Supporting Information



# Flexibility at the Fringes: Conformations of the Steroid Hormone *β*-Estradiol

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# Contents

# 1 Calculated rotational constants of the 16 diastereomers of estradiol

Table S1: Calculated rotational constants, dipole moment components and energy differences of the 16 diastereomers of estradiol. The first column gives the configuration of the five chiral centers C8/C9/C13/C14/C17. $\alpha$- and $\beta$-estradiol are specially marked.

| Stereoisomers | A [MHz] | B [MHz] | C [MHz] | $\|\mu_a\|$ [D] | $\|\mu_b\|$ [D] | $\|\mu_c\|$ [D] | $\|\mu_{tot}\|$ [D] | ΔE [kJ/mol] |
|---|---|---|---|---|---|---|---|---|
| RSRSS | 932.91 | 174.23 | 162.46 | 0.1 | -2.2 | 0.1 | 2.2 | 0.0 |
| RSSSS ($\beta$) | 939.89 | 172.97 | 153.73 | 0.5 | -1.5 | -1.2 | 1.9 | 1.9 |
| RSSRS | 820.60 | 189.92 | 173.44 | -1.0 | -1.8 | -1.6 | 2.6 | 2.0 |
| RSSSR ($\alpha$) | 899.95 | 178.42 | 160.68 | -1.9 | -0.4 | 0.5 | 2.0 | 2.1 |
| SSRSS | 778.84 | 195.16 | 177.68 | 0.5 | -1.3 | -1.7 | 2.2 | 4.5 |
| SRRSS | 952.09 | 173.03 | 155.36 | 0.4 | -1.5 | -1.1 | 1.9 | 5.5 |
| RRSRS | 706.18 | 219.94 | 202.63 | 0.6 | -2.0 | 0.4 | 2.1 | 5.7 |
| RRSSS | 960.25 | 172.24 | 153.90 | 0.6 | -1.4 | -0.8 | 1.7 | 6.4 |
| RRRSS | 977.30 | 172.53 | 157.58 | -0.7 | -0.9 | 0.4 | 1.2 | 6.6 |
| SSSSS | 1005.57 | 171.65 | 164.44 | 0.7 | -1.8 | -1.3 | 2.3 | 6.8 |
| SSSRS | 744.33 | 203.08 | 193.20 | -1.0 | 0.6 | -1.2 | 1.7 | 7.1 |
| SSRRS | 896.22 | 181.22 | 169.74 | -0.2 | -2.2 | -1.3 | 2.6 | 7.3 |
| SRSRS | 814.91 | 192.19 | 175.20 | 0.7 | -1.3 | 1.2 | 1.9 | 7.9 |
| RSRRS | 905.37 | 179.01 | 161.16 | 0.3 | -1.4 | 1.3 | 1.9 | 11.6 |
| RRRRS | 739.33 | 215.63 | 198.04 | 0.5 | -1.5 | -0.1 | 1.6 | 11.7 |
| SRSSS | 952.86 | 175.02 | 160.39 | 0.4 | -1.9 | -0.8 | 2.1 | 12.0 |
| SRRRS | 806.71 | 192.48 | 175.56 | 0.2 | -1.7 | 0.7 | 1.9 | 13.9 |

# 2 Simulations of different stereoisomers of estradiol

Figure S1 shows a comparison between the simulated spectra of $\alpha$- and $\beta$-estradiol at a rotational temperature of 1 K. Even though the two stereoisomers only differ in the configuration at one chiral center (C17), their rotational spectra differ significantly. The spectrum of $\alpha$-estradiol is dominated by a typical a-type pattern, caused by the strong dipole moment component in the direction of the a-axes, while the spectrum of $\beta$-estradiol shows mainly b- and c-type transitions. A zoom into the region around 4 GHz (Figure S2) underlines the clear difference between the well recognizable a-type pattern of $\alpha$-estradiol and a congested q-branch in the spectrum of $\beta$-estradiol.

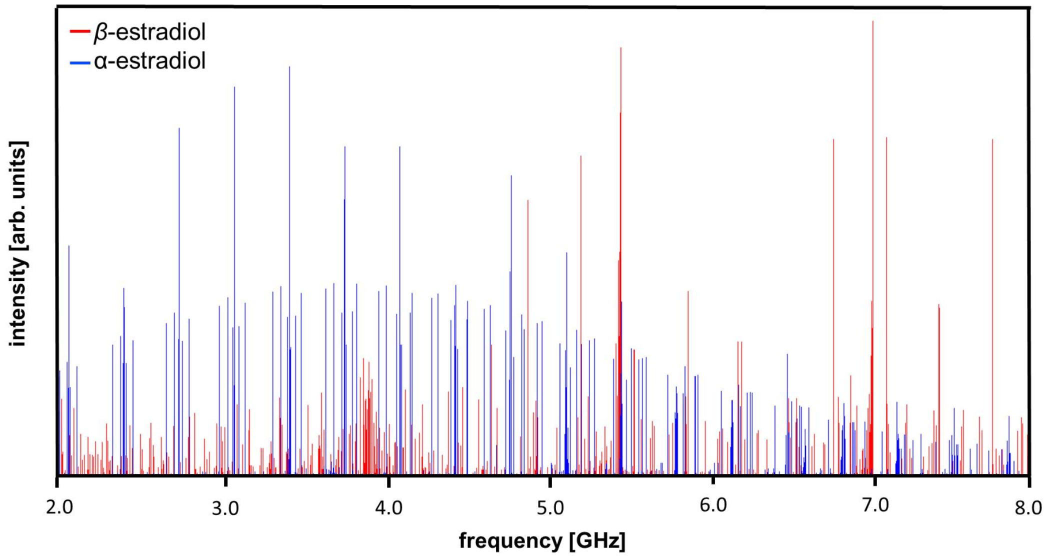


Figure S1: Simulations of the rotational spectra of $\alpha$- and $\beta$-estradiol at a rotational temperature of 1 K

