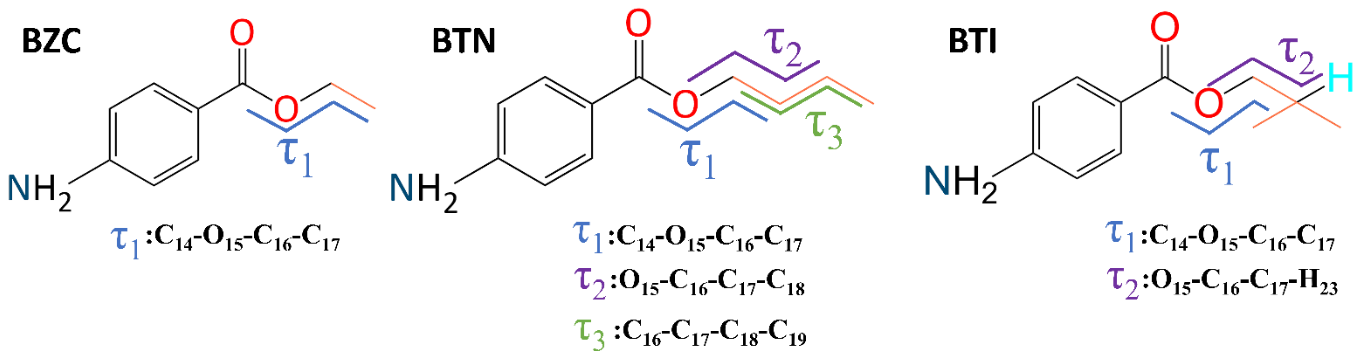
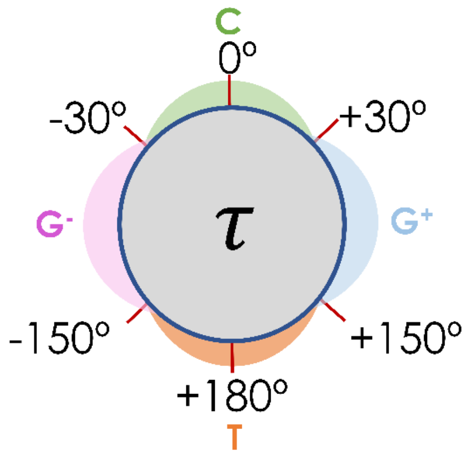


Figure S1. General molecular structure of benzocaine (BZC), butamben (BTN) and isobutamben (BTI).



C =*cis*/ G$^-$ = *gauche* $^-$/ G$^+$ = *gauche* $^+$/ T = *trans*

Figure S2. Nomenclature used for the dihedral angles,τ, represented in Figure S1.

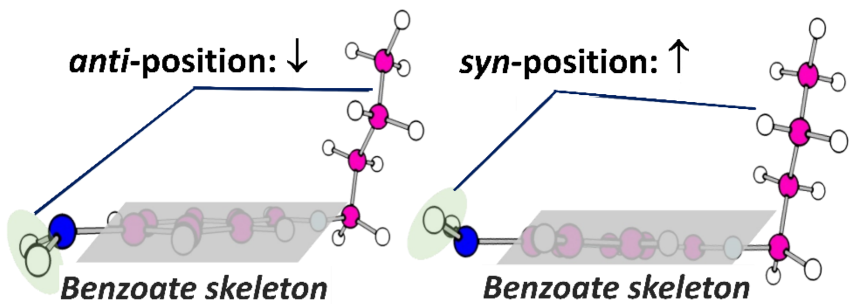


Figure S3. Nomenclature used for the amine hydrogens position with respect to the alkyl chain of each conformer.

2. Computational Methods

The first step involves an exhaustive conformational search of the system using a molecular mechanics method (Merck Molecular Force Field: MMFFs[1]). Thus, the relative energy of the three studied molecules in each conformation was estimated within an energy window of 20 kJ mol^{-1}. All the geometries found were later fully re-optimized by quantum mechanical methods, such as the MP2[2] *ab initio* method and Density Functional Theory (DFT) procedures (M06-2X[3,4] and B3LYP- D3BJ[5,6]). In both cases, the basis-set used was the *Popple's triple zeta* 6-311 basis increased with polarization and diffusion functions (6-311++G(d,p))[7,8,9]. On the other hand, harmonic frequency calculations were also carried out. All the theoretical calculations were implemented in Gaussian 16.[10]

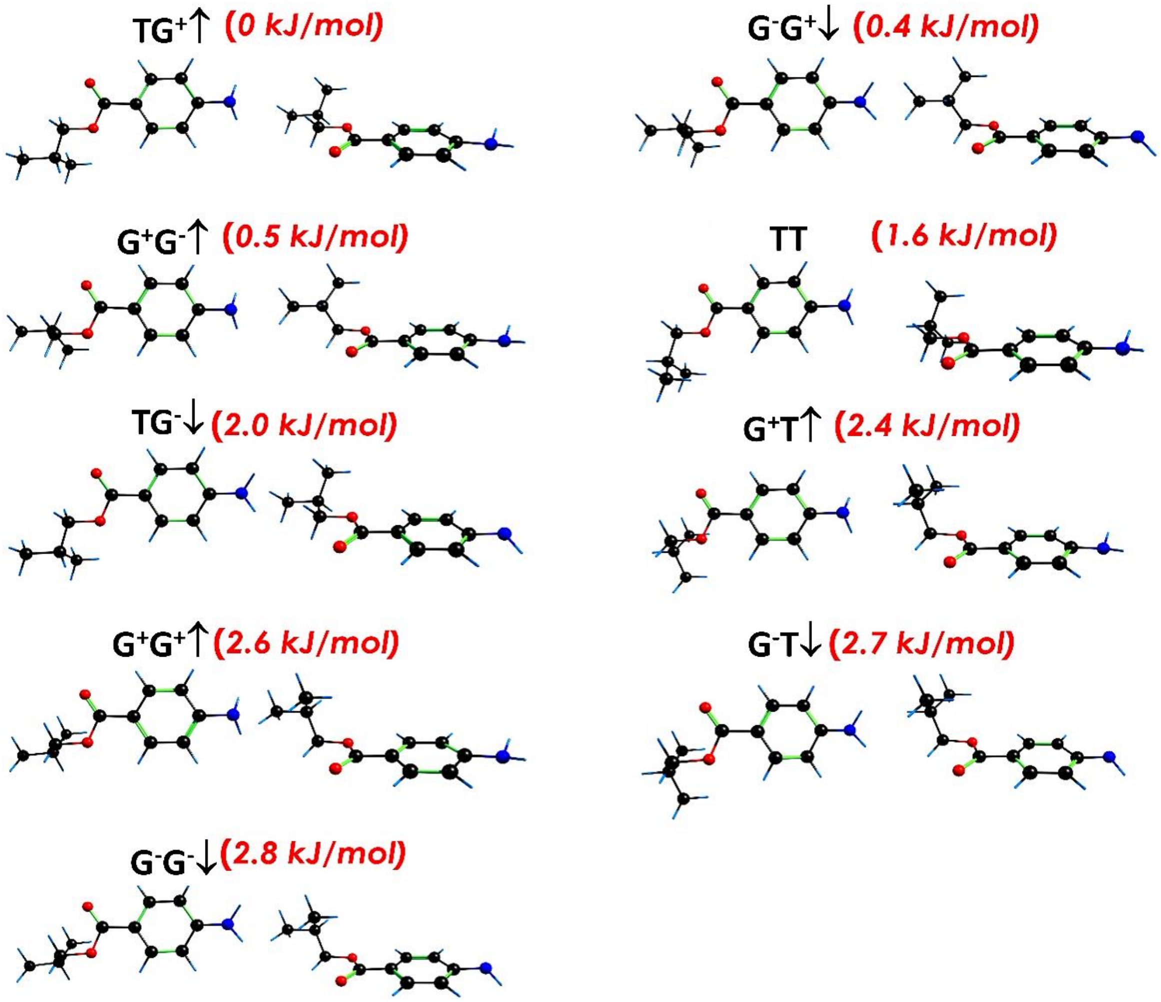


Figure S4. MP2 computed structures of the most stable conformers of BTI in two points of view and with their respective relative energies (ΔE_0/kJ·mol^{-1}) with respect to the most stable conformer. The conformers are labelled following the nomenclature displayed in Figure S2 and S3.

Table S1. Predicted parameters for BTI at MP2, M06-2X and B3LYP-D3BJ level using 6-311++G(d,p) basis.

MP2 / 6-311++G(d,p)

	A/MHz	B/MHz	C/MHz	μ_A/D	μ_B/D	μ_C/D	ΔE_0 /kJ·mol^{-1}	ΔG_0/ kJ·mol^{-1}	τ_1	τ_2	NH_2 (↑/↓)*
BTI 1 (TG$^+$↑)	1828.7	281.7	250.7	**-1.4**	**-2.6**	**-0.7**	0.0	0.0	178.1	57.8	↑
BTI 2 (G$^-$G$^+$↓)	1996.5	287.0	267.6	**-2.0**	**-1.5**	**1.0**	0.4	2.1	-80.0	+62.7	↓
BTI 3 (G$^+$G$^-$↑)	1977.8	288.3	268.4	**-1.6**	**-2.2**	**1.0**	0.5	2.3	79.8	-62.9	↑
BTI 4 (TT)	1501.9	314.6	276.2	**-1.3**	**-2.4**	**1.1**	1.6	2.0	-179.5	-180.0	↑=↓
BTI 5 (TG$^-$↓)	1829.7	281.6	250.6	**-1.5**	**-2.2**	**1.4**	2.0	2.9	-178.2	-57.8	↓
BTI 6 (G$^+$T↑)	1593.5	324.1	295.8	**-1.4**	**-2.3**	**1.1**	2.4	4.4	102.7	179.4	↑
BTI 7 (G$^+$G$^+$↑)	2014.0	285.8	271.8	**-1.5**	**-2.2**	**1.4**	2.6	4.2	103.7	58.7	↑
BTI 8 (G$^-$T↓)	1603.5	323.1	295.0	**-1.8**	**-1.8**	**-0.9**	2.7	4.8	-102.8	-179.4	↓
BTI 9 (G$^-$G$^-$↓)	2021.5	285.4	271.3	**-1.9**	**-1.9**	**0.7**	2.8	4.3	-104.1	-58.8	↓

B3LYP-D3BJ / 6-311++G(d,p)

	A/MHz	B/MHz	C/MHz	μ_A/D	μ_B/D	μ_C/D	ΔE_0 /kJ·mol^{-1}	ΔG_0/ kJ·mol^{-1}	τ_1	τ_2	NH_2 (↑/↓)*
BTI 1 (TG$^+$↑)	1816.4	282.4	251.0	**-2.1**	**-3.0**	**-0.5**	0.3	0.0	176.0	56.7	↑
BTI 2 (G$^-$G$^+$↓)	1978.4	286.2	265.3	**-2.7**	**-1.9**	**0.8**	0.0	0.5	-83.6	+61.2	↓
BTI 3 (G$^+$G$^-$↑)	1979.7	286.2	265.2	**-2.4**	**-2.5**	**0.8**	0.0	0.6	83.6	-61.2	↑
BTI 4 (TT)	1496.7	314.3	275.8	**-1.9**	**-2.9**	**0.8**	1.2	1.0	-179.8	-180.0	↑=↓
BTI 5 (TG$^-$↓)	1815.7	282.4	250.9	**-2.1**	**-2.7**	**1.2**	0.3	0.0	-176.4	-56.8	↓
BTI 6 (G$^+$T↑)	1586.8	321.8	292.3	**-2.1**	**-2.7**	**1.0**	2.3	2.9	106.5	178.6	↑
BTI 7 (G$^+$G$^+$↑)	1993.5	283.6	268.9	**-2.3**	**-2.6**	**1.1**	1.8	1.9	108.6	56.9	↑
BTI 8 (G$^-$T↓)	1585.9	321.9	292.4	**-2.5**	**-2.3**	**-0.6**	2.2	2.9	-106.4	-178.6	↓
BTI 9 (G$^-$G$^-$↓)	1992.1	283.7	269.0	**-2.6**	**-2.3**	**-0.5**	1.7	1.9	-108.6	-56.9	↓

M06-2X / 6-311++G(d,p)

	A/MHz	B/MHz	C/MHz	μ_A/D	μ_B/D	μ_C/D	ΔE_0 /kJ·mol^{-1}	ΔG_0/ kJ·mol^{-1}	τ_1	τ_2	NH_2 (↑/↓)*
BTI 1 (TG$^+$↑)	1836.9	284.3	252.2	**-1.8**	**-2.8**	**-0.5**	0.0	0.0	178.4	57.8	↑
BTI 2 (G$^-$G$^+$↓)	2012.3	288.0	268.0	**-2.4**	**-1.8**	**0.8**	0.5	1.2	-81.0	61.5	↓
BTI 3 (G$^+$G$^-$↑)	2012.4	288.0	267.9	**-2.1**	**-2.3**	**0.8**	0.5	1.3	81.0	-61.5	↑
BTI 4 (TT)	1509.1	317.2	278.3	**-1.7**	**-2.8**	**0.9**	0.9	1.1	-180.0	-180.0	↑=↓
BTI 5 (TG$^-$↓)	1836.7	284.3	252.1	**-1.9**	**-2.6**	**1.2**	0.2	0.5	-178.7	-57.9	↓
BTI 6 (G$^+$T↑)	1612.6	326.4	297.6	**-1.9**	**-2.5**	**1.0**	2.7	4.0	101.1	179.3	↑
BTI 7 (G$^+$G$^+$↑)	2060.2	286.6	272.6	**-2.0**	**-2.3**	**1.3**	2.5	4.0	101.5	58.6	↑
BTI 8 (G$^-$T↓)	1612.9	326.4	297.7	**-2.2**	**-2.1**	**-0.7**	2.6	3.9	-101.0	-179.3	↓
BTI 9 (G$^-$G$^-$↓)	2060.1	286.6	272.6	**-1.9**	**0.7**	**2.8**	2.5	4.1	-101.5	-58.6	↓

Table S2. Predicted nuclear quadrupolar constants of ^{14}N (expressed in MHz) for BTI at MP2, M06-2X and B3LYP-D3BJ level using 6-311++G(d,p) basis.

	MP2			B3LYP-D3BJ			M06-2X		
	χ_{aa}	χ_{bb}	χ_{cc}	χ_{aa}	χ_{bb}	χ_{cc}	χ_{aa}	χ_{bb}	χ_{cc}
BTI 1 (TG$^+$↑)	2.202	1.999	-4.201	2.378	2.258	-4.636	2.300	2.200	-4.500
BTI 5 (TG$^-$↓)	2.467	1.638	-4.105	2.601	1.974	-4.576	2.500	2.000	-4.500
Planar	2.846	2.208	-5.054	2.811	2.352	-5.163	2.749	2.314	-5.064
BTI 2 (G$^-$G$^+$↓)	2.673	1.122	-3.795	2.758	1.364	-4.122	2.700	1.300	-4.000
BTI 3 (G$^+$G$^-$↑)	1.660	1.546	-3.206	1.878	1.771	-3.649	1.800	1.700	-3.500
Planar	2.656	1.626	-4.281	2.687	1.682	-4.369	2.534	1.685	-4.219
BTI 4 (TT)	2.342	2.005	-4.347	2.496	2.283	-4.779	2.400	2.200	-4.600
Planar	2.785	2.366	-5.150	2.820	2.529	-5.349	2.757	2.470	-5.227
BTI 6 (G$^+$T↑)	1.499	1.832	-3.331	1.740	2.113	-3.853	1.700	2.000	-3.700
BTI 8 (G$^-$T↓)	2.661	1.448	-4.109	2.734	1.757	-4.491	2.700	1.700	-4.400
BTI 7 (G$^+$G$^+$↑)	1.655	1.944	-3.599	1.875	2.173	-4.048	1.800	2.200	-4.000
BTI 9 (G$^-$G$^-$↓)	2.669	1.778	-4.448	2.753	1.955	-4.708	2.700	2.100	-4.800

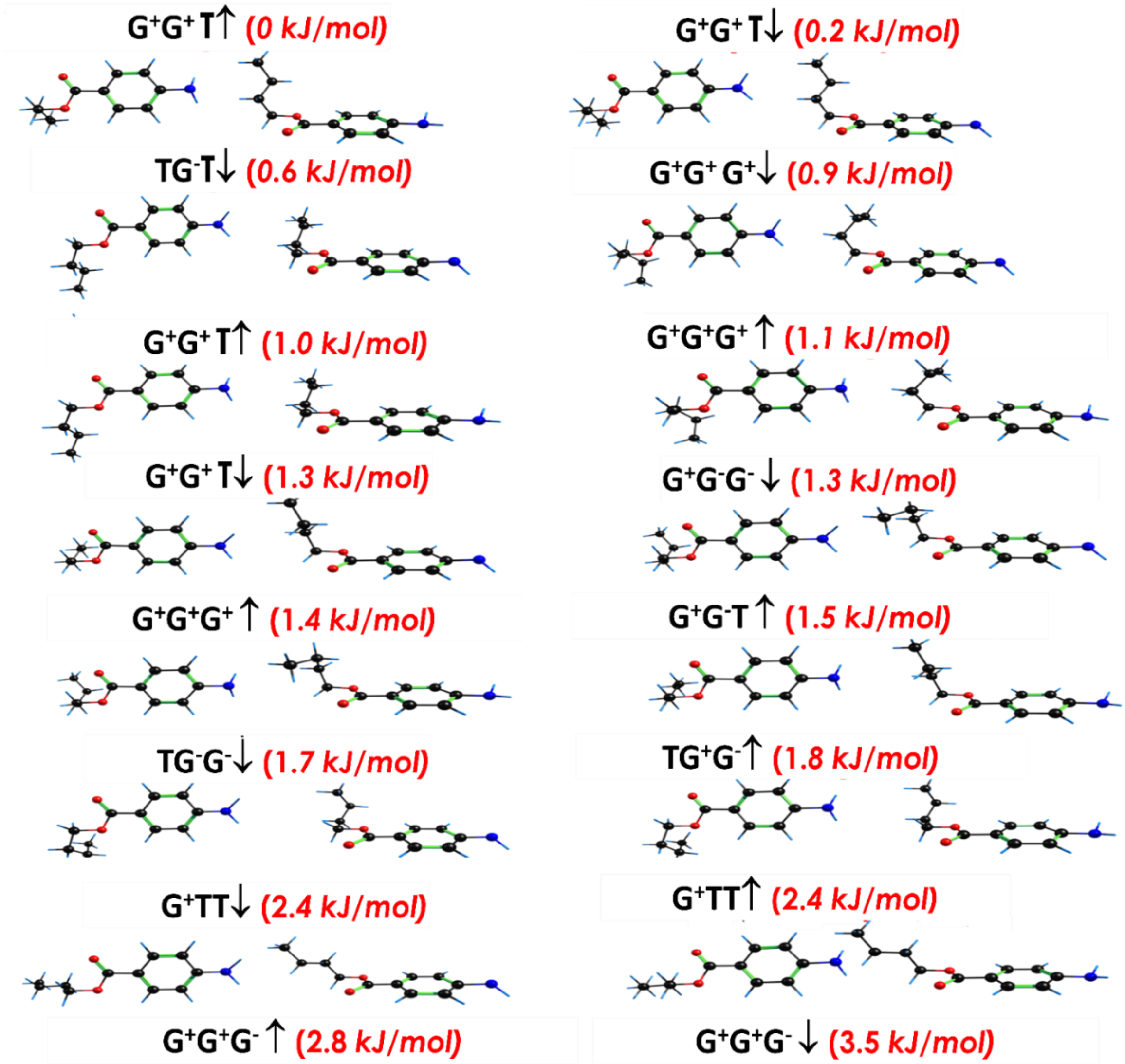


Figure S5. MP2 computed structures of the most stable conformers of BTN in two points of view and with their respective relative energies (ΔE_0/kJ·mol^{-1}) with respect to the most stable conformer. The conformers are labelled following the nomenclature displayed in Figure S2 and S3.

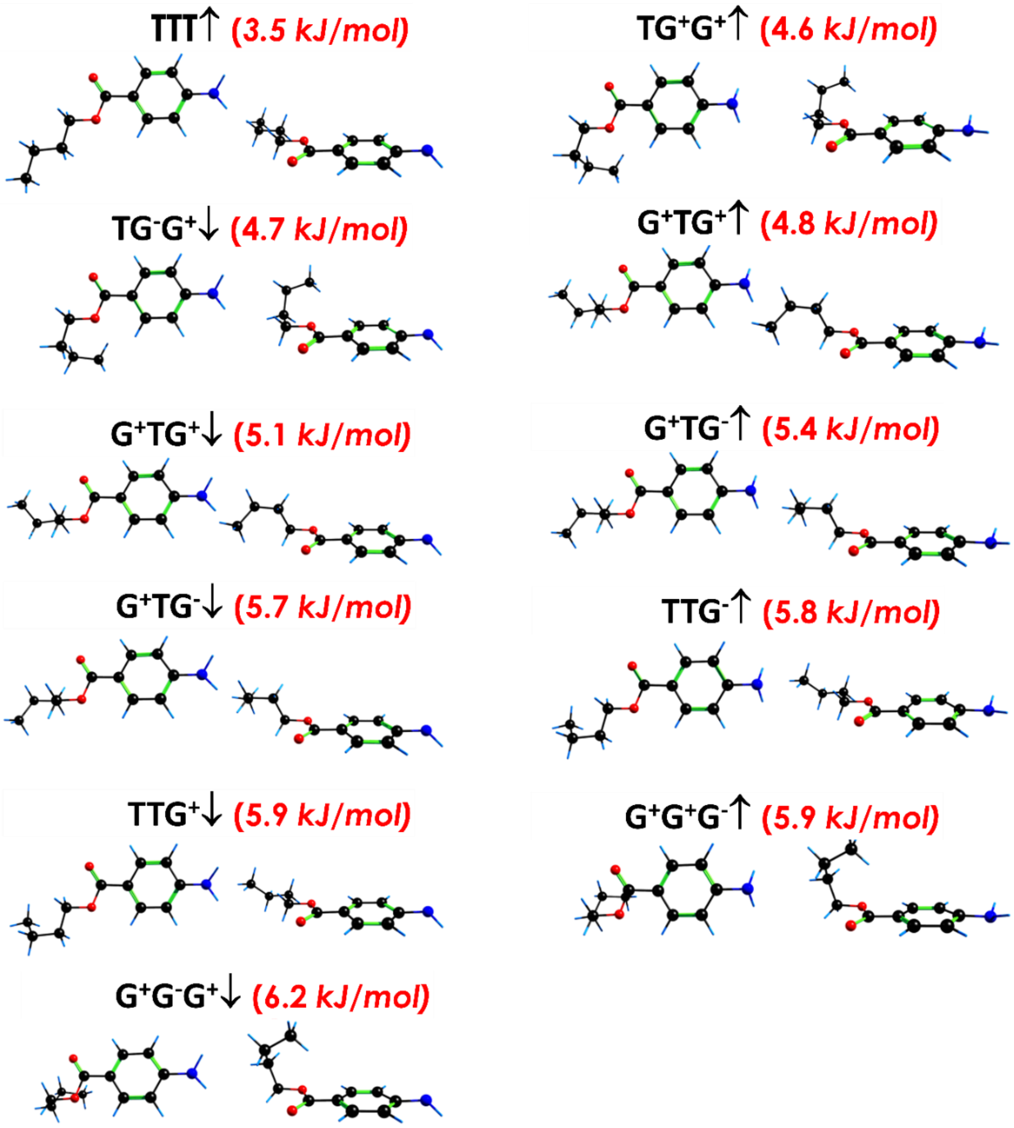


Figure S5. Continue to previous page.

Table S3. Predicted parameters for BTN at MP2, M06-2X and B3LYP-D3BJ level using 6-311++G(d,p) basis.

MP2 / 6-311++G(d,p)												
	A/MHz	**B/MHz**	**C/MHz**	**μ_A/D**	**μ_B/D**	**μ_C/D**	**ΔE_0 /kJ·mol^{-1}**	**ΔG_0/ kJ·mol^{-1}**	τ_1	τ_2	τ_3	**NH_2 (↑/↓)***
BTN 1 (G^+G^+T↑)	1420.1	299.8	279.3	-1.3	2.7	-0.1	0.0	0.1	78.5	56.2	179.1	↑
BTN 2 (G^+ G^+T↓)	1437.6	297.6	278.1	-1.9	-1.3	-1.5	0.2	0.5	78.8	56.4	179.2	↓
BTN 3 (T G^-T↓)	1376.7	292.1	247.0	-1.2	-2.3	-1.3	0.6	0.0	-178.3	63.3	179.3	↓
BTN 4 ($G^+G^+G^+$↓)	1469.7	329.0	291.1	1.8	-1.7	1.1	0.9	2.1	75.1	46.2	56.5	↓
BTN 5 (TG^+T↑)	1373.3	292.5	246.8	-1.0	2.7	0.8	1.0	0.9	-179.2	63.3	179.3	↑
BTN 6 ($G^+G^+G^+$↑)	1457.3	331.2	292.2	1.4	-2.5	-0.8	1.1	2.7	75.0	46.1	56.6	↑
BTN 7 (G^+G^-T↓)	1489.1	293.3	289.8	-2.0	0.6	-1.7	1.3	1.7	101.0	-62.2	-178.0	↓
BTN 8 ($G^-G^-G^-$↓)	1669.8	308.7	293.2	2.2	1.8	-0.1	1.3	2.9	106.3	-64.5	-67.5	↓
BTN 9 ($G^+G^-G^-$↑)	1662.1	309.2	293.8	1.7	1.5	2.0	1.4	3.2	105.9	-64.7	-67.7	↑
BTN 10 (G^+G^+T↑)	1478.3	294.4	290.4	-1.4	2.4	-0.9	1.5	2.1	100.7	-62.4	-177.9	↑
BTN 11 (TG^+G^+↓)	1451.4	309.5	274.2	-1.5	-2.2	-1.5	1.7	1.3	-177.4	55.9	55.7	↓
BTN 12 (TG^+G^+↑)	1448.8	309.4	273.5	-1.2	-2.7	-0.5	1.8	1.8	-178.5	56.1	55.8	↑
BTN 13 (G^+TT↓)	2193.3	241.5	233.0	-1.9	-1.7	-0.6	2.4	2.5	80.6	177.5	-179.3	↓
BTN 14 (G^+TT↑)	2158.1	242.1	233.8	1.4	-1.9	1.5	2.4	2.6	80.6	177.4	-179.2	↑
BTN 15 ($G^+G^+G^-$↑)	1481.7	340.4	312.0	-1.4	2.7	0.2	2.8	3.3	77.3	59.7	-76.9	↑
BTN 16 ($G^+G^+G^-$↓)	1493.0	338.3	310.1	-1.9	1.3	-1.4	3.5	4.4	77.5	60.2	-76.3	↓
BTN 17 (TTT)	2001.6	237.5	213.5	-1.2	-2.4	-1.1	3.5	2.7	179.2	179.9	-180.0	↑
BTN 18 (TG^-G^+↑)	1404.0	327.8	275.7	1.1	-2.6	-0.5	4.6	4.1	179.6	-73.9	67.5	↑
BTN 19 (TG^-G^+↓)	1407.6	327.4	276.9	1.4	-2.1	1.5	4.7	4.0	177.8	-73.8	67.3	↓
BTN 20 (G^+T G^+↑)	2476.1	251.0	236.2	1.6	-1.8	1.4	4.8	5.1	81.6	173.7	64.2	↑
BTN 21 (G^+TG^+↓)	2502.1	250.6	235.6	1.9	-1.6	-0.7	5.1	5.4	81.7	173.8	64.2	↓
BTN 22 (G^+T G^-↑)	2420.3	246.8	231.9	1.4	-1.9	1.4	5.4	6.2	81.0	-176.9	-62.2	↑
BTN 23 (G^+T G^-↓)	2444.5	246.4	231.3	1.7	-1.8	-0.7	5.7	6.3	81.1	-176.9	-62.2	↓
BTN 24 (TTG^+↑)	2234.3	243.2	223.2	-1.3	2.2	-1.1	5.8	5.8	179.8	174.4	62.0	↑
BTN 25 (TTG^+↓)	2242.8	243.2	223.1	-1.4	-2.3	-1.0	5.9	5.8	178.1	174.2	61.8	↓
BTN 26 ($G^+G^-G^+$↑)	1550.5	327.9	324.9	-1.5	-2.5	0.0	5.9	7.5	102.6	-63.5	86.0	↑
BTN 27 ($G^+G^-G^+$↓)	1563.7	325.6	323.6	-2.0	-1.2	-1.3	6.2	8.1	102.8	-63.6	85.8	↓