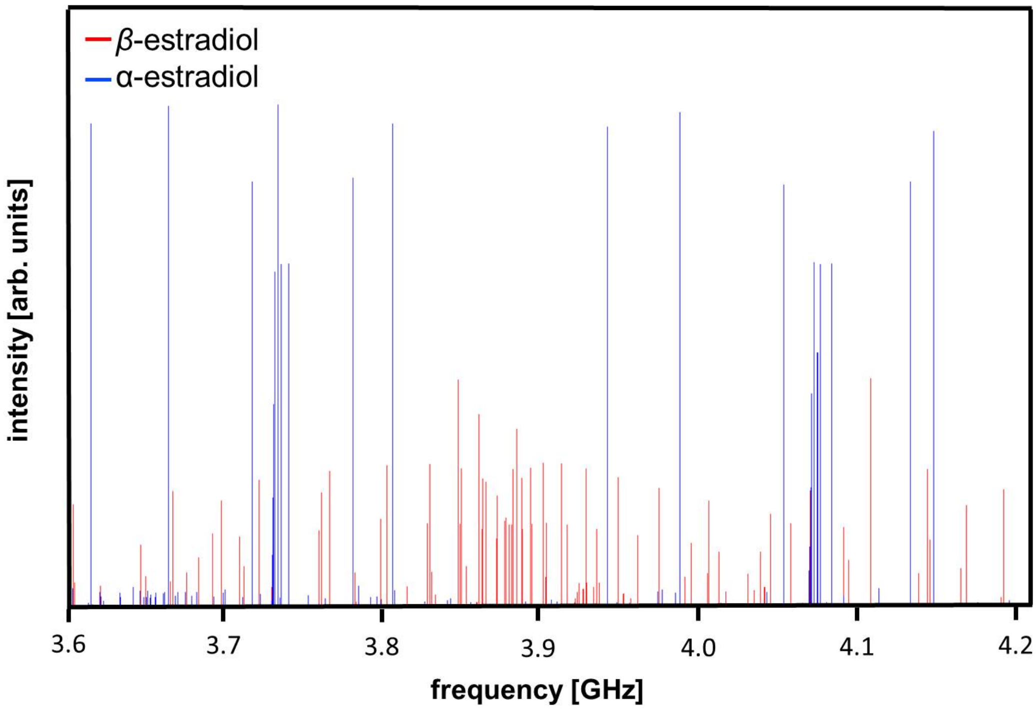


Figure S2: Zoom into the simulated spectra of $\alpha$- and $\beta$-estradiol at around 4 GHz.

## 3 Rotational Constants of the $^{13}$C isotopologues

Table S2: Experimentally determined rotational constants for all single $^{13}$C substituted species of the *trans-gauche(+)* conformer of $\beta$-estradiol, number of assigned lines and the error of the fit. The distortion constant $D_K$ of the parent molecule was used for the fits of the isotopologues.

| Isotopologue | A (MHz) | B (MHz) | C (MHz) | assigned lines | error (kHz) |
|---|---|---|---|---|---|
| C1 | 935.4420(10) | 174.3960(18) | 154.91436(58) | 7 | 7.0 |
| C2 | 935.81985(49) | 173.87482(42) | 154.49729(16) | 8 | 3.9 |
| C3 | 939.39846(72) | 173.6033(11) | 154.36545(36) | 6 | 4.6 |
| C4 | 938.09559(64) | 173.94533(55) | 154.61979(22) | 7 | 4.9 |
| C5 | 938.27788(84) | 174.50734(61) | 155.04509(29) | 7 | 6.6 |
| C6 | 931.43437(75) | 174.70332(49) | 154.98799(23) | 6 | 5.2 |
| C7 | 931.74640(97) | 174.8079(17) | 155.13409(54) | 6 | 6.2 |
| C8 | 938.46308(73) | 174.79723(161) | 155.30446(53) | 6 | 4.6 |
| C9 | 938.6545(12) | 174.795095(84) | 155.33604(38) | 6 | 8.5 |
| C10 | 939.2348(11) | 174.6183(18) | 155.18657(59) | 8 | 7.8 |
| C11 | 934.28166(93) | 174.8095(11) | 155.19413(39) | 7 | 6.6 |
| C12 | 933.78937(53) | 174.59453(34) | 155.02786(17) | 9 | 4.5 |
| C13 | 939.01256(86) | 174.42697(63) | 155.01551(26) | 9 | 7.5 |
| C14 | 938.44316(86) | 174.58268(71) | 155.14569(28) | 6 | 5.8 |
| C15 | 933.71626(81) | 174.31684(63) | 154.79017(33) | 7 | 5.8 |
| C16 | 937.18377(95) | 173.7113(18) | 154.4074(6) | 7 | 6.4 |
| C17 | 939.1732(12) | 173.8547(18) | 154.5694(6) | 7 | 8.2 |
| C18 | 933.99017(76) | 174.2851(13) | 155.01268(43) | 5 | 4.3 |

# 4 Coordinates from the least squares fit method

Table S3: Experimentally determined atom positions, calculated with the least squares fit method.