B3LYP-D3BJ / 6-311++G(d.p)												
	A/MHz	**B/MHz**	**C/MHz**	**μ_A/D**	**μ_B/D**	**μ_C/D**	**ΔE_0 /kJ·mol^{-1}**	**ΔG_0/ kJ·mol^{-1}**	τ_1	τ_2	τ_3	**NH_2 (↑/↓)***
BTN 1 (G^+G^+T↑)	1434.1	294.9	272.1	-2.1	2.9	-0.2	0.4	1.1	83.2	59.1	-179.8	↑
BTN 2 (G^+ G^+T↓)	1433.0	295.0	272.3	-2.5	1.9	-1.4	0.3	1.1	83.2	59.1	-179.8	↓
BTN 3 (T G^-T↓)	1367.4	292.7	247.0	-1.8	2.9	-1.2	0.0	0.0	-176.7	64.3	179.9	↓
BTN 4 ($G^+G^+G^+$↓)	1485.1	313.3	276.4	2.4	-2.3	0.9	2.0	2.7	81.9	53.7	61.1	↓
BTN 5 (TG^+T↑)	1367.9	292.6	247.0	-1.6	3.2	0.5	0.0	0.0	176.8	64.3	179.9	↑
BTN 6 ($G^+G^+G^+$↑)	1486.0	313.2	276.2	2.0	-2.9	-0.7	2.1	2.7	81.9	53.7	61.1	↑
BTN 7 (G^+G^-T↓)	1480.4	290.7	283.5	-2.7	1.5	-1.6	1.2	1.9	105.8	-64.8	-178.6	↓
BTN 8 ($G^-G^-G^-$↓)	1677.3	305.3	290.2	2.9	2.0	0.3	1.3	3.4	108.2	-65.1	-65.3	↓
BTN 9 ($G^+G^-G^-$↑)	1678.5	305.2	290.1	2.5	1.8	1.9	1.3	3.4	108.2	-65.1	-65.3	↑
BTN 10 (G^+G^+T↑)	1482.5	290.5	283.3	-2.2	2.7	-0.5	1.3	1.9	105.9	-64.8	-178.6	↑
BTN 11 (TG^+G^+↓)	1464.6	301.4	269.7	2.2	-2.7	-1.3	1.5	1.0	-173.8	60.5	61.5	↓
BTN 12 (TG^+G^+↑)	1465.0	301.4	269.6	1.9	-3.2	0.3	1.5	1.0	-174.0	-60.4	-61.5	↑
BTN 13 (G^+TT↓)	2191.5	240.1	231.3	2.6	-2.0	-0.4	1.3	2.0	84.0	177.5	-179.7	↓
BTN 14 (G^+TT↑)	2194.1	240.1	231.2	2.2	-2.2	1.3	1.3	2.0	84.0	-177.5	-179.7	↑
BTN 15 ($G^+G^+G^-$↑)	1484.9	333.9	299.7	-2.1	2.8	0.1	3.9	5.0	80.9	65.0	-72.3	↑
BTN 16 ($G^+G^+G^-$↓)	1484.2	334.0	299.8	-2.5	1.9	-1.3	3.9	5.0	80.8	65.0	-72.2	↓
BTN 17 (TTT)	1978.1	238.1	213.7	1.8	-2.9	0.8	1.3	1.2	179.8	-179.9	180.0	↑
BTN 18 (TG^-G^+↑)	1385.7	329.7	275.9	1.8	-3.1	-0.3	3.8	4.6	178.9	-72.2	70.3	↑
BTN 19 (TG^-G^+↓)	1385.3	329.7	275.9	1.9	-2.7	1.3	3.8	4.6	178.8	-72.1	70.3	↓
BTN 20 (G^+T G^+↑)	2493.1	249.2	234.1	2.4	-2.1	1.2	3.9	4.6	84.9	-174.6	65.7	↑
BTN 21 (G^+TG^+↓)	2492.1	249.2	234.1	2.6	-1.9	-0.5	3.9	4.6	84.9	174.6	65.7	↓
BTN 22 (G^+T G^-↑)	2396.4	245.3	229.8	2.2	-2.3	1.3	4.2	5.0	84.1	-179.4	-64.7	↑
BTN 23 (G^+T G^-↓)	2395.0	245.3	229.9	2.4	-2.1	-0.4	4.1	4.9	84.1	-179.4	-64.7	↓
BTN 24 (TTG^+↑)	2199.7	243.1	223.1	-2.0	2.7	-0.9	3.8	3.7	178.9	176.6	64.5	↑
BTN 25 (TTG^+↓)	2198.9	243.2	223.1	-2.1	2.7	0.7	3.8	3.7	178.6	176.6	64.5	↓
BTN 26 ($G^+G^-G^+$↑)	1536.9	326.5	316.7	-2.3	-2.7	-0.3	6.4	6.8	107.6	-65.6	84.6	↑
BTN 27 ($G^+G^-G^+$↓)	1536.9	326.4	316.7	-2.7	-1.6	-1.5	6.4	6.8	107.7	-65.7	84.5	↓

M06-2X / 6-311++G(d.p)												
	A/MHz	B/MHz	C/MHz	μ_A/D	μ_B/D	μ_C/D	ΔE_0 /kJ·mol^{-1}	ΔG_0/ kJ·mol^{-1}	τ_1	τ_2	τ_3	NH_2 (↑/↓)*
BTN 1 (G^+G^+T↑)	1456.7	296.8	276.4	-1.8	2.8	-0.2	1.0	1.7	80.4	58.9	179.8	↑
BTN 2 (G^+G^+T↓)	1456.1	296.8	276.4	-2.3	1.7	-1.4	1.0	1.7	80.4	58.9	179.8	↓
BTN 3 (TG^-T↓)	1379.6	295.0	248.6	-1.6	2.7	-1.2	0.0	0.0	-178.4	63.4	179.8	↓
BTN 4 ($G^+G^+G^+$↓)	1479.9	330.1	291.4	2.2	-2.1	1.0	1.8	2.3	76.3	47.5	55.2	↓
BTN 5 (TG^+T↑)	1380.1	294.9	248.6	-1.4	3.1	0.6	0.1	0.2	-178.4	63.4	179.7	↑
BTN 6 ($G^+G^+G^+$↑)	1480.4	329.9	291.2	1.9	-2.7	-0.7	1.9	2.5	76.4	47.5	55.2	↑
BTN 7 (G^+G^-T↓)	1524.4	292.1	289.6	-2.5	1.0	-1.7	1.9	3.1	100.3	-63.2	-177.7	↓
BTN 8 ($G^-G^-G^-$↓)	1750.2	307.5	289.4	2.7	1.9	0.1	1.5	4.2	102.3	-66.5	-67.5	↓
BTN 9 ($G^+G^-G^-$↑)	1752.6	307.2	289.1	2.3	1.6	1.8	1.5	4.2	102.3	-66.5	-67.5	↑
BTN 10 (G^+G^+T↑)	1526.6	291.8	289.4	-2.0	2.5	-0.8	2.0	3.2	100.3	-63.2	-177.7	↑
BTN 11 (TG^+G^+↓)	1460.5	310.0	274.7	1.9	-2.5	-1.3	1.4	1.6	-178.3	56.6	56.6	↓
BTN 12 (TG^+G^+↑)	1460.9	310.0	274.6	-1.6	-3.0	-0.3	1.5	1.6	-178.4	56.6	56.6	↑
BTN 13 (G^+TT↓)	2239.9	242.0	233.2	2.3	-1.9	-0.4	1.7	2.4	81.0	177.8	-179.4	↓
BTN 14 (G^+TT↑)	2241.8	242.0	233.1	2.0	-2.0	1.4	1.6	2.2	81.0	177.8	-179.4	↑
BTN 15 ($G^+G^+G^-$↑)	1501.3	338.6	300.2	-1.8	2.7	0.3	4.5	4.4	78.8	70.2	-63.8	↑
BTN 16 ($G^+G^+G^-$↓)	1500.5	338.6	300.2	-2.2	1.9	-1.2	4.5	4.5	78.8	70.3	-63.6	↓
BTN 17 (TTT)	2009.9	239.2	214.9	1.6	-2.7	0.9	1.3	1.1	-179.9	179.9	-180.0	↑
BTN 18 (TG^-G^+↑)	1408.7	332.5	278.3	-1.5	2.9	0.4	3.9	4.5	-179.1	-73.3	66.2	↑
BTN 19 (TG^-G^+↓)	1408.3	332.7	278.4	-1.7	2.5	-1.4	3.8	4.4	-179.3	-73.2	66.3	↓
BTN 20 (G^+TG^+↑)	2551.0	250.9	236.1	2.2	-2.0	1.2	4.0	4.6	81.4	173.0	62.7	↑
BTN 21 (G^+TG^+↓)	2551.0	250.9	236.1	2.4	-1.8	-0.6	4.1	4.6	81.4	173.0	62.7	↓
BTN 22 (G^+TG^-↑)	2470.5	247.5	232.2	2.0	-2.1	1.3	4.3	5.0	81.1	-177.2	-61.5	↑
BTN 23 ($G^+T\ G^-$↓)	2470.6	247.5	232.3	2.2	-2.0	-0.5	4.3	5.0	81.1	-177.1	-61.4	↓
BTN 24 (TTG^+↑)	2248.8	244.9	224.6	-1.8	2.6	-1.0	3.6	3.7	179.7	174.5	61.4	↑
BTN 25 (TTG^+↓)	2249.2	244.9	224.6	-1.8	2.6	0.8	3.6	3.6	179.7	174.5	61.3	↓
BTN 26 ($G^+G^-G^+$↑)	1581.8	329.1	324.4	-2.1	-2.5	0.0	7.4	9.5	100.8	-63.6	87.1	↑
BTN 27 ($G^+G^-G^+$↓)	1582.2	329.0	324.4	-2.5	-1.5	-1.3	7.4	9.6	100.8	-63.6	87.1	↓

Table S4. Predicted nuclear quadrupolar constants of ^{14}N (expressed in MHz) for BTN at MP2, M06-2X and B3LYP-D3BJ level using 6-311++G(d,p) basis.

	MP2			B3LYP-D3BJ			M06-2X		
	χ_{aa}	χ_{bb}	χ_{cc}	χ_{aa}	χ_{bb}	χ_{cc}	χ_{aa}	χ_{bb}	χ_{cc}
BTN 3 (TG$^-$T↓)	2.579	1.770	-4.349	2.579	1.770	-4.349	2.579	1.770	-4.349
BTN 5 (TG$^+$T↑)	2.094	2.251	-4.346	2.094	2.251	-4.346	2.094	2.251	-4.346
Planar	2.607	2.218	-4.825	2.607	2.218	-4.825	2.607	2.218	-4.825
BTN 1 (G$^+$G$^+$T↑)	1.011	-0.041	-0.970	2.647	1.784	-4.432	1.165	0.122	-1.287
BTN 2 (G$^+$G$^+$T↓)	2.613	-1.396	-1.216	2.137	2.290	-4.427	2.607	-1.117	-1.490
BTN 4 (G$^+$G$^+$G$^+$↓)	2.645	0.735	-3.381	2.732	2.221	-4.953	2.667	0.962	-3.629
BTN 6 (G$^+$G$^+$G$^+$↑)	1.452	1.504	-2.956	1.247	0.348	-1.595	1.581	1.664	-3.244
BTN 7 (G$^+$G$^-$T↓)	2.634	-3.490	0.856	2.643	-0.865	-1.778	2.633	-3.280	0.647
BTN 10 (G$^+$G$^+$T↑)	1.022	-1.938	0.916	2.711	1.147	-3.858	1.189	-1.775	0.585
BTN 8 (G$^-$G$^-$G$^-$↓)	2.690	1.888	-4.578	1.665	1.817	-3.482	2.710	2.058	-4.768
BTN 9 (G$^+$G$^-$G$^-$↑)	1.384	1.827	-3.210	2.653	-2.295	-0.358	1.598	2.017	-3.615
BTN 11 (TG$^+$G$^+$↓)	2.573	1.234	-3.808	1.210	-0.912	-0.298	2.640	1.402	-4.042
BTN 12 (TG$^+$G$^+$↑)	1.871	1.907	-3.778	2.747	2.178	-4.925	1.951	2.011	-3.962
BTN 13 (G$^+$TT↓)	2.688	1.885	-4.572	1.585	2.125	-3.710	2.710	2.109	-4.819
BTN 14 (G$^+$TT↑)	1.487	1.951	-3.438	2.707	1.343	-4.050	1.656	2.174	-3.830
BTN 15 (G$^+$G$^+$G$^-$↑)	1.241	-0.001	-1.239	1.927	1.992	-3.918	1.537	1.090 -2.627	1.537
BTN 16 (G$^+$G$^+$G$^-$↓)	2.658	-1.072	-1.586	2.758	2.065	-4.823	2.672	0.239 -2.911	2.672
BTN 17 (TTT)	2.342	1.996	-4.338	1.705	2.192	-3.897	2.420	2.219 -4.638	2.420
BTN 18 (TG$^-$G$^+$↑)	1.995	1.962	-3.957	1.547	0.709	-2.256	2.143	2.146 -4.289	2.143

BTN 19 (TG^{-}G^{+}↓)	2.545	1.192	-3.737	2.716	-0.252	-2.464	2.587	1.628	-4.215	2.587
BTN 20 (G^{+}TG^{+}↑)	1.907	1.930	-3.837	2.503	2.282	-4.785	2.075	2.140	-4.215	2.075
BTN 21 (G^{+}TG^{+}↓)	2.632	1.860	-4.492	2.165	2.148	-4.313	2.673	2.070	-4.743	2.673
BTN 22 (G^{+}TG^{-}↑)	1.887	1.987	-3.874	2.663	1.588	-4.251	2.023	2.198	-4.221	2.023
BTN 23 (G^{+}T G^{-}↓)	2.626	1.924	-4.550	2.112	2.201	-4.314	2.675	2.143	-4.818	2.675
BTN 24 (TTG^{+}↑)	2.253	1.957	-4.210	2.746	2.126	-4.871	2.337	2.186	-4.522	2.337
BTN 25 (TTG^{+}↓)	2.438	2.001	-4.438	2.078	2.259	-4.337	2.528	2.209	-4.737	2.528
BTN 26 (G^{+}G^{-}G^{+}↑)	1.280	-0.593	-0.688	2.738	2.173	-4.911	1.507	0.198	-1.704	1.507
BTN 27 (G^{+}G^{-}G^{+}↓)	2.677	-0.991	-1.686	2.382	2.263	-4.645	2.690	-0.638	-2.052	2.690

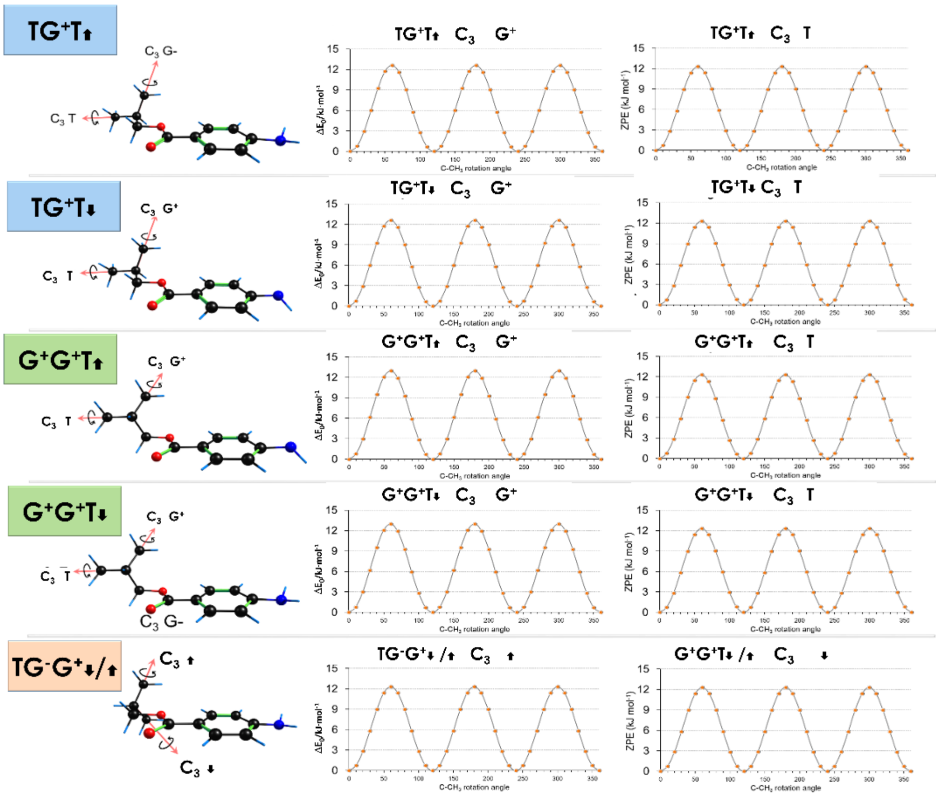


Figure S6. Methyl rotation energy of the assigned structures of BTI.

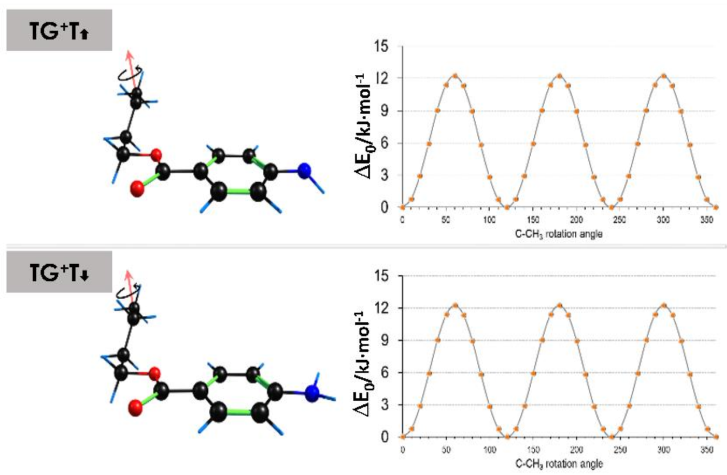


Figure S7. Methyl rotation energy of the assigned structures of BTN.

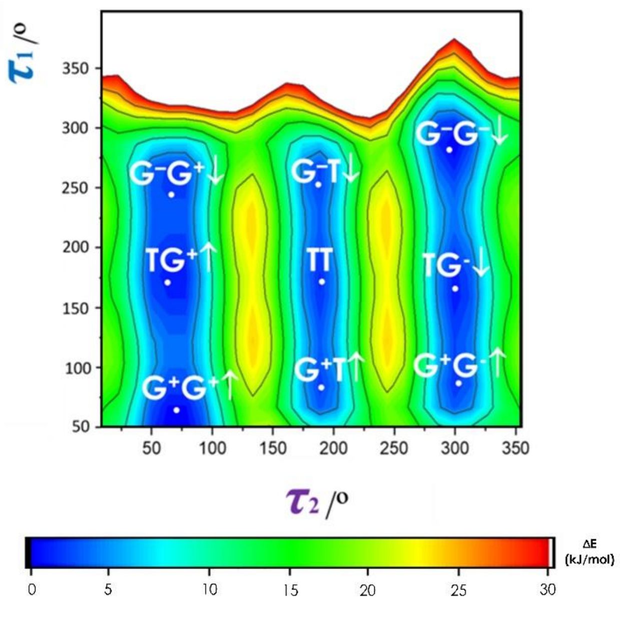


Figure S8. PES of BTI computed at B3LYP-D3BJ / 6-311++G(d,p) level.

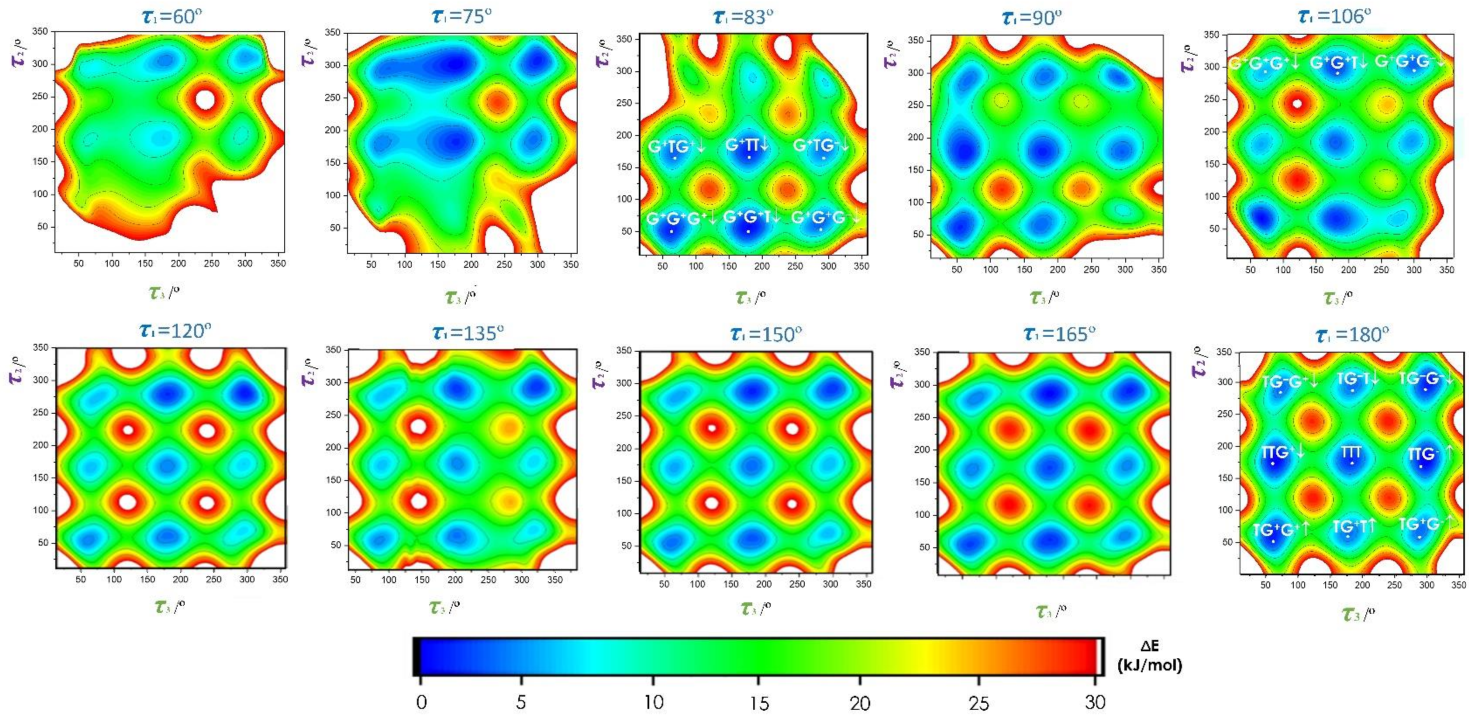


Figure S9. PES of BTN computed at B3LYP-D3BJ / 6-311++G(d,p) level.

3. Experimental Methods

Two different microwave spectrometers (working in the millimetre and centimetre region) and vaporization systems were employed in this work with the objective of obtaining the rotational spectra of BTI and BTN.

The Fourier Transform Microwave spectrometer (FTMW) consists of a Fabry-Pérot resonator where a microwave pulse is guided through two antennas. One of them is fixed to a movable mirror making possible the tuning of all the frequencies in the operating range [4-18] GHz and polarizing the sample previously injected in the vacuum chamber (10^{-7}mmbar) using an inert gas through a solenoid pulse valve.[11,12,13] The subsequent free induced decay is recorded in the time domain and Fourier transformed to the frequency domain. The accuracy of the measurements is better than 3 kHz and rotational transitions separated by more than 10 kHz are resolvable.

A Stark and pulse modulated free jet absorption millimetre-wave spectrometer (described elsewhere)[14] working in the region [60-78] GHz has been used to record the transitions corresponding to the higher rotational energy levels in BTN. The spectrometer consists of a vacuum chamber where the sample is injected via Ne carrier gas through a pulsed valve. In order to provide Stark modulation, the valve has two attached parallel discs to which a modulation voltage is applied. Millimetre waves propagate through the expanding plume of vapour causing the polarization of the molecules.

The chemicals used are:

- BTI: Isobutyl 4-Aminobenzoate (193.24 g/mol), purchased by TCI Europe N.V, 25g, >98.0%(GC)(T). It appears as a white to light yellow to dark green powder to crystal. Melting point: 65 °C.
- BTN: Butyl 4-aminobenzoate (193.24 g/mol), purchased by Fluka™, 100g, ≥98.0% (NT). It appears as a white, odourless, crystalline powder. Melting point: 58 °C.

In the sample vaporization process two different systems have been employed. When measuring BTI, a conventional home-made heating system was used consisting of an electric resistance wrapped around the sample holder through which the current is driven. After vaporization, the sample is guided into the vacuum chamber where the supersonic expansion takes place. For BTN, the solid sample was prepared under pressure as a solid stick and vaporized by laser ablation from a picosecond Nd-YAG laser operating in the third harmonic.[15] This method avoids the problems of sample decomposition due to heating.

The centimeter-range spectrometers provide higher resolution, so that hyperfine effects due to the quadrupolar coupling can be resolved and analyzed. The millimeter spectrometer allows monitoring transitions with higher rotational energy, so more accurate centrifugal distortion effects can be measured.

As regards BTI, an estimation of the relative population of the observed conformers can be obtained by relative intensities (*I*) measurements. This can be done because there is a direct relation between the intensities and the population of each conformer in the jet (N_i). The relation between them also includes the values of the dipole moment component involved along each axis (μ_g with *g*=*a*,*b* and/or *c*) according to the following expression:

$$\frac{N_i}{N_0} \propto \frac{I_i \omega_0 \Delta\upsilon_i \mu_g(0) \lambda_0 \upsilon_0^2}{I_0 \omega_i \Delta\upsilon_0 \mu_g(i) \lambda_i \upsilon_i^2} \propto \frac{I_i}{I_0} \cdot \frac{\mu_g(0)}{\mu_g(i)}$$

where ω is the conformational degeneration, Δυ the line width at half height and γ the line strength.[16] In this way, if the transition intensities are well-known for the different conformers, it is possible to estimate the abundance of each conformer respect to the most stable one.

The analysis was performed considering nearby in frequency μ_a and μ_b-type transitions (see Table S3) in order to minimize the errors of the estimation, taking into account the MP2 dipole moments values of Table S1. The average of the data corresponding to a single conformer were used to obtain the final ratio in percentage. A visual example of a measured transition is reported in Figure S10.

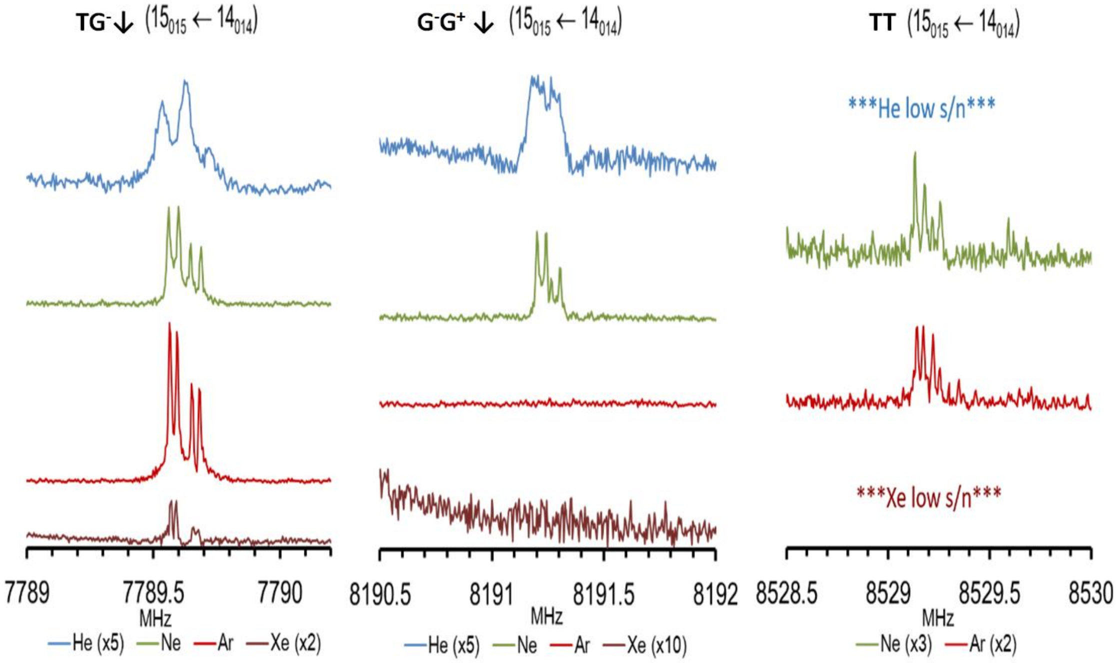


Figure S10. $15_{015} \leftarrow 14_{014}$ transition of the assigned rotamers of BTI measured using different carrier gases in the Bilbao spectrometer with laser vaporization. The number of accumulations for each line were 2000 for Ne (6+1 bar), Ar (4+1 bar) and Xe (2+1 bar) and 10000 for He (~30+1 bar).

Table S5. Comparison between the predicted (MP2/6-311++G**) data and the experimental spectroscopic parameters and conformational energies for the BTI and BTN rotationally observed conformers.

	ISOBUTAMBEN (BTI)						BUTAMBEN (BTN)	
	BTI I		BTI II		BTI III		BTN I	
	Experiment	**$TG^{-}\downarrow$**	Experiment	**$G^{-}G^{+}\downarrow$**	Experiment	**$TT\downarrow$**	Experiment	**$TG^{-}T\downarrow$**
***A* / MHz**	1831.7471(2)[a]	1830	1988.596(3)	1997	1509.466(3)	1502	1384.5107(1)	1373
***B* / MHz**	282.57280(3)	282	286.80516(9)	287	314.2755(1)	315	292.04655(6)	293
***C* / MHz**	251.02606(2)	251	265.83363(6)	268	276.27507(8)	276	246.75153(2)	247
D_J / kHz	0.00449(3)		0.01013(7)		0.0045(1)		0.01379(8)	
D_{JK} / kHz	-0.0480(7)		-0.150(5)				-0.171(1)	
D_K / kHz	0.83(2)				18.(1)		1.157(2)	
d_1 / kHz	-0.00084(2)		-0.00045(8)				-0.00364(4)	
d_2 / kHz							-0.00033(3)	
χ_{aa} / MHz	2.320(6)	2.5	2.47(7)	2.7	1.3(3)	2.3	2.24(2)	2.5
χ_{bb} / MHz	1.818(5)	1.6	1.18(4)	1.1	2.4(2)	2.0	2.01(2)	1.5
χ_{cc} / MHz	-4.128(5)	-4.1	-3.65(4)	-3.8	-3.7(2)	-4.3	-4.01(2)	-4.0
ΔE_0^{MP2}/kJmol^{-1}		2.0		0.4		1.6		0.6
ΔG_0^{MP2}/kJmol^{-1} (298K)		2.9		2.1		2.0		0.0
$\Delta E_{exp.}^{Ne}$ /kJmol^{-1}	0		1.5 (5)		2.8 (5)			
N [b]	261		130		87		212	
σ [c] **/ kHz**	2.9		3.3		3.6		26.4	
σ / σ_{exp} [d]	0.6		0.7		0.7		0.7	

[a] Standard error in parentheses in the units of the last digits. [b] Number of distinct frequencies in fit. [c] Root mean square error of the fit. [d] Reduced deviation of the fit, relative to measurement errors of 200 and 5 kHz for the mmw and FTMW spectrometers, respectively.

Table S6. BTI relative population results obtained measuring several rotational transitions for each conformer using different carrier gases.