| Atom number | x | dx | y | dy | z | dz |
|---|---|---|---|---|---|---|
| C1 | 2.63092 | 0.04446 | -1.48883 | 0.02026 | -0.35852 | 0.03547 |
| C2 | 3.98353 | 0.03462 | -1.44616 | 0.02121 | -0.16255 | 0.04944 |
| C3 | 4.54289 | 0.02698 | -0.24022 | 0.02434 | 0.17819 | 0.03477 |
| C4 | 3.82771 | 0.02971 | 0.89754 | 0.08194 | 0.21788 | 0.02770 |
| C5 | 2.34868 | 0.05901 | 0.85042 | 0.07506 | 0.00537 | 0.01731 |
| C6 | 1.57600 | 0.08548 | 2.18902 | 0.03936 | 0.07759 | 0.07264 |
| C7 | 0.29083 | 0.12058 | 2.11698 | 0.04273 | -0.43956 | 0.03142 |
| C8 | -0.42073 | 0.09720 | 0.78131 | 0.03946 | 0.03881 | 0.03284 |
| C9 | 0.31386 | 0.13939 | -0.41139 | 0.09362 | -0.54642 | 0.02063 |
| C10 | 1.83376 | 0.06408 | -0.35919 | 0.09784 | -0.26973 | 0.01252 |
| C11 | -0.39212 | 0.27817 | -1.74107 | 0.05167 | -0.18143 | 0.05731 |
| C12 | -1.82521 | 0.05712 | -1.77914 | 0.05479 | -0.45578 | 0.03462 |
| C13 | -2.56314 | 0.02714 | -0.56429 | 0.03428 | 0.14932 | 0.01498 |
| C14 | -1.90362 | 0.04338 | 0.68762 | 0.03786 | -0.35115 | 0.01372 |
| C15 | -2.90671 | 0.04478 | 1.83192 | 0.05958 | 0.04316 | 0.04456 |
| C16 | -4.30485 | 0.02263 | 1.17193 | 0.09413 | -0.10885 | 0.05563 |
| C17 | -4.04026 | 0.02601 | -0.30889 | 0.02793 | -0.40094 | 0.02412 |
| C18 | -2.59863 | 0.03273 | -0.66927 | 0.06049 | 1.70348 | 0.03693 |
| O1 | -5.07918 | 0.02819 | -1.09989 | 0.03641 | 0.17666 | 0.03445 |
| O2 | 5.88826 | 0.02884 | -0.15631 | 0.06821 | 0.43411 | 0.09377 |
| H1 | -5.02300 | 0.03513 | -1.99313 | 0.03424 | -0.17692 | 0.03806 |
| H2 | 6.36512 | 0.03545 | -0.96244 | 0.04643 | 0.24725 | 0.07275 |
| H3 | -1.92887 | 0.04972 | 0.62096 | 0.04390 | -1.45097 | 0.01381 |
| H4 | -0.33921 | 0.09838 | 0.73748 | 0.05320 | 1.13378 | 0.03368 |
| H5 | 0.18837 | 0.14757 | -0.32932 | 0.11044 | -1.63856 | 0.02159 |
| H6 | -2.72069 | 0.04648 | 2.18266 | 0.05668 | 1.06275 | 0.04818 |
| H7 | -2.81544 | 0.05110 | 2.70090 | 0.06370 | -0.61175 | 0.05781 |
| H8 | 0.32222 | 0.11821 | 2.13705 | 0.05495 | -1.53664 | 0.03169 |
| H9 | -0.27914 | 0.12769 | 2.99616 | 0.04167 | -0.12473 | 0.02882 |
| H10 | -2.23912 | 0.06396 | -2.72139 | 0.05289 | -0.07592 | 0.04013 |
| H11 | -1.97846 | 0.06280 | -1.78244 | 0.06724 | -1.54338 | 0.03294 |
| H12 | -4.02889 | 0.03339 | -0.47484 | 0.02889 | -1.48766 | 0.02313 |
| H13 | -3.06030 | 0.03949 | 0.20399 | 0.06649 | 2.16809 | 0.02106 |
| H14 | -3.19047 | 0.03535 | -1.53779 | 0.06283 | 2.00090 | 0.04357 |
| H15 | -1.60100 | 0.03619 | -0.78023 | 0.07467 | 2.13078 | 0.05163 |
| H16 | -4.92429 | 0.02518 | 1.61992 | 0.10093 | -0.88832 | 0.06951 |
| H17 | -4.86766 | 0.02817 | 1.24667 | 0.09300 | 0.82426 | 0.06309 |
| H18 | 0.07746 | 0.27902 | -2.57147 | 0.05558 | -0.71503 | 0.06325 |
| H19 | -0.20461 | 0.28181 | -1.92045 | 0.05158 | 0.88256 | 0.05886 |
| H20 | 2.13514 | 0.08678 | 3.00250 | 0.04229 | -0.39552 | 0.07470 |
| H21 | 1.51640 | 0.08845 | 2.44615 | 0.04460 | 1.14357 | 0.07064 |
| H22 | 2.18436 | 0.05031 | -2.44701 | 0.02533 | -0.59322 | 0.04966 |
| H23 | 4.31783 | 0.03495 | 1.83872 | 0.08638 | 0.44365 | 0.03482 |
| H24 | 4.57511 | 0.03751 | -2.35397 | 0.02492 | -0.23926 | 0.07158 |

# 5 Coordinates from the substitution method

The substitution fit reveals imaginary coordinates for several atoms, which are close to the inertial axis. These imaginary coordinates were set to zero.