Conformer	Line	*J´´*	*K*	*K*	*F´´*	*J´*	*K*	*K*	*F´*	$\nu_{exp.}$	I_{Ne}	I_{Ar}
TG-↓	μa - lines	14	0	14	15	13	0	13	14	7288.3014	3.91	2.37
					13				12			
					14				13	7288.3938	2.14	1.23
		14	1	14	15	13	1	13	14	7205.19	3.66	3.96
					13				12			
					14				13	7205.22	2.62	3.3
		15	0	15	14	14	0	14	13	7789.581	5.39	8.16
					16				15			
					15				14	7789.6676	3.35	5.4
		16	0	16	17	15	0	15	16	8289.637	2.15	4.42
					15				14			
					16				15	8289.720	1.33	2.62
	μb - lines	15	0	15	16	14	1	14	15	7858.315	0.98	1.65
					15				14	7858.542	1.08	3.61
					14				13	7858.567	1.02	3.51
		16	0	16	16	15	1	15	15	7282.770	0.51	0.58
					17				16	7383.050	0.90	1.32
					15				14	7283.090	0.88	1.38
		17	0	17	17	16	1	16	16	8424.963	0.88	0.77
					18				17	8425.145	0.87	1.6
					16				15	8425.165	0.81	1.36
G⁻G⁺↓	μa - lines	14	0	14	15	13	0	13	14	7655.33	5.34	0
					13				12			
					14				13	7655.40	2.65	0
		14	1	14	15	13	1	13	14	7570.77	2.37	0
					13				12	7570.78	1.55	0
					14				13	7570.80	2.19	0
		15	0	15	14	14	0	14	13	8191.22	3.22	0
					16				15			
					15				14	8191.28	1.74	0
		16	0	16	17	15	0	15	16	8725.66	1.23	0
					15				14			
					16				15	8725.72	0.59	0
	μb - lines	15	0	15	16	14	1	14	15	7938.90	0.35	0
					15				14	7939.30	0.43	0
					14				13	7939.30	0.42	0
		16	0	16	16	15	1	15	15	7322.10	0.48	0
					17				16	7322.50	0.70	0
					15				14	7322.50	0.47	0
		17	0	17	17	16	1	16	16	8551.44	0.35	0
					18				17	8551.77	0.27	0
					16				15	8551.77	0.29	0
TT	μa - lines	14	0	14	15	13	0	13	14	7980.53	1.25	0.88
					13				12			
					14				13	7980.62	0.96	0.63
		14	1	14	15	13	1	13	14	7926.69	0.85	0.31
					13				12	7926.71	0.85	0.41
					14				13	7926.73	0.55	0.36
		15	0	15	14	14	0	14	13	8529.16	0.52	0.62
					16				15			
					15				14	8529.24	0.31	0.44
		16	0	16	17	15	0	15	16	9077.81	0.57	0.73
					15				14			
					16				15	9077.89	0.34	0.63
	μb - lines	15	0	15	16	14	1	14	15	8909.50	0.42	0.79
					15				14	8909.57	0.26	0.66
					14				13	8909.59	0.27	0.47
		16	0	16	16	15	1	15	15	8316.10	0.34	0.27
					17				16	8316.20	0.30	0.47
					15				14	8316.24	0.20	0.59
		17	0	17	17	16	1	16	16	9494.98	0.27	0.37
					18				17	9495.03	0.38	0.43
					16				15	9495.05	0.36	0.39

Final Results	Ne %	Ar %
TG-↓	54(5)	82(5)
G⁻G⁺↓	30(5)	0
TT	16	18

Table S7. Rotational transitions of BTI (**TG$^-$↓**)

J´´	*K*	*K*	*F´´*	*J´*	*K*	*K*	*F´*	$\nu_{exp.}$	$\nu_{calc.}$	$\nu_{exp.}-\nu_{calc.}$
12	0	12	11	11	0	11	10	6280.101	6280.102	-0.001
12	0	12	13	11	0	11	12	6280.101	6280.100	0.001
12	0	12	12	11	0	11	11	6280.202	6280.199	0.003
13	0	13	14	12	0	12	13	6785.308	6785.310	-0.002
13	0	13	12	12	0	12	11	6785.316	6785.317	-0.001
13	0	13	13	12	0	12	12	6785.411	6785.411	0.000
14	0	14	15	13	0	13	14	7288.301	7288.302	0.000
14	0	14	13	13	0	13	12	7288.301	7288.302	-0.001
14	0	14	14	13	0	13	13	7288.394	7288.394	0.000
15	0	15	14	14	0	14	13	7789.581	7789.581	0.000
15	0	15	16	14	0	14	15	7789.581	7789.579	0.002
15	0	15	15	14	0	14	14	7789.668	7789.667	0.000
16	0	16	17	15	0	15	16	8289.637	8289.636	0.001
16	0	16	15	15	0	15	14	8289.637	8289.639	-0.002
16	0	16	16	15	0	15	15	8289.720	8289.719	0.002
17	0	17	18	16	0	16	17	8788.923	8788.921	0.002
17	0	17	16	16	0	16	15	8788.923	8788.924	-0.001
17	0	17	17	16	0	16	16	8788.996	8788.997	0.000
18	0	18	19	17	0	17	18	9287.804	9287.802	0.001
18	0	18	17	17	0	17	16	9287.804	9287.805	-0.001
18	0	18	18	17	0	17	17	9287.869	9287.871	-0.002
19	0	19	20	18	0	18	19	9786.564	9786.562	0.002
19	0	19	18	18	0	18	17	9786.564	9786.565	-0.001
19	0	19	19	18	0	18	18	9786.624	9786.624	0.000
20	0	20	21	19	0	19	20	10285.404	10285.402	0.002
20	0	20	19	19	0	19	18	10285.404	10285.405	-0.001
20	0	20	20	19	0	19	19	10285.458	10285.458	0.001
21	0	21	22	20	0	20	21	10784.450	10784.449	0.000
21	0	21	20	20	0	20	19	10784.450	10784.452	-0.003
21	0	21	21	20	0	20	20	10784.499	10784.499	0.000
22	0	22	23	21	0	21	22	11283.777	11283.776	0.002
22	0	22	21	21	0	21	20	11283.777	11283.779	-0.001
22	0	22	22	21	0	21	21	11283.819	11283.820	-0.001
23	0	23	24	22	0	22	23	11783.414	11783.412	0.002
23	0	23	22	22	0	22	21	11783.414	11783.415	0.000
23	0	23	23	22	0	22	22	11783.443	11783.452	-0.009
14	1	14	13	13	1	13	12	7205.193	7205.194	-0.001
14	1	14	15	13	1	13	14	7205.193	7205.190	0.003
14	1	14	14	13	1	13	13	7205.220	7205.222	-0.002
15	1	15	14	14	1	14	13	7714.167	7714.163	0.004
15	1	15	15	14	1	14	14	7714.181	7714.182	-0.002
15	1	15	16	14	1	14	15	7714.150	7714.150	-0.001
16	1	16	17	15	1	15	16	8222.324	8222.319	0.005
16	1	16	15	15	1	15	14	8222.324	8222.326	-0.002
16	1	16	16	15	1	15	15	8222.354	8222.350	0.004
17	1	17	18	16	1	16	17	8729.742	8729.742	0.000

17	1	17	16	16	1	16	15	8729.742	8729.748	-0.006
17	1	17	17	16	1	16	16	8729.775	8729.772	0.003
18	1	18	19	17	1	17	18	9236.469	9236.470	-0.001
18	1	18	17	17	1	17	16	9236.469	9236.476	-0.007
18	1	18	18	17	1	17	17	9236.505	9236.500	0.004
19	1	19	20	18	1	18	19	9742.567	9742.562	0.004
19	1	19	18	18	1	18	17	9742.567	9742.567	-0.001
20	1	20	21	19	1	19	20	10248.079	10248.076	0.003
20	1	20	19	19	1	19	18	10248.079	10248.081	-0.002
20	1	20	20	19	1	19	19	10248.102	10248.104	-0.003
19	1	19	19	18	1	18	18	9742.587	9742.591	-0.004
21	1	21	22	20	1	20	21	10753.076	10753.072	0.004
21	1	21	20	20	1	20	19	10753.076	10753.076	0.000
21	1	21	21	20	1	20	20	10753.106	10753.099	0.007
22	1	22	23	21	1	21	22	11257.607	11257.607	0.000
22	1	22	21	21	1	21	20	11257.607	11257.611	-0.004
22	1	22	22	21	1	21	21	11257.628	11257.633	-0.005
23	1	23	24	22	1	22	23	11761.740	11761.739	0.001
23	1	23	22	22	1	22	21	11761.740	11761.742	-0.003
23	1	23	23	22	1	22	22	11761.765	11761.764	0.001
13	1	12	12	12	1	11	11	7092.281	7092.276	0.005
13	1	12	14	12	1	11	13	7092.281	7092.280	0.001
13	1	12	13	12	1	11	12	7092.326	7092.328	-0.002
14	1	13	13	13	1	12	12	7627.765	7627.762	0.003
14	1	13	15	13	1	12	14	7627.765	7627.765	-0.001
14	1	13	14	13	1	12	13	7627.817	7627.819	-0.002
15	1	14	14	14	1	13	13	8160.614	8160.610	0.005
15	1	14	16	14	1	13	15	8160.614	8160.613	0.001
15	1	14	15	14	1	13	14	8160.667	8160.672	-0.005
16	1	15	15	15	1	14	14	8690.538	8690.535	0.003
16	1	15	17	15	1	14	16	8690.538	8690.538	0.000
16	1	15	16	15	1	14	15	8690.600	8690.603	-0.002
17	1	16	16	16	1	15	15	9217.272	9217.269	0.003
17	1	16	18	16	1	15	17	9217.272	9217.272	0.000
17	1	16	17	16	1	15	16	9217.342	9217.342	-0.001
18	1	17	17	17	1	16	16	9740.583	9740.579	0.004
18	1	17	19	17	1	16	18	9740.583	9740.582	0.001
18	1	17	18	17	1	16	17	9740.658	9740.658	0.000
19	1	18	18	18	1	17	17	10260.294	10260.290	0.004
19	1	18	20	18	1	17	19	10260.294	10260.293	0.000
19	1	18	19	18	1	17	18	10260.375	10260.374	0.001
20	1	19	19	19	1	18	18	10776.317	10776.314	0.003
20	1	19	21	19	1	18	20	10776.317	10776.315	0.002
20	1	19	20	19	1	18	19	10776.405	10776.402	0.002
21	1	20	20	20	1	19	19	11288.662	11288.658	0.004
21	1	20	22	20	1	19	21	11288.662	11288.662	0.000
21	1	20	21	20	1	19	20	11288.744	11288.750	-0.007
22	1	21	21	21	1	20	20	11797.474	11797.470	0.004
22	1	21	23	21	1	20	22	11797.474	11797.473	0.001
22	1	21	22	21	1	20	21	11797.569	11797.565	0.003

13	2	12	14	12	2	11	13	6909.355	6909.353	0.003
13	2	12	12	12	2	11	11	6909.355	6909.354	0.001
13	2	12	13	12	2	11	12	6909.387	6909.388	0.000
14	2	13	15	13	2	12	14	7435.933	7435.931	0.003
14	2	13	13	13	2	12	12	7435.933	7435.933	0.000
14	2	13	14	13	2	12	13	7435.964	7435.965	-0.001
15	2	14	16	14	2	13	15	7961.463	7961.458	0.006
15	2	14	16	14	2	13	15	7961.463	7961.458	0.006
15	2	14	16	14	2	13	15	7961.454	7961.458	-0.003
19	2	18	20	18	2	17	19	10052.066	10052.061	0.004
19	2	18	18	18	2	17	17	10052.066	10052.063	0.003
19	2	18	19	18	2	17	18	10052.100	10052.098	0.003
20	2	19	21	19	2	18	20	10571.665	10571.661	0.004
20	2	19	19	19	2	18	18	10571.665	10571.662	0.003
20	2	19	20	19	2	18	19	10571.701	10571.698	0.003
21	2	20	22	20	2	19	21	11090.007	11090.003	0.004
21	2	20	20	20	2	19	19	11090.007	11090.004	0.003
21	2	20	21	20	2	19	20	11090.046	11090.040	0.006
22	2	21	23	21	2	20	22	11607.096	11607.088	0.008
22	2	21	21	21	2	20	20	11607.096	11607.089	0.007
22	2	21	22	21	2	20	21	11607.128	11607.126	0.002
13	2	11	12	12	2	10	11	7060.384	7060.389	-0.005
13	2	11	14	12	2	10	13	7060.384	7060.384	0.000
13	2	11	13	12	2	10	12	7060.323	7060.323	0.000
17	2	15	17	16	2	14	16	9288.597	9288.596	0.001
17	2	15	16	16	2	14	15	9288.630	9288.631	-0.002
17	2	15	18	16	2	14	17	9288.630	9288.631	-0.002
18	2	16	18	17	2	15	17	9844.055	9844.059	-0.004
18	2	16	19	17	2	15	18	9844.090	9844.086	0.005
18	2	16	17	17	2	15	16	9844.090	9844.089	0.002
19	2	17	19	18	2	16	18	10397.901	10397.905	-0.005
19	2	17	20	18	2	16	19	10397.924	10397.923	0.001
19	2	17	18	18	2	16	17	10397.924	10397.924	0.000
20	2	18	20	19	2	17	19	10949.777	10949.767	0.009
20	2	18	21	19	2	17	20	10949.777	10949.777	0.000
20	2	18	19	19	2	17	18	10949.777	10949.777	0.000
21	2	19	21	20	2	18	20	11499.330	11499.331	-0.001
21	2	19	20	20	2	18	19	11499.330	11499.332	-0.002
21	2	19	22	20	2	18	21	11499.330	11499.332	-0.002
13	3	10	13	12	3	9	12	6966.476	6966.478	-0.002
13	3	10	14	12	3	9	13	6966.476	6966.485	-0.008
13	3	10	12	12	3	9	11	6966.488	6966.489	-0.001
13	3	11	14	12	3	10	13	6953.263	6953.265	-0.002
13	3	11	12	12	3	10	11	6953.275	6953.273	0.002
13	3	11	13	12	3	10	12	6953.290	6953.285	0.005
15	3	12	16	15	2	13	16	7200.438	7200.435	0.003
15	3	12	15	15	2	13	15	7200.948	7200.944	0.003
15	3	12	14	15	2	13	14	7200.405	7200.401	0.004
15	3	13	16	14	3	12	15	8025.940	8025.947	-0.008
15	3	13	14	14	3	12	13	8025.947	8025.950	-0.003

15	3	13	15	14	3	12	14	8025.955	8025.956	-0.001
19	3	17	20	18	3	16	19	10169.151	10169.149	0.002
19	3	17	18	18	3	16	17	10169.151	10169.152	-0.001
19	3	17	19	18	3	16	18	10169.151	10169.156	-0.006
19	3	16	19	18	3	15	18	10250.514	10250.516	-0.001
19	3	16	20	18	3	15	19	10250.563	10250.562	0.001
19	3	16	18	18	3	15	17	10250.563	10250.566	-0.003
20	3	17	20	19	3	16	19	10806.129	10806.133	-0.004
20	3	17	21	19	3	16	20	10806.183	10806.184	-0.001
20	3	17	19	19	3	16	18	10806.183	10806.187	-0.004
20	3	18	21	19	3	17	20	10703.863	10703.863	0.001
20	3	18	19	19	3	17	18	10703.863	10703.863	0.001
20	3	18	20	19	3	17	19	10703.877	10703.872	0.005
21	3	19	22	20	3	18	21	11237.907	11237.907	0.000
21	3	19	20	20	3	18	19	11237.907	11237.908	-0.001
21	3	19	21	20	3	18	20	11237.923	11237.917	0.006
21	3	18	21	20	3	17	20	11364.179	11364.182	-0.003
21	3	18	22	20	3	17	21	11364.236	11364.236	0.000
21	3	18	20	20	3	17	19	11364.236	11364.239	-0.003
22	3	20	23	21	3	19	22	11771.178	11771.175	0.003
22	3	20	21	21	3	19	20	11771.178	11771.176	0.002
22	3	20	22	21	3	19	21	11771.195	11771.187	0.008
22	3	19	22	21	3	18	21	11924.445	11924.448	-0.003
22	3	19	23	21	3	18	22	11924.502	11924.504	-0.002
22	3	19	21	21	3	18	20	11924.502	11924.507	-0.005
13	4	10	14	12	4	9	13	6949.262	6949.261	0.001
13	4	10	12	12	4	9	11	6949.262	6949.262	0.000
13	4	10	13	12	4	9	12	6949.286	6949.290	-0.004
13	4	9	14	12	4	8	13	6949.662	6949.662	0.000
13	4	9	12	12	4	8	11	6949.662	6949.664	-0.001
13	4	9	13	12	4	8	12	6949.689	6949.691	-0.002
19	4	16	20	18	4	15	19	10173.701	10173.700	0.001
19	4	16	19	18	4	15	18	10173.701	10173.702	-0.001
20	4	17	20	19	4	16	19	10712.379	10712.378	0.001
20	4	17	21	19	4	16	20	10712.379	10712.378	0.001
20	4	17	19	19	4	16	18	10712.379	10712.379	0.000
20	4	16	20	19	4	15	19	10720.671	10720.676	-0.005
20	4	16	21	19	4	15	20	10720.687	10720.685	0.002
20	4	16	19	19	4	15	18	10720.687	10720.687	0.000
19	4	16	18	18	4	15	17	10173.701	10173.702	-0.001
21	4	18	21	20	4	17	20	11251.351	11251.349	0.002
21	4	18	22	20	4	17	21	11251.351	11251.350	0.000
21	4	18	20	20	4	17	19	11251.351	11251.352	-0.001
21	4	17	21	20	4	16	20	11262.951	11262.956	-0.005
21	4	17	22	20	4	16	21	11262.969	11262.968	0.001
21	4	17	20	20	4	16	19	11262.969	11262.970	-0.001
13	5	9	13	12	5	8	12	6945.129	6945.125	0.004
13	5	9	12	12	5	8	11	6945.074	6945.071	0.003
13	5	9	14	12	5	8	13	6945.074	6945.072	0.002
19	5	15	20	18	5	14	19	10162.513	10162.515	-0.001

19	5	15	18	18	5	14	17	10162.513	10162.516	-0.002
19	5	15	19	18	5	14	18	10162.529	10162.525	0.004
19	5	14	20	18	5	13	19	10162.714	10162.716	-0.002
19	5	14	18	18	5	13	17	10162.714	10162.718	-0.003
19	5	14	19	18	5	13	18	10162.730	10162.727	0.003
21	5	17	22	20	5	16	21	11237.741	11237.739	0.002
21	5	17	20	20	5	16	19	11237.741	11237.740	0.001
21	5	17	21	20	5	16	20	11237.741	11237.744	-0.003
21	5	16	22	20	5	15	21	11238.224	11238.232	-0.008
21	5	16	20	20	5	15	19	11238.242	11238.241	0.001
21	5	16	21	20	5	15	20	11238.242	11238.244	-0.002
13	7	7	12	12	7	6	11	6941.444	6941.437	0.007
13	7	7	14	12	7	6	13	6941.444	6941.445	-0.001
13	7	7	13	12	7	6	12	6941.551	6941.555	-0.003
15	0	15	16	14	1	14	15	7283.059	7283.055	0.004
15	0	15	15	14	1	14	14	7282.782	7282.778	0.004
15	0	15	14	14	1	14	13	7283.090	7283.089	0.001
16	0	16	16	15	1	15	15	7858.315	7858.315	0.000
16	0	16	17	15	1	15	16	7858.542	7858.541	0.001
16	0	16	15	15	1	15	14	7858.567	7858.565	0.003
17	0	17	17	16	1	16	16	8424.963	8424.961	0.001
17	0	17	18	16	1	16	17	8425.145	8425.143	0.002
17	0	17	16	16	1	16	15	8425.165	8425.162	0.002
21	0	21	21	20	1	20	20	10612.447	10612.445	0.002
21	0	21	22	20	1	20	21	10612.505	10612.509	-0.004
21	0	21	20	20	1	20	19	10612.523	10612.517	0.006
22	0	22	22	21	1	21	21	11143.169	11143.167	0.002
22	0	22	23	21	1	21	22	11143.210	11143.213	-0.003
22	0	22	21	21	1	21	20	11143.210	11143.220	-0.010
23	0	23	23	22	1	22	22	11668.989	11668.986	0.003
23	0	23	24	22	1	22	23	11669.016	11669.018	-0.002
23	0	23	22	22	1	22	21	11669.016	11669.024	-0.008
11	1	11	10	10	0	10	9	6547.047	6547.050	-0.003
11	1	11	12	10	0	10	11	6547.098	6547.097	0.001
11	1	11	11	10	0	10	10	6547.756	6547.755	0.001
12	1	12	11	11	0	11	10	6959.604	6959.605	-0.001
12	1	12	13	11	0	11	12	6959.643	6959.643	0.000
12	1	12	12	11	0	11	11	6960.232	6960.236	-0.004
12	1	12	11	11	0	11	10	6959.600	6959.605	-0.005
12	1	12	13	11	0	11	12	6959.645	6959.643	0.002
12	1	12	12	11	0	11	11	6960.234	6960.236	-0.002
13	1	13	12	12	0	12	11	7374.918	7374.916	0.002
13	1	13	13	12	0	12	12	7375.469	7375.472	-0.003
13	1	13	14	12	0	12	13	7374.941	7374.945	-0.004
14	1	14	13	13	0	13	12	7794.795	7794.794	0.001
14	1	14	15	13	0	13	14	7794.823	7794.825	-0.003
14	1	14	14	13	0	13	13	7795.281	7795.283	-0.003
15	1	15	14	14	0	14	13	8220.653	8220.655	-0.002
15	1	15	16	14	0	14	15	8220.673	8220.674	-0.001
15	1	15	15	14	0	14	14	8221.071	8221.071	0.000

16	1	16	15	15	0	15	14	8653.397	8653.400	-0.003
16	1	16	17	15	0	15	16	8653.414	8653.414	0.000
16	1	16	16	15	0	15	15	8653.753	8653.754	-0.001
17	1	17	16	16	0	16	15	9093.505	9093.509	-0.004
17	1	17	18	16	0	16	17	9093.521	9093.519	0.001
17	1	17	17	16	0	16	16	9093.805	9093.807	-0.002
20	1	20	19	19	0	19	18	10457.341	10457.340	0.001
20	1	20	21	19	0	19	20	10457.341	10457.343	-0.002
20	1	20	20	19	0	19	19	10457.510	10457.511	-0.002
21	1	21	20	20	0	20	19	10925.010	10925.011	-0.001
21	1	21	22	20	0	20	21	10925.010	10925.012	-0.002
21	1	21	21	20	0	20	20	10925.152	10925.152	0.000
22	1	22	21	21	0	21	20	11398.171	11398.170	0.001
22	1	22	23	21	0	21	22	11398.171	11398.170	0.001
22	1	22	22	21	0	21	21	11398.286	11398.286	-0.001
23	1	23	24	22	0	22	23	11876.133	11876.133	0.000
23	1	23	22	22	0	22	21	11876.133	11876.133	0.000
23	1	23	23	22	0	22	22	11876.228	11876.230	-0.001
7	2	6	8	6	1	5	7	8098.584	8098.581	0.003
7	2	6	6	6	1	5	5	8098.437	8098.443	-0.006
7	2	6	7	6	1	5	6	8099.499	8099.497	0.001
8	2	6	8	7	1	7	7	9502.780	9502.780	-0.001
8	2	6	9	7	1	7	8	9504.293	9504.288	0.005
8	2	6	7	7	1	7	6	9504.515	9504.512	0.003
9	2	8	8	8	1	7	7	8931.311	8931.312	-0.001
9	2	8	10	8	1	7	9	8931.425	8931.422	0.002
9	2	8	9	8	1	7	8	8932.381	8932.379	0.002
5	3	2	5	4	2	3	4	10495.814	10495.815	-0.001
5	3	2	6	4	2	3	5	10496.084	10496.082	0.002
5	3	2	4	4	2	3	3	10496.155	10496.154	0.001
5	3	3	5	4	2	2	4	10488.608	10488.611	-0.003
5	3	3	6	4	2	2	5	10488.784	10488.785	-0.001
5	3	3	4	4	2	2	3	10488.829	10488.833	-0.004
6	3	3	6	5	2	4	5	11033.245	11033.246	-0.001
6	3	3	7	5	2	4	6	11033.488	11033.487	0.001
6	3	3	5	5	2	4	4	11033.547	11033.545	0.002
6	3	4	6	5	2	3	5	11016.321	11016.323	-0.002
6	3	4	7	5	2	3	6	11016.416	11016.417	-0.001
6	3	4	5	5	2	3	4	11016.442	11016.445	-0.002
7	3	4	7	6	2	5	6	11573.256	11573.256	0.000
7	3	4	8	6	2	5	7	11573.486	11573.482	0.004
7	3	4	6	6	2	5	5	11573.528	11573.530	-0.002
10	2	9	9	9	1	8	8	9325.750	9325.755	-0.005
10	2	9	11	9	1	8	10	9325.859	9325.854	0.005
10	2	9	10	9	1	8	9	9326.819	9326.819	0.000
11	2	10	10	10	1	9	9	9706.252	9706.249	0.003
11	2	10	12	10	1	9	11	9706.340	9706.339	0.000
11	2	10	11	10	1	9	10	9707.303	9707.306	-0.002
13	2	12	12	12	1	11	11	10428.434	10428.427	0.008
13	2	12	14	12	1	11	13	10428.498	10428.500	-0.002

13	2	12	13	12	1	11	12	10429.454	10429.453	0.001
15	2	14	14	14	1	13	13	11105.786	11105.782	0.004
15	2	14	16	14	1	13	15	11105.840	11105.843	-0.003
15	2	14	15	14	1	13	14	11106.761	11106.763	-0.002
16	2	15	15	15	1	14	14	11431.052	11431.053	-0.001
16	2	15	17	15	1	14	16	11431.112	11431.108	0.003
16	2	15	16	15	1	14	15	11432.004	11432.004	0.000
14	3	11	13	14	2	12	13	7322.448	7322.445	0.002
14	3	11	15	14	2	12	15	7322.476	7322.480	-0.003
14	3	11	14	14	2	12	14	7322.963	7322.961	0.003
6	3	3	6	6	2	4	6	7800.651	7800.652	-0.001
6	3	3	7	6	2	4	7	7800.794	7800.795	-0.001
6	3	3	5	6	2	4	5	7800.821	7800.819	0.002
7	3	4	7	7	2	5	7	7782.350	7782.349	0.002
7	3	4	8	7	2	5	8	7782.374	7782.372	0.002
7	3	4	6	7	2	5	6	7782.374	7782.375	-0.001
7	3	5	7	7	2	6	7	7840.786	7840.785	0.001
7	3	5	8	7	2	6	8	7841.079	7841.080	-0.001
8	3	5	7	8	2	6	7	7755.292	7755.296	-0.004
8	3	5	9	8	2	6	9	7755.310	7755.306	0.004
8	3	5	8	8	2	6	8	7755.383	7755.383	0.000
8	3	6	8	8	2	7	8	7851.800	7851.798	0.002
8	3	6	9	8	2	7	9	7852.072	7852.069	0.003
8	3	6	7	8	2	7	7	7852.102	7852.103	-0.001
9	3	7	9	9	2	8	9	7867.325	7867.326	-0.002
9	3	7	10	9	2	8	10	7867.590	7867.589	0.001
9	3	7	8	9	2	8	8	7867.616	7867.619	-0.003
10	3	8	10	10	2	9	10	7888.364	7888.366	-0.002
10	3	8	11	10	2	9	11	7888.633	7888.631	0.002
10	3	8	9	10	2	9	9	7888.652	7888.658	-0.006
11	3	9	11	11	2	10	11	7915.954	7915.954	0.000
11	3	9	12	11	2	10	12	7916.230	7916.230	0.000
11	3	9	10	11	2	10	10	7916.250	7916.256	-0.006
12	3	9	11	12	2	10	11	7524.963	7524.961	0.003
12	3	9	13	12	2	10	13	7524.990	7524.993	-0.003
12	3	9	12	12	2	10	12	7525.377	7525.378	0.000
12	3	10	12	12	2	11	12	7951.163	7951.165	-0.002
12	3	10	13	12	2	11	13	7951.456	7951.460	-0.004
12	3	10	11	12	2	11	11	7951.481	7951.477	0.003
18	4	14	17	18	3	15	17	10704.609	10704.612	-0.003
18	4	14	19	18	3	15	19	10704.625	10704.622	0.003
18	4	14	18	18	3	15	18	10704.806	10704.806	0.000

Table S8. Rotational transitions of BTI (**G^-G^+**↓)

J´´	*K*	*K*	*F´´*	*J´*	*K*	*K*	*F´*	$\nu_{exp.}$	$\nu_{calc.}$	$\nu_{exp.}-\nu_{calc.}$
12	0	12	13	11	0	11	12	6578.691	6578.688	0.003
12	0	12	11	11	0	11	10	6578.691	6578.692	-0.001
12	0	12	12	11	0	11	11	6578.742	6578.748	-0.006
13	0	13	14	12	0	12	13	7117.854	7117.852	0.002
13	0	13	12	12	0	12	11	7117.854	7117.859	-0.005
13	0	13	13	12	0	12	12	7117.917	7117.917	0.000
14	0	14	15	13	0	13	14	7655.333	7655.332	0.000
14	0	14	13	13	0	13	12	7655.333	7655.333	0.000
14	0	14	14	13	0	13	13	7655.398	7655.394	0.004
15	0	15	16	14	0	14	15	8191.222	8191.221	0.001
15	0	15	14	14	0	14	13	8191.222	8191.223	-0.002
15	0	15	15	14	0	14	14	8191.285	8191.284	0.000
16	0	16	17	15	0	15	16	8725.660	8725.655	0.004
16	0	16	15	15	0	15	14	8725.660	8725.657	0.002
16	0	16	16	15	0	15	15	8725.719	8725.718	0.000
17	0	17	18	16	0	16	17	9258.806	9258.807	-0.001
17	0	17	16	16	0	16	15	9258.806	9258.809	-0.003
17	0	17	17	16	0	16	16	9258.868	9258.869	-0.002
18	0	18	19	17	0	17	18	9790.873	9790.872	0.000
18	0	18	17	17	0	17	16	9790.873	9790.874	-0.002
18	0	18	18	17	0	17	17	9790.934	9790.932	0.002
19	0	19	20	18	0	18	19	10322.056	322.055	0.001
19	0	19	18	18	0	18	17	10322.056	322.057	-0.001
19	0	19	19	18	0	18	18	10322.113	322.113	0.001
20	0	20	21	19	0	19	20	10852.561	852.558	0.003
20	0	20	19	19	0	19	18	10852.561	852.560	0.001
20	0	20	20	19	0	19	19	10852.607	852.612	-0.006
21	0	21	22	20	0	20	21	11382.570	1382.569	0.001
21	0	21	20	20	0	20	19	11382.570	1382.571	-0.001
21	0	21	21	20	0	20	20	11382.619	1382.620	-0.001
22	0	22	23	21	0	21	22	11912.254	1912.254	0.001
22	0	22	21	21	0	21	20	11912.254	1912.255	-0.001
22	0	22	22	21	0	21	21	11912.302	1912.301	0.001
13	1	13	14	12	1	12	13	7032.282	7032.285	-0.003
13	1	13	12	12	1	12	11	7032.295	7032.295	0.000
13	1	13	13	12	1	12	12	7032.310	7032.306	0.003
14	1	14	15	13	1	13	14	7570.768	7570.771	-0.003
14	1	14	13	13	1	13	12	7570.781	7570.782	-0.001
14	1	14	14	13	1	13	13	7570.796	7570.792	0.004
15	1	15	14	14	1	14	13	8108.808	8108.813	-0.005
15	1	15	16	14	1	14	15	8108.808	8108.807	0.001
15	1	15	15	14	1	14	14	8108.830	8108.828	0.002
16	1	16	17	15	1	15	16	8646.392	8646.390	0.002
16	1	16	15	15	1	15	14	8646.392	8646.397	-0.005
16	1	16	16	15	1	15	15	8646.416	8646.411	0.005
17	1	17	18	16	1	16	17	9183.525	9183.524	0.000