Table S4: Experimentally determined atom positions, calculated with the substitution method.

| Atom number | x | dx | y | dy | z | dz |
|---|---|---|---|---|---|---|
| C1 | 2.60742 | 0.00143 | -1.48830 | 0.00251 | -0.42314 | 0.00887 |
| C2 | 3.95590 | 0.00090 | -1.47497 | 0.00244 | -0.08907 | 0.04050 |
| C3 | 4.51246 | 0.00158 | -0.50827 | 0.01417 | 0.0 | 0.01883 |
| C4 | 3.79844 | 0.00440 | 0.89648 | 0.01875 | 0.24511 | 0.06868 |
| C5 | 2.30640 | 0.00146 | 0.97200 | 0.00347 | 0.0 | 0.00776 |
| C6 | 1.52086 | 0.00158 | 2.27121 | 0.00106 | 0.0 | 0.00366 |
| C7 | 0.08504 | 0.04941 | 2.09380 | 0.00201 | -0.38316 | 0.01110 |
| C8 | -0.49939 | 0.00373 | 0.75394 | 0.00247 | 0.28133 | 0.00663 |
| C9 | 0.0 | 0.01876 | -0.40611 | 0.00433 | -0.61049 | 0.00288 |
| C10 | 1.78578 | 0.00231 | -0.31875 | 0.01295 | -0.32175 | 0.01283 |
| C11 | -0.31530 | 0.00767 | -1.74141 | 0.00139 | -0.16145 | 0.01508 |
| C12 | -1.86527 | 0.00173 | -1.77330 | 0.00182 | -0.45170 | 0.00720 |
| C13 | -2.55139 | 0.00139 | -0.61341 | 0.00581 | 0.0 | 0.01718 |
| C14 | -1.91977 | 0.00228 | 0.68054 | 0.00645 | -0.44361 | 0.00991 |
| C15 | -2.87422 | 0.00132 | 1.83628 | 0.00207 | 0.16146 | 0.02375 |
| C16 | -4.28575 | 0.00074 | 1.16734 | 0.00275 | -0.17586 | 0.01830 |
| C17 | -4.00383 | 0.00521 | -0.51677 | 0.04065 | -0.0 | 0.13221 |
| C18 | -2.50293 | 0.00231 | -0.81847 | 0.00703 | 1.60160 | 0.00362 |

# 6 Calculated coordinates using the B3LYP/6-311++g(d,p) method

Table S5: Calculated atom positions using the B3LYP/6-311++g(d,p) method.

| Atom number | x | y | z |
|---|---|---|---|
| C1 | -1.917971 | 0.720306 | -0.370334 |
| C2 | -0.444798 | 0.806179 | 0.028129 |
| C3 | -2.611075 | -0.565309 | 0.148154 |
| C4 | 0.302084 | -0.419955 | -0.557647 |
| C5 | -4.040405 | -0.310892 | -0.398323 |
| C6 | 2.603396 | -1.507653 | -0.347586 |
| C7 | 3.823545 | 0.898459 | 0.231033 |
| C | 3.978676 | -1.471952 | -0.138173 |
| C | -2.658226 | -0.660844 | 1.686610 |
| C1 | -5.035555 | -1.987621 | -0.172780 |
| C11 | 6.360227 | -1.001254 | 0.286745 |
| C1 | 4.593469 | -0.256498 | 0.155302 |
| C1 | -2.897883 | 1.851450 | 0.003381 |
| 14 | 0.253293 | 2.087861 | -0.435003 |
| C15 | -1.880745 | -1.780941 | -0.441651 |
| C16 | -4.299774 | 1.185399 | -0.113630 |

Table S5: Calculated atom positions using the B3LYP/6-311++g(d,p) method.

| Atom number | x | y | z |
|---|---|---|---|
| C17 | -0.367624 | -1.748809 | -0.140579 |
| C18 | 1.666555 | 2.161271 | 0.145285 |
| O1 | -5.088616 | -1.092184 | 0.175693 |
| O2 | 5.942920 | -0.138055 | 0.373265 |
| H1 | 1.804375 | -0.360319 | -0.269811 |
| H2 | 2.442639 | 0.862187 | 0.022422 |
| H3 | -1.935529 | 0.647997 | -1.469953 |
| H4 | -0.371647 | 0.767621 | 1.123892 |
| H5 | 0.185195 | -0.342858 | -1.651103 |
| H6 | -2.717160 | 2.206383 | 1.022470 |
| H7 | -2.796210 | 2.716355 | -0.655379 |
| H8 | 0.292911 | 2.101924 | -1.531908 |
| H9 | -0.313335 | 2.972308 | -0.129028 |
| H10 | -2.303490 | -2.718506 | -0.059936 |
| H11 | -2.025974 | -1.789010 | -1.530325 |
| H12 | -4.022069 | -0.482653 | -1.484042 |
| H13 | -3.117704 | 0.217785 | 2.143198 |
| H14 | -3.257799 | -1.523990 | 1.984185 |
| H15 | -1.664515 | -0.775906 | 2.121879 |
| H16 | -4.910562 | 1.633207 | -0.900016 |
| H17 | -4.868970 | 1.268666 | 0.814878 |
| H18 | 0.100555 | -2.585000 | -0.666320 |
| H19 | -0.189126 | -1.923756 | 0.925696 |
| H20 | 2.234375 | 2.968665 | -0.327921 |
| H21 | 1.600734 | 2.424416 | 1.209434 |
| H22 | 2.152447 | -2.464197 | -0.580574 |
| H23 | 4.318015 | 1.837676 | 0.455498 |
| H24 | 4.564976 | -2.383908 | -0.205731 |

# 7 Comparison between the experimentally determined and calculated bond lengths

Table S6: Experimentally determined bond lengths of $\beta$-estradiol (*trans-gauche(+)* conformer) ($r_0$-structure) compared to values from quantum-chemical calculations.

| bond | exp. $r_0$-structure (Å) | B3LYP/6-311++g(d,p) |
|---|---|---|
| 1-2 | 1.36(3) | 1.39 |
| 2-3 | 1.31(4) | 1.39 |
| 3-4 | 1.30(3) | 1.39 |
| 4-5 | 1.49(3) | 1.40 |
| 5-6 | 1.45(13) | 1.52 |
| 6-7 | 1.39(8) | 1.53 |
| 7-8 | 1.59(4) | 1.53 |
| 8-9 | 1.50(8) | 1.55 |
| 9-10 | 1.54(5) | 1.53 |
| 1-10 | 1.40(6) | 1.40 |
| 9-11 | 1.59(5) | 1.55 |
| 11-12 | 1.51(13) | 1.54 |
| 12-13 | 1.55(4) | 1.54 |
| 13-18 | 1.56(1) | 1.54 |
| 13-14 | 1.49(3) | 1.55 |
| 8-14 | 1.57(5) | 1.53 |
| 14-15 | 1.56(3) | 1.54 |
| 15-16 | 1.56(2) | 1.56 |
| 16-17 | 1.56(5) | 1.55 |
| 13-17 | 1.56(2) | 1.55 |

# 8 Line List of Observed Transitions

Assigned transitions for the three estradiol conformers and the singly substituted isotopologues of the *trans-gauche(+)* conformer. The quantum numbers describe a transition from $J'_{K'_a K'_c} \leftarrow J_{K_a K_c}$. The observed and the calculated frequencies and their differences for each transition are given.

Table S7: Observed transitions for the *trans-gauche(+)* conformer (Conf1)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 9 | 2 | 7 | 9 | 1 | 8 | 2016.161 | 2016.167 | -6.4 |
| 6 | 1 | 5 | 5 | 1 | 4 | 2036.325 | 2036.324 | 0.8 |
| 7 | 2 | 6 | 7 | 1 | 6 | 2056.092 | 2056.090 | 2.2 |
| 8 | 2 | 6 | 8 | 1 | 7 | 2057.047 | 2057.052 | -4.9 |
| 8 | 0 | 8 | 7 | 1 | 7 | 2073.825 | 2073.820 | 5.3 |
| 9 | 4 | 6 | 10 | 3 | 7 | 2100.357 | 2100.368 | -10.6 |
| 9 | 4 | 5 | 10 | 3 | 7 | 2100.430 | 2100.422 | 7.8 |
| 7 | 2 | 5 | 7 | 1 | 6 | 2101.747 | 2101.742 | 5.0 |
| 9 | 4 | 5 | 10 | 3 | 8 | 2107.782 | 2107.780 | 2.3 |

Table S7: Observed transitions for the *trans-gauche(+)* conformer (Conf1)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 6 | 2 | 5 | 6 | 1 | 5 | 2122.000 | 2122.006 | -5.8 |
| 17 | 2 | 15 | 17 | 1 | 16 | 2127.145 | 2127.138 | 6.3 |
| 6 | 2 | 4 | 6 | 1 | 5 | 2147.514 | 2147.516 | -1.9 |
| 5 | 2 | 4 | 5 | 1 | 4 | 2179.015 | 2179.018 | -3.4 |
| 5 | 2 | 3 | 5 | 1 | 4 | 2191.817 | 2191.821 | -4.3 |
| 4 | 1 | 3 | 3 | 0 | 3 | 2193.385 | 2193.380 | 5.7 |
| 4 | 2 | 3 | 4 | 1 | 3 | 2226.866 | 2226.866 | 0.0 |
| 4 | 2 | 2 | 4 | 1 | 3 | 2232.367 | 2232.365 | 2.3 |
| 7 | 1 | 7 | 6 | 1 | 6 | 2238.421 | 2238.414 | 7.0 |
| 3 | 2 | 2 | 3 | 1 | 2 | 2265.350 | 2265.351 | -1.3 |
| 3 | 2 | 1 | 3 | 1 | 2 | 2267.179 | 2267.186 | -6.9 |
| 5 | 1 | 5 | 4 | 0 | 4 | 2282.255 | 2282.253 | 1.8 |
| 7 | 0 | 7 | 6 | 0 | 6 | 2290.974 | 2290.977 | -3.8 |
| 7 | 2 | 6 | 6 | 2 | 5 | 2308.274 | 2308.270 | 4.0 |
| 7 | 5 | 3 | 6 | 5 | 2 | 2312.428 | 2312.427 | 1.3 |
| 7 | 5 | 2 | 6 | 5 | 1 | 2312.428 | 2312.427 | 1.3 |
| 7 | 4 | 4 | 6 | 4 | 3 | 2312.958 | 2312.949 | 8.2 |
| 7 | 4 | 3 | 6 | 4 | 2 | 2312.958 | 2312.955 | 3.1 |
| 7 | 3 | 4 | 6 | 3 | 3 | 2314.461 | 2314.452 | 8.5 |
| 7 | 2 | 5 | 6 | 2 | 4 | 2328.420 | 2328.411 | 8.8 |
| 12 | 1 | 11 | 11 | 2 | 10 | 2336.946 | 2336.936 | 9.8 |
| 7 | 1 | 6 | 6 | 1 | 5 | 2374.188 | 2374.185 | 2.3 |
| 4 | 2 | 3 | 4 | 1 | 4 | 2421.587 | 2421.571 | 15.6 |
| 8 | 4 | 5 | 9 | 3 | 6 | 2437.025 | 2437.023 | 2.7 |
| 8 | 4 | 4 | 9 | 3 | 6 | 2437.025 | 2437.044 | -18.2 |
| 8 | 4 | 5 | 9 | 3 | 7 | 2441.003 | 2440.997 | 6.0 |
| 8 | 4 | 4 | 9 | 3 | 7 | 2441.003 | 2441.018 | -14.9 |
| 9 | 0 | 9 | 8 | 1 | 8 | 2446.940 | 2446.932 | 8.0 |
| 5 | 2 | 3 | 5 | 1 | 5 | 2483.812 | 2483.804 | 8.2 |
| 6 | 2 | 5 | 6 | 1 | 6 | 2530.589 | 2530.588 | 1.3 |
| 6 | 2 | 4 | 6 | 1 | 6 | 2556.104 | 2556.098 | 5.9 |
| 8 | 1 | 8 | 7 | 1 | 7 | 2556.579 | 2556.577 | 1.6 |
| 6 | 1 | 6 | 5 | 0 | 5 | 2558.474 | 2558.479 | -5.0 |
| 5 | 1 | 4 | 4 | 0 | 4 | 2574.240 | 2574.236 | 4.8 |
| 7 | 2 | 6 | 7 | 1 | 7 | 2600.447 | 2600.443 | 3.3 |
| 8 | 0 | 8 | 7 | 0 | 7 | 2611.480 | 2611.481 | -1.9 |
| 8 | 2 | 7 | 7 | 2 | 6 | 2636.802 | 2636.802 | 0.4 |
| 8 | 5 | 4 | 7 | 5 | 3 | 2643.095 | 2643.080 | 15.5 |
| 8 | 5 | 3 | 7 | 5 | 2 | 2643.095 | 2643.080 | 15.4 |
| 8 | 3 | 6 | 7 | 3 | 5 | 2645.170 | 2645.159 | 10.7 |
| 7 | 2 | 5 | 7 | 1 | 7 | 2646.101 | 2646.095 | 6.6 |
| 8 | 3 | 5 | 7 | 3 | 4 | 2646.253 | 2646.244 | 9.2 |
| 8 | 2 | 6 | 7 | 2 | 5 | 2666.587 | 2666.591 | -3.2 |
| 8 | 2 | 7 | 8 | 1 | 8 | 2680.676 | 2680.668 | 7.6 |
| 8 | 1 | 7 | 7 | 1 | 6 | 2711.288 | 2711.281 | 7.4 |
| 8 | 2 | 6 | 8 | 1 | 8 | 2756.122 | 2756.108 | 13.7 |
| 14 | 1 | 13 | 13 | 2 | 11 | 2763.447 | 2763.444 | 3.0 |
| 13 | 1 | 12 | 12 | 2 | 11 | 2770.713 | 2770.715 | -1.9 |
| 9 | 2 | 8 | 9 | 1 | 9 | 2771.341 | 2771.341 | 0.3 |
| 10 | 0 | 10 | 9 | 1 | 9 | 2818.414 | 2818.409 | 4.4 |
| 7 | 1 | 7 | 6 | 0 | 6 | 2828.638 | 2828.639 | -1.1 |

Table S7: Observed transitions for the *trans-gauche(+)* conformer (Conf1)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 19 | 0 | 19 | 18 | 1 | 17 | 2837.259 | 2837.252 | 7.0 |
| 10 | 2 | 9 | 10 | 1 | 10 | 2872.514 | 2872.506 | 8.6 |
| 9 | 1 | 9 | 8 | 1 | 8 | 2874.183 | 2874.176 | 6.2 |
| 9 | 2 | 7 | 9 | 1 | 9 | 2888.510 | 2888.503 | 7.5 |
| 9 | 0 | 9 | 8 | 0 | 8 | 2929.686 | 2929.689 | -2.8 |
| 6 | 1 | 5 | 5 | 0 | 5 | 2967.062 | 2967.061 | 1.3 |
| 9 | 6 | 4 | 8 | 6 | 3 | 2973.275 | 2973.270 | 5.0 |
| 9 | 6 | 3 | 8 | 6 | 2 | 2973.275 | 2973.270 | 5.0 |
| 9 | 5 | 5 | 8 | 5 | 4 | 2973.860 | 2973.855 | 5.4 |
| 9 | 5 | 4 | 8 | 5 | 3 | 2973.860 | 2973.855 | 5.2 |
| 2 | 2 | 1 | 1 | 1 | 0 | 2974.120 | 2974.124 | -4.5 |
| 2 | 2 | 0 | 1 | 1 | 0 | 2974.494 | 2974.492 | 2.1 |
| 9 | 3 | 7 | 8 | 3 | 6 | 2976.612 | 2976.606 | 5.5 |
| 9 | 3 | 6 | 8 | 3 | 5 | 2978.593 | 2978.589 | 4.0 |
| 2 | 2 | 1 | 1 | 1 | 1 | 2993.594 | 2993.598 | -3.8 |
| 2 | 2 | 0 | 1 | 1 | 1 | 2993.952 | 2993.965 | -13.7 |
| 9 | 2 | 7 | 8 | 2 | 6 | 3006.576 | 3006.571 | 4.7 |
| 21 | 3 | 18 | 21 | 2 | 19 | 3009.694 | 3009.679 | 15.0 |
| 9 | 1 | 8 | 8 | 1 | 7 | 3047.459 | 3047.456 | 3.1 |
| 20 | 3 | 17 | 20 | 2 | 18 | 3061.927 | 3061.918 | 9.0 |
| 15 | 1 | 14 | 14 | 2 | 12 | 3072.907 | 3072.910 | -2.5 |
| 8 | 1 | 8 | 7 | 0 | 7 | 3094.238 | 3094.238 | -0.7 |
| 17 | 3 | 15 | 17 | 2 | 15 | 3123.668 | 3123.661 | 6.6 |
| 19 | 3 | 16 | 19 | 2 | 17 | 3126.351 | 3126.341 | 10.3 |
| 11 | 0 | 11 | 10 | 1 | 10 | 3186.786 | 3186.781 | 4.6 |
| 10 | 1 | 10 | 9 | 1 | 9 | 3191.193 | 3191.188 | 5.0 |
| 18 | 3 | 15 | 18 | 2 | 16 | 3199.760 | 3199.753 | 7.3 |
| 14 | 1 | 13 | 13 | 2 | 12 | 3207.648 | 3207.645 | 3.9 |
| 13 | 2 | 12 | 13 | 1 | 13 | 3238.676 | 3238.675 | 0.5 |
| 10 | 0 | 10 | 9 | 0 | 9 | 3245.654 | 3245.654 | 0.5 |
| 17 | 3 | 14 | 17 | 2 | 15 | 3278.868 | 3278.861 | 6.8 |
| 3 | 2 | 2 | 2 | 1 | 1 | 3284.808 | 3284.811 | -3.0 |
| 3 | 2 | 1 | 2 | 1 | 1 | 3286.645 | 3286.646 | -1.1 |
| 10 | 2 | 9 | 9 | 2 | 8 | 3292.349 | 3292.353 | -4.3 |
| 10 | 5 | 6 | 9 | 5 | 5 | 3304.768 | 3304.768 | -0.1 |
| 10 | 5 | 5 | 9 | 5 | 4 | 3304.768 | 3304.769 | -0.8 |
| 10 | 4 | 7 | 9 | 4 | 6 | 3306.268 | 3306.267 | 1.2 |
| 10 | 4 | 6 | 9 | 4 | 5 | 3306.340 | 3306.339 | 0.7 |
| 10 | 3 | 8 | 9 | 3 | 7 | 3308.230 | 3308.227 | 3.1 |
| 10 | 3 | 7 | 9 | 3 | 6 | 3311.608 | 3311.611 | -2.6 |
| 3 | 2 | 2 | 2 | 1 | 2 | 3343.237 | 3343.232 | 4.6 |
| 10 | 2 | 8 | 9 | 2 | 7 | 3348.251 | 3348.233 | 18.0 |
| 9 | 1 | 9 | 8 | 0 | 8 | 3356.935 | 3356.933 | 1.8 |
| 16 | 3 | 13 | 16 | 2 | 14 | 3360.403 | 3360.397 | 5.3 |
| 16 | 1 | 15 | 15 | 2 | 13 | 3362.063 | 3362.059 | 4.8 |
| 15 | 3 | 13 | 15 | 2 | 13 | 3364.593 | 3364.587 | 5.9 |
| 7 | 1 | 6 | 6 | 0 | 6 | 3372.995 | 3372.992 | 3.3 |
| 14 | 2 | 13 | 14 | 1 | 14 | 3381.233 | 3381.226 | 6.9 |
| 10 | 1 | 9 | 9 | 1 | 8 | 3382.537 | 3382.540 | -2.5 |
| 15 | 3 | 12 | 15 | 2 | 13 | 3441.266 | 3441.264 | 2.1 |
| 14 | 3 | 12 | 14 | 2 | 12 | 3466.976 | 3466.971 | 5.1 |

Table S7: Observed transitions for the *trans-gauche(+)* conformer (Conf1)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 11 | 1 | 11 | 10 | 1 | 10 | 3507.600 | 3507.602 | -1.3 |
| 14 | 3 | 11 | 14 | 2 | 12 | 3518.677 | 3518.672 | 5.7 |
| 15 | 2 | 14 | 15 | 1 | 15 | 3533.658 | 3533.653 | 4.5 |
| 12 | 0 | 12 | 11 | 1 | 11 | 3550.889 | 3550.886 | 3.3 |
| 13 | 3 | 11 | 13 | 2 | 11 | 3556.515 | 3556.513 | 1.9 |
| 11 | 0 | 11 | 10 | 0 | 10 | 3559.575 | 3559.560 | 14.5 |
| 14 | 2 | 13 | 14 | 0 | 14 | 3571.061 | 3571.074 | -12.5 |
| 4 | 2 | 3 | 3 | 1 | 2 | 3585.705 | 3585.708 | -2.6 |
| 13 | 3 | 10 | 13 | 2 | 11 | 3590.269 | 3590.271 | -2.1 |
| 4 | 2 | 2 | 3 | 1 | 2 | 3591.203 | 3591.207 | -3.2 |
| 10 | 1 | 10 | 9 | 0 | 9 | 3618.431 | 3618.433 | -1.5 |
| 11 | 2 | 10 | 10 | 2 | 9 | 3619.266 | 3619.259 | 6.2 |
| 12 | 3 | 10 | 12 | 2 | 10 | 3633.007 | 3633.010 | -2.2 |
| 11 | 6 | 6 | 10 | 6 | 5 | 3634.775 | 3634.767 | 7.7 |
| 11 | 6 | 5 | 10 | 6 | 4 | 3634.775 | 3634.767 | 7.7 |
| 11 | 5 | 7 | 10 | 5 | 6 | 3635.843 | 3635.834 | 8.3 |
| 11 | 5 | 6 | 10 | 5 | 5 | 3635.843 | 3635.836 | 6.5 |
| 11 | 4 | 8 | 10 | 4 | 7 | 3637.817 | 3637.808 | 8.4 |
| 11 | 4 | 7 | 10 | 4 | 6 | 3637.956 | 3637.953 | 2.9 |
| 11 | 3 | 8 | 10 | 3 | 7 | 3645.452 | 3645.451 | 0.7 |
| 15 | 1 | 14 | 14 | 2 | 13 | 3646.333 | 3646.337 | -4.4 |
| 12 | 3 | 9 | 12 | 2 | 10 | 3654.255 | 3654.260 | -4.8 |
| 11 | 2 | 9 | 10 | 2 | 8 | 3691.325 | 3691.321 | 4.9 |
| 16 | 2 | 15 | 16 | 1 | 16 | 3695.626 | 3695.628 | -2.3 |
| 11 | 3 | 9 | 11 | 2 | 9 | 3696.630 | 3696.635 | -5.2 |
| 4 | 2 | 3 | 3 | 1 | 3 | 3702.554 | 3702.545 | 9.7 |
| 11 | 3 | 8 | 11 | 2 | 9 | 3709.461 | 3709.457 | 4.5 |
| 11 | 1 | 10 | 10 | 1 | 9 | 3716.352 | 3716.345 | 7.0 |
| 10 | 3 | 8 | 10 | 2 | 8 | 3747.966 | 3747.969 | -2.1 |
| 10 | 3 | 7 | 10 | 2 | 8 | 3755.326 | 3755.326 | 0.1 |
| 9 | 3 | 7 | 9 | 2 | 7 | 3787.967 | 3787.974 | -7.1 |
| 9 | 3 | 6 | 9 | 2 | 7 | 3791.948 | 3791.948 | -0.5 |
| 8 | 1 | 7 | 7 | 0 | 7 | 3793.302 | 3793.295 | 6.9 |
| 8 | 3 | 6 | 8 | 2 | 6 | 3817.936 | 3817.939 | -3.1 |
| 12 | 1 | 12 | 11 | 1 | 11 | 3823.416 | 3823.419 | -3.0 |
| 7 | 3 | 5 | 7 | 2 | 5 | 3839.366 | 3839.370 | -4.6 |
| 7 | 3 | 4 | 7 | 2 | 5 | 3840.278 | 3840.277 | 0.4 |
| 6 | 3 | 4 | 6 | 2 | 4 | 3853.868 | 3853.873 | -4.9 |
| 6 | 3 | 3 | 6 | 2 | 4 | 3854.234 | 3854.236 | -1.6 |
| 5 | 3 | 3 | 5 | 2 | 3 | 3863.026 | 3863.028 | -2.2 |
| 5 | 3 | 2 | 5 | 2 | 3 | 3863.143 | 3863.149 | -6.2 |
| 4 | 3 | 1 | 4 | 2 | 2 | 3868.315 | 3868.329 | -14.2 |
| 12 | 0 | 12 | 11 | 0 | 11 | 3871.708 | 3871.706 | 1.6 |
| 4 | 3 | 2 | 4 | 2 | 3 | 3873.806 | 3873.798 | 8.6 |
| 5 | 3 | 3 | 5 | 2 | 4 | 3875.825 | 3875.831 | -5.9 |
| 5 | 3 | 2 | 5 | 2 | 4 | 3875.951 | 3875.952 | -1.4 |
| 5 | 2 | 4 | 4 | 1 | 3 | 3876.852 | 3876.853 | -0.5 |
| 6 | 3 | 4 | 6 | 2 | 5 | 3879.373 | 3879.383 | -9.4 |
| 11 | 1 | 11 | 10 | 0 | 10 | 3880.382 | 3880.381 | 1.5 |
| 7 | 3 | 4 | 7 | 2 | 6 | 3885.923 | 3885.928 | -5.9 |
| 5 | 2 | 3 | 4 | 1 | 3 | 3889.648 | 3889.655 | -6.9 |

Table S7: Observed transitions for the *trans-gauche(+)* conformer (Conf1)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 8 | 3 | 6 | 8 | 2 | 7 | 3893.375 | 3893.379 | -3.5 |
| 8 | 3 | 5 | 8 | 2 | 7 | 3895.367 | 3895.371 | -3.7 |
| 9 | 3 | 7 | 9 | 2 | 8 | 3905.139 | 3905.136 | 3.1 |
| 9 | 3 | 6 | 9 | 2 | 8 | 3909.105 | 3909.110 | -5.9 |
| 10 | 3 | 8 | 10 | 2 | 9 | 3921.013 | 3921.010 | 3.0 |
| 10 | 3 | 7 | 10 | 2 | 9 | 3928.366 | 3928.368 | -1.5 |
| 11 | 3 | 9 | 11 | 2 | 10 | 3941.742 | 3941.738 | 3.7 |
| 12 | 2 | 11 | 11 | 2 | 10 | 3945.518 | 3945.515 | 2.8 |
| 11 | 3 | 8 | 11 | 2 | 10 | 3954.559 | 3954.560 | -0.6 |
| 12 | 5 | 8 | 11 | 5 | 7 | 3967.069 | 3967.069 | -0.2 |
| 12 | 5 | 7 | 11 | 5 | 6 | 3967.069 | 3967.073 | -4.5 |
| 12 | 3 | 10 | 12 | 2 | 11 | 3968.055 | 3968.062 | -7.3 |
| 12 | 4 | 9 | 11 | 4 | 8 | 3969.596 | 3969.597 | -0.3 |
| 12 | 3 | 10 | 11 | 3 | 9 | 3971.838 | 3971.839 | -0.8 |
| 12 | 3 | 9 | 11 | 3 | 8 | 3980.266 | 3980.268 | -1.6 |
| 12 | 3 | 9 | 12 | 2 | 11 | 3989.312 | 3989.313 | -0.5 |
| 13 | 3 | 11 | 13 | 2 | 12 | 4000.714 | 4000.713 | 0.7 |
| 13 | 3 | 10 | 13 | 2 | 12 | 4034.474 | 4034.472 | 1.8 |
| 12 | 2 | 