17	1	17	16	16	1	16	15	9183.525	9183.530	-0.006
17	1	17	17	16	1	16	16	9183.550	9183.545	0.005
18	1	18	19	17	1	17	18	9720.210	9720.216	-0.006
18	1	18	17	17	1	17	16	9720.225	9720.221	0.004
18	1	18	18	17	1	17	17	9720.240	9720.236	0.004
19	1	19	20	18	1	18	19	10256.476	256.476	0.000
19	1	19	18	18	1	18	17	10256.476	256.481	-0.005
19	1	19	19	18	1	18	18	10256.499	256.496	0.003
20	1	20	21	19	1	19	20	10792.319	792.319	0.000
20	1	20	19	19	1	19	18	10792.319	792.324	-0.004
20	1	20	20	19	1	19	19	10792.344	792.339	0.005
21	1	21	22	20	1	20	21	11327.763	1327.762	0.000
21	1	21	20	20	1	20	19	11327.763	1327.766	-0.004
21	1	21	21	20	1	20	20	11327.786	1327.782	0.004
22	1	22	23	21	1	21	22	11862.823	1862.825	-0.002
22	1	22	21	21	1	21	20	11862.823	1862.829	-0.006
22	1	22	22	21	1	21	21	11862.845	1862.844	0.001
12	1	11	11	11	1	10	10	6742.811	6742.808	0.003
12	1	11	13	11	1	10	12	6742.811	6742.809	0.002
12	1	11	12	11	1	10	11	6742.826	6742.831	-0.005
13	1	12	12	12	1	11	11	7301.618	7301.616	0.002
13	1	12	14	12	1	11	13	7301.618	7301.617	0.001
13	1	12	13	12	1	11	12	7301.644	7301.640	0.004
14	1	13	13	13	1	12	12	7859.590	7859.589	0.002
14	1	13	15	13	1	12	14	7859.590	7859.590	0.000
14	1	13	14	13	1	12	13	7859.612	7859.615	-0.003
15	1	14	14	14	1	13	13	8416.630	8416.629	0.001
15	1	14	16	14	1	13	15	8416.630	8416.630	0.000
15	1	14	15	14	1	13	14	8416.660	8416.657	0.003
16	1	15	15	15	1	14	14	8972.634	8972.632	0.002
16	1	15	17	15	1	14	16	8972.634	8972.633	0.001
16	1	15	16	15	1	14	15	8972.658	8972.663	-0.005
17	1	16	16	16	1	15	15	9527.492	9527.489	0.003
17	1	16	18	16	1	15	17	9527.492	9527.490	0.002
17	1	16	17	16	1	15	16	9527.515	9527.522	-0.006
18	1	17	17	17	1	16	16	10081.087	81.085	0.002
18	1	17	19	17	1	16	18	10081.087	81.086	0.001
18	1	17	18	17	1	16	17	10081.119	81.120	-0.001
19	1	18	18	18	1	17	17	10633.305	633.304	0.001
19	1	18	20	18	1	17	19	10633.305	633.305	0.000
19	1	18	19	18	1	17	18	10633.339	633.342	-0.003
20	1	19	19	19	1	18	18	11184.032	1184.032	0.000
20	1	19	21	19	1	18	20	11184.032	1184.033	-0.001
20	1	19	20	19	1	18	19	11184.068	1184.072	-0.004
21	1	20	20	20	1	19	19	11733.157	1733.155	0.002
21	1	20	22	20	1	19	21	11733.157	1733.156	0.000
21	1	20	21	20	1	19	20	11733.192	1733.199	-0.006
12	2	11	13	11	2	10	12	6622.950	6622.943	0.006
12	2	11	11	11	2	10	10	6622.950	6622.951	-0.001
12	2	11	12	11	2	10	11	6622.973	6622.969	0.005

13	2	12	14	12	2	11	13	7173.122	7173.119	0.002
13	2	12	12	12	2	11	11	7173.122	7173.122	0.000
13	2	12	13	12	2	11	12	7173.146	7173.144	0.003
14	2	13	15	13	2	12	14	7722.879	7722.875	0.004
14	2	13	13	13	2	12	12	7722.879	7722.879	0.001
14	2	13	14	13	2	12	13	7722.896	7722.898	-0.002
15	2	14	14	14	2	13	13	8272.191	8272.192	-0.001
15	2	14	16	14	2	13	15	8272.191	8272.189	0.002
15	2	14	15	14	2	13	14	8272.214	8272.211	0.003
16	2	15	17	15	2	14	16	8821.032	8821.031	0.000
16	2	15	15	15	2	14	14	8821.032	8821.034	-0.002
16	2	15	16	15	2	14	15	8821.032	8821.052	-0.021
17	2	16	18	16	2	15	17	9369.375	9369.374	0.001
17	2	16	16	16	2	15	15	9369.375	9369.377	-0.001
17	2	16	17	16	2	15	16	9369.399	9369.395	0.004
18	2	17	19	17	2	16	18	9917.194	9917.192	0.002
18	2	17	17	17	2	16	16	9917.194	9917.194	0.000
18	2	17	18	17	2	16	17	9917.217	9917.213	0.004
19	2	18	20	18	2	17	19	10464.462	464.461	0.001
19	2	18	18	18	2	17	17	10464.462	464.463	-0.001
19	2	18	19	18	2	17	18	10464.487	464.482	0.005
20	2	19	21	19	2	18	20	11011.158	1011.158	0.000
20	2	19	19	19	2	18	18	11011.158	1011.160	-0.002
20	2	19	20	19	2	18	19	11011.182	1011.179	0.002
21	2	20	22	20	2	19	21	11557.264	1557.263	0.001
21	2	20	20	20	2	19	19	11557.264	1557.264	0.000
21	2	20	21	20	2	19	20	11557.288	1557.285	0.003
12	2	10	12	11	2	9	11	6675.788	6675.786	0.002
12	2	10	13	11	2	9	12	6675.816	6675.817	-0.001
12	2	10	11	11	2	9	10	6675.829	6675.824	0.005
13	2	11	13	12	2	10	12	7239.380	7239.382	-0.002
13	2	11	14	12	2	10	13	7239.414	7239.418	-0.005
13	2	11	12	12	2	10	11	7239.421	7239.424	-0.004
14	2	12	14	13	2	11	13	7804.232	7804.232	0.000
14	2	12	15	13	2	11	14	7804.270	7804.270	0.000
14	2	12	13	13	2	11	12	7804.270	7804.276	-0.006
15	2	13	15	14	2	12	14	8370.207	8370.205	0.002
15	2	13	14	14	2	12	13	8370.245	8370.249	-0.004
15	2	13	16	14	2	12	15	8370.245	8370.244	0.000
16	2	14	16	15	2	13	15	8937.126	8937.125	0.001
16	2	14	17	15	2	13	16	8937.165	8937.165	0.000
16	2	14	15	15	2	13	14	8937.165	8937.169	-0.005
17	2	15	17	16	2	14	16	9504.785	9504.782	0.003
17	2	15	18	16	2	14	17	9504.818	9504.820	-0.003
17	2	15	16	16	2	14	15	9504.818	9504.824	-0.007
18	2	16	18	17	2	15	17	10072.941	72.937	0.004
18	2	16	19	17	2	15	18	10072.978	72.974	0.005
18	2	16	17	17	2	15	16	10072.978	72.977	0.002
19	2	17	19	18	2	16	18	10641.346	641.342	0.004
19	2	17	20	18	2	16	19	10641.374	641.376	-0.002

19	2	17	18	18	2	16	17	10641.374	641.378	-0.005
20	2	18	20	19	2	17	19	11209.748	1209.748	0.001
20	2	18	21	19	2	17	20	11209.775	1209.778	-0.003
20	2	18	19	19	2	17	20	11209.775	1209.767	0.008
21	2	19	21	20	2	18	20	11777.921	1777.916	0.005
21	2	19	22	20	2	18	21	11777.940	1777.942	-0.002
21	2	19	20	20	2	18	19	11777.940	1777.944	-0.004
13	3	10	14	12	3	9	13	7195.170	7195.168	0.002
13	3	10	12	12	3	9	11	7195.170	7195.172	-0.001
13	3	10	13	12	3	9	12	7195.181	7195.181	0.001
13	3	11	14	12	3	10	13	7191.876	7191.876	0.000
13	3	11	12	12	3	10	11	7191.876	7191.878	-0.001
13	3	11	13	12	3	10	12	7191.894	7191.893	0.001
13	5	9	14	12	5	8	13	7187.648	7187.650	-0.003
13	5	9	12	12	5	8	11	7187.648	7187.649	-0.001
13	5	9	13	12	5	8	12	7187.707	7187.711	-0.004
15	0	15	16	14	1	14	15	7322.501	7322.503	-0.002
15	0	15	15	14	1	14	14	7322.094	7322.096	-0.002
15	0	15	14	14	1	14	13	7322.533	7322.538	-0.005
16	0	16	16	15	1	15	15	7938.986	7938.987	-0.001
16	0	16	17	15	1	15	16	7939.361	7939.352	0.009
16	0	16	15	15	1	15	14	7939.383	7939.383	0.000
17	0	17	17	16	1	16	16	8551.447	8551.445	0.002
17	0	17	18	16	1	16	17	8551.774	8551.769	0.006
17	0	17	16	16	1	16	15	8551.792	8551.795	-0.003
19	0	19	19	18	1	18	18	9760.702	9760.709	-0.007
19	0	19	20	18	1	18	19	9760.947	9760.956	-0.009
19	0	19	18	18	1	18	17	9760.979	9760.975	0.004
13	1	13	12	12	0	12	11	8071.089	8071.096	-0.006
13	1	13	13	12	0	12	12	8071.706	8071.707	-0.001
13	1	13	14	12	0	12	13	8071.136	8071.131	0.005
18	1	18	17	17	0	17	16	10351.955	351.957	-0.002
18	1	18	19	17	0	17	18	10351.973	351.972	0.001
18	1	18	18	17	0	17	17	10352.333	352.336	-0.003

Table S9. Rotational transitions of BTI (**TT**)

J´´	*K*	*K*	*F´´*	*J´*	*K*	*K*	*F´*	$\nu_{exp.}$	$\nu_{calc.}$	$\nu_{exp.}-\nu_{calc.}$
12	0	12	13	11	0	11	12	6881.403	6881.401	0.001
12	0	12	11	11	0	11	10	6881.403	6881.403	0.000
12	0	12	12	11	0	11	11	6881.517	6881.515	0.001
13	0	13	14	12	0	12	13	7431.496	7431.492	0.005
13	0	13	12	12	0	12	11	7431.496	7431.493	0.003
13	0	13	13	12	0	12	12	7431.598	7431.595	0.003
14	0	14	15	13	0	13	14	7980.532	7980.530	0.002
14	0	14	13	13	0	13	12	7980.532	7980.532	-0.001
14	0	14	14	13	0	13	13	7980.623	7980.623	0.000
15	0	15	16	14	0	14	15	8529.158	8529.157	0.001
15	0	15	14	14	0	14	13	8529.158	8529.160	-0.002

15	0	15	15	14	0	14	14	8529.238	8529.239	-0.001
16	0	16	17	15	0	15	16	9077.813	9077.814	-0.001
16	0	16	15	15	0	15	14	9077.813	9077.817	-0.004
16	0	16	16	15	0	15	15	9077.894	9077.886	0.008
12	1	12	13	11	1	11	12	6808.059	6808.063	-0.004
12	1	12	11	11	1	11	10	6808.078	6808.073	0.005
12	1	12	12	11	1	11	11	6808.109	6808.103	0.005
13	1	13	14	12	1	12	13	7367.932	7367.934	-0.002
13	1	13	12	12	1	12	11	7367.947	7367.942	0.004
13	1	13	13	12	1	12	12	7367.971	7367.973	-0.003
14	1	14	15	13	1	13	14	7926.693	7926.697	-0.004
14	1	14	13	13	1	13	12	7926.710	7926.705	0.006
14	1	14	14	13	1	13	13	7926.734	7926.736	-0.001
15	1	15	16	14	1	14	15	8484.462	8484.454	0.008
15	1	15	14	14	1	14	13	8484.462	8484.461	0.002
15	1	15	15	14	1	14	14	8484.485	8484.491	-0.007
16	1	16	17	15	1	15	16	9041.316	9041.313	0.003
16	1	16	15	15	1	15	14	9041.316	9041.319	-0.003
16	1	16	16	15	1	15	15	9041.342	9041.349	-0.008
12	1	11	11	11	1	10	10	7238.939	7238.941	-0.002
12	1	11	13	11	1	10	12	7238.954	7238.949	0.005
12	1	11	12	11	1	10	11	7239.027	7239.022	0.005
13	1	12	12	12	1	11	11	7824.890	7824.882	0.008
13	1	12	14	12	1	11	13	7824.890	7824.890	0.000
13	1	12	13	12	1	11	12	7824.976	7824.972	0.004
14	1	13	13	13	1	12	12	8405.958	8405.961	-0.003
14	1	13	15	13	1	12	14	8405.978	8405.975	0.004
14	1	13	14	13	1	12	13	8406.059	8406.061	-0.002
15	1	14	16	14	1	13	15	8981.792	8981.798	-0.006
15	1	14	14	14	1	13	13	8981.792	8981.798	-0.006
15	1	14	15	14	1	13	14	8981.900	8981.904	-0.004
16	1	15	15	15	1	14	14	9552.112	9552.110	0.001
16	1	15	17	15	1	14	16	9552.112	9552.117	-0.006
16	1	15	16	15	1	14	15	9552.227	9552.225	0.002
13	2	12	14	12	2	11	13	7626.304	7626.300	0.004
13	2	12	12	12	2	11	11	7626.304	7626.300	0.004
13	2	12	13	12	2	11	12	7626.337	7626.343	-0.006
13	2	11	13	12	2	10	12	7870.077	7870.076	0.001
13	2	11	14	12	2	10	13	7870.131	7870.132	-0.001
13	2	11	12	12	2	10	11	7870.131	7870.134	-0.003
14	2	13	15	13	2	12	14	8204.022	8204.018	0.004
14	2	13	13	13	2	12	12	8204.022	8204.020	0.002
14	2	13	14	13	2	12	13	8204.065	8204.062	0.003
15	2	14	16	14	2	13	15	8779.919	8779.919	0.000
15	2	14	14	14	2	13	13	8779.919	8779.920	-0.001
15	2	14	15	14	2	13	14	8779.965	8779.965	0.001
16	2	15	17	15	2	14	16	9353.953	9353.955	-0.003
16	2	15	15	15	2	14	14	9353.953	9353.956	-0.003
16	2	15	16	15	2	14	15	9354.000	9354.002	-0.002
14	2	12	14	13	2	11	13	8488.069	8488.073	-0.004

14	2	12	15	13	2	11	14	8488.109	8488.116	-0.006
14	2	12	13	13	2	11	12	8488.109	8488.116	-0.007
15	2	13	15	14	2	12	14	9104.010	9104.011	-0.001
15	2	13	16	14	2	12	15	9104.042	9104.039	0.003
15	2	13	14	14	2	12	13	9104.042	9104.038	0.004
16	2	14	16	15	2	13	15	9717.141	9717.144	-0.003
16	2	14	17	15	2	13	16	9717.162	9717.158	0.004
16	2	14	15	15	2	13	14	9717.162	9717.157	0.005
13	3	11	14	12	3	10	13	7702.301	7702.297	0.004
13	3	11	12	12	3	10	11	7702.301	7702.293	0.008
13	3	11	13	12	3	10	12	7702.301	7702.306	-0.004
13	0	13	13	12	1	12	12	7100.951	7100.951	0.000
13	0	13	14	12	1	12	13	7101.156	7101.160	-0.004
13	0	13	12	12	1	12	11	7101.188	7101.188	-0.001
15	0	15	15	14	1	14	14	8316.100	8316.103	-0.004
15	0	15	16	14	1	14	15	8316.217	8316.217	0.000
15	0	15	14	14	1	14	13	8316.241	8316.233	0.007
16	0	16	16	15	1	15	15	8909.499	8909.498	0.001
16	0	16	17	15	1	15	16	8909.571	8909.577	-0.006
16	0	16	15	15	1	15	14	8909.590	8909.590	0.000
17	0	17	17	16	1	16	16	9494.977	9494.980	-0.003
17	0	17	18	16	1	16	17	9495.026	9495.032	-0.006
17	0	17	16	16	1	16	15	9495.045	9495.042	0.003
19	0	19	19	18	1	18	18	10647.000	10646.996	0.004
19	0	19	20	18	1	18	19	10647.020	10647.014	0.007
19	0	19	18	18	1	18	17	10647.024	10647.021	0.003
20	0	20	20	19	1	19	19	11215.702	11215.706	-0.004
20	0	20	21	19	1	19	20	11215.718	11215.713	0.006
20	0	20	19	19	1	19	18	11215.718	11215.718	0.000
13	1	13	12	12	0	12	11	7698.246	7698.247	-0.002
13	1	13	14	12	0	12	13	7698.268	7698.265	0.003
13	1	13	13	12	0	12	12	7698.612	7698.618	-0.006
14	1	14	13	13	0	13	12	8193.457	8193.458	-0.001
14	1	14	15	13	0	13	14	8193.472	8193.470	0.002
14	1	14	14	13	0	13	13	8193.758	8193.758	0.000
15	1	15	14	14	0	14	13	8697.389	8697.387	0.003
15	1	15	16	14	0	14	15	8697.389	8697.394	-0.005
15	1	15	15	14	0	14	14	8697.629	8697.627	0.002
16	1	16	15	15	0	15	14	9209.548	9209.546	0.002
16	1	16	17	15	0	15	16	9209.548	9209.551	-0.003
16	1	16	16	15	0	15	15	9209.739	9209.737	0.002
17	1	17	16	16	0	16	15	9729.120	9729.121	-0.002
17	1	17	18	16	0	16	17	9729.120	9729.123	-0.003
17	1	17	17	16	0	16	16	9729.272	9729.273	-0.001
18	1	18	19	17	0	17	18	10255.137	10255.139	-0.003
18	1	18	17	17	0	17	16	10255.137	10255.139	-0.002
18	1	18	18	17	0	17	17	10255.259	10255.259	0.000
19	1	19	20	18	0	18	19	10786.595	10786.597	-0.002
19	1	19	18	18	0	18	17	10786.595	10786.598	-0.003
19	1	19	19	18	0	18	18	10786.690	10786.693	-0.003

20	1	20	21	19	0	19	20	11322.550	11322.548	0.002
20	1	20	19	19	0	19	18	11322.550	11322.550	0.000
20	1	20	20	19	0	19	19	11322.631	11322.626	0.005

Table S10. Rotational transitions of BTN (**TG^{-}T↓**)

J´´	*K*	*K*	*F´´*	*J´*	*K*	*K*	*F´*	$\nu_{exp.}$	$\nu_{calc.}$	$\nu_{exp.} - \nu_{calc.}$
39	18	21	40	38	17	22	39	60024.980	60024.770	0.210
39	18	21	38	38	17	22	37	60024.980	60024.771	0.209
39	18	21	39	38	17	22	38	60024.980	60024.742	0.238
35	19	16	36	34	18	17	35	60100.400	60100.396	0.004
35	19	16	35	34	18	17	34	60100.400	60100.363	0.037
35	19	16	34	34	18	17	33	60100.400	60100.397	0.003
31	20	12	32	30	19	11	31	60170.590	60170.658	-0.067
31	20	12	31	30	19	11	30	60170.590	60170.622	-0.032
31	20	12	30	30	19	11	29	60170.590	60170.658	-0.068
27	21	6	28	26	20	7	27	60238.060	60237.974	0.086
27	21	6	27	26	20	7	26	60238.060	60237.941	0.119
27	21	6	26	26	20	7	25	60238.060	60237.974	0.086
23	22	1	24	22	21	2	23	60303.730	60303.694	0.037
23	22	1	23	22	21	2	22	60303.730	60303.680	0.050
23	22	1	22	22	21	2	21	60303.730	60303.691	0.039
40	18	23	41	39	17	22	40	60562.180	60562.306	-0.126
40	18	23	40	39	17	22	39	60562.180	60562.279	-0.099
40	18	23	39	39	17	22	38	60562.180	60562.307	-0.127
36	19	18	37	35	18	17	36	60639.250	60639.057	0.193
36	19	18	36	35	18	17	35	60639.250	60639.025	0.225
36	19	18	35	35	18	17	34	60639.250	60639.058	0.192
32	20	12	33	31	19	13	32	60709.900	60709.927	-0.027
32	20	12	32	31	19	13	31	60709.900	60709.892	0.008
32	20	12	31	31	19	13	30	60709.900	60709.928	-0.028
28	21	8	29	27	20	7	28	60777.490	60777.537	-0.047
28	21	8	28	27	20	7	27	60777.490	60777.503	-0.013
28	21	8	27	27	20	7	26	60777.490	60777.537	-0.047
24	22	3	25	23	21	2	24	60843.300	60843.360	-0.060
24	22	3	24	23	21	2	23	60843.300	60843.341	-0.041
24	22	3	23	23	21	2	22	60843.300	60843.359	-0.059
41	18	23	42	40	17	24	41	61099.500	61099.604	-0.104
41	18	23	41	40	17	24	40	61099.500	61099.579	-0.079
41	18	23	40	40	17	24	39	61099.500	61099.605	-0.105
37	19	18	38	36	18	19	37	61177.580	61177.579	0.001
37	19	18	37	36	18	19	36	61177.580	61177.548	0.032
37	19	18	36	36	18	19	35	61177.580	61177.580	0.000
29	21	8	30	28	20	9	29	61316.990	61317.070	-0.080
29	21	8	29	28	20	9	28	61316.990	61317.035	-0.045
29	21	8	28	28	20	9	27	61316.990	61317.070	-0.080
25	22	4	26	24	21	3	25	61382.940	61383.025	-0.085

25	22	4	25	24	21	3	24	61382.940	61383.001	-0.061
25	22	4	24	24	21	3	23	61382.940	61383.024	-0.084
7	4	3	7	6	3	4	6	11577.995	11577.992	0.004
7	4	3	8	6	3	4	7	11578.152	11578.148	0.004
7	4	3	6	6	3	4	5	11578.179	11578.176	0.003
8	4	5	8	7	3	4	7	12111.050	12111.052	-0.002
8	4	5	9	7	3	4	8	12111.156	12111.158	-0.002
8	4	5	7	7	3	4	6	12111.174	12111.177	-0.003
8	4	4	8	7	3	5	7	12116.721	12116.720	0.000
8	4	4	9	7	3	5	8	12116.855	12116.854	0.001
8	4	4	7	7	3	5	6	12116.876	12116.876	-0.001
9	4	6	9	8	3	5	8	12643.073	12643.075	-0.002
9	4	6	10	8	3	5	9	12643.142	12643.143	-0.001
9	4	6	8	8	3	5	7	12643.156	12643.155	0.000
9	4	5	9	8	3	6	8	12655.585	12655.585	0.000
9	4	5	10	8	3	6	9	12655.699	12655.699	0.000
9	4	5	8	8	3	6	7	12655.717	12655.718	-0.001
18	2	16	17	17	2	15	16	10035.030	10035.030	0.000
18	2	16	19	17	2	15	18	10035.034	10035.033	0.001
18	2	16	18	17	2	15	17	10035.080	10035.080	0.000
20	1	20	21	19	1	19	20	10094.573	10094.573	0.000
20	1	20	19	19	1	19	18	10094.578	10094.578	0.001
20	1	20	20	19	1	19	19	10094.600	10094.600	0.000
20	0	20	21	19	0	19	20	10101.831	10101.831	0.000
20	0	20	19	19	0	19	18	10101.836	10101.836	0.001
20	0	20	20	19	0	19	19	10101.864	10101.864	0.000
21	0	21	22	20	0	20	21	10594.167	10594.167	-0.001
21	0	21	20	20	0	20	19	10594.172	10594.171	0.001
21	0	21	21	20	0	20	20	10594.196	10594.197	0.000
20	1	19	19	19	1	18	18	10619.056	10619.054	0.002
20	1	19	21	19	1	18	20	10619.056	10619.057	-0.001
20	1	19	20	19	1	18	19	10619.168	10619.167	0.000
20	3	18	21	19	3	17	20	10784.707	10784.707	0.001
20	3	18	19	19	3	17	18	10784.707	10784.707	0.000
20	3	18	20	19	3	17	19	10784.740	10784.740	0.000
20	4	17	21	19	4	16	20	10868.055	10868.056	0.000
20	4	17	20	19	4	16	19	10868.055	10868.059	-0.003
20	4	17	19	19	4	16	18	10868.055	10868.056	-0.001
20	5	16	21	19	5	15	20	10854.996	10854.996	0.000
20	5	15	20	19	5	14	19	10862.190	10862.192	-0.001
20	5	15	21	19	5	14	20	10862.199	10862.198	0.001
21	1	20	22	20	1	19	21	11103.180	11103.181	0.000
21	1	20	20	20	1	19	19	11103.180	11103.179	0.002
21	1	20	21	20	1	19	20	11103.281	11103.281	0.000
21	3	19	22	20	3	18	21	11310.613	11310.612	0.000
21	3	19	20	20	3	18	19	11310.613	11310.612	0.000
21	3	19	21	20	3	18	20	11310.648	11310.649	0.000
21	4	18	22	20	4	17	21	11413.972	11413.972	0.000
21	4	18	20	20	4	17	19	11413.972	11413.973	-0.001
21	4	18	21	20	4	17	20	11413.976	11413.976	0.001

22	2	21	23	21	2	20	22	11514.654	11514.653	0.001
22	2	21	21	21	2	20	20	11514.654	11514.654	0.000
22	2	21	22	21	2	20	21	11514.706	11514.705	0.001
23	0	23	24	22	0	22	23	11579.579	11579.580	0.000
23	0	23	22	22	0	22	21	11579.584	11579.584	0.001
23	0	23	23	22	0	22	22	11579.604	11579.604	0.000
22	1	21	23	21	1	20	22	11587.514	11587.515	-0.001
22	1	21	21	21	1	20	20	11587.514	11587.513	0.001
22	1	21	22	21	1	20	21	11587.605	11587.606	0.000
21	2	19	20	20	2	18	19	11619.221	11619.223	-0.002
21	2	19	22	20	2	18	21	11619.221	11619.227	-0.006
21	2	19	21	20	2	18	20	11619.311	11619.311	0.000
22	3	20	23	21	3	19	22	11833.653	11833.652	0.001
22	3	20	21	21	3	19	20	11833.653	11833.652	0.001
22	3	20	22	21	3	19	21	11833.691	11833.691	0.000
22	5	18	23	21	5	17	22	11955.330	11955.328	0.002
22	5	18	22	21	5	17	21	11955.330	11955.325	0.005
22	5	18	21	21	5	17	20	11955.330	11955.330	0.000
22	6	16	23	21	6	15	22	11929.642	11929.643	-0.001
22	6	16	22	21	6	15	21	11929.642	11929.646	-0.004
22	6	16	21	21	6	15	20	11929.642	11929.644	-0.002
22	4	19	23	21	4	18	22	11958.693	11958.693	-0.001
22	4	19	21	21	4	18	20	11958.693	11958.694	-0.001
22	4	19	22	21	4	18	21	11958.700	11958.700	0.001
28	2	27	29	27	2	26	28	14497.770	14497.769	0.000
28	2	27	27	27	2	26	26	14497.770	14497.770	0.000
28	2	27	28	27	2	26	27	14497.810	14497.810	0.000
28	3	26	29	27	3	25	28	14912.881	14912.881	0.000
28	3	26	27	27	3	25	26	14912.881	14912.880	0.000
28	3	26	28	27	3	25	27	14912.928	14912.928	0.000
21	3	18	21	20	3	17	20	11736.086	11736.084	0.002
21	3	18	22	20	3	17	21	11736.117	11736.116	0.000
21	3	18	20	20	3	17	19	11736.117	11736.117	-0.001
24	0	24	25	23	0	23	24	12072.543	12072.544	-0.001
24	0	24	23	23	0	23	22	12072.548	12072.548	0.001
24	0	24	24	23	0	23	23	12072.565	12072.566	-0.001
23	1	22	24	22	1	21	23	12072.610	12072.610	-0.001
23	1	22	22	22	1	21	21	12072.610	12072.610	0.000
23	1	22	23	22	1	21	22	12072.694	12072.692	0.001
8	4	5	8	7	3	4	7	12111.049	12111.052	-0.003
8	4	5	9	7	3	4	8	12111.158	12111.158	0.000
8	4	5	7	7	3	4	6	12111.172	12111.177	-0.005
7	4	4	7	6	3	3	6	11575.729	11575.734	-0.005
7	4	4	8	6	3	3	7	11575.872	11575.876	-0.005
7	4	4	6	6	3	3	5	11575.896	11575.902	-0.006
9	5	5	9	8	4	4	8	14884.762	14884.764	-0.002
9	5	5	10	8	4	4	9	14884.879	14884.883	-0.004
9	5	5	8	8	4	4	7	14884.879	14884.899	-0.020
9	5	4	9	8	4	5	8	14884.975	14884.974	0.001
9	5	4	10	8	4	5	9	14885.094	14885.094	0.000

9	5	4	8	8	4	5	7	14885.109	14885.110	-0.001
10	5	6	10	9	4	5	9	15422.047	15422.049	-0.002
10	5	6	11	9	4	5	10	15422.148	15422.149	-0.002
10	5	6	9	9	4	5	8	15422.148	15422.163	-0.015
10	5	5	10	9	4	6	9	15422.594	15422.596	-0.002
10	5	5	11	9	4	6	10	15422.698	15422.699	-0.001
10	5	5	9	9	4	6	8	15422.709	15422.713	-0.003
11	5	7	11	10	4	6	10	15958.131	15958.134	-0.003
11	5	7	12	10	4	6	11	15958.213	15958.215	-0.002
11	5	7	10	10	4	6	9	15958.213	15958.226	-0.013
12	5	8	12	11	4	7	11	16492.542	16492.543	-0.001
12	5	8	13	11	4	7	12	16492.605	16492.607	-0.002
12	5	8	11	11	4	7	10	16492.615	16492.616	0.000
32	2	31	33	31	1	30	32	16492.864	16492.864	0.000
32	2	31	31	31	1	30	30	16492.864	16492.865	-0.001
32	2	31	32	31	1	30	31	16492.905	16492.905	0.000
12	5	7	12	11	4	8	11	16495.297	16495.291	0.005
12	5	7	13	11	4	8	12	16495.369	16495.363	0.006
12	5	7	11	11	4	8	10	16495.379	16495.372	0.007

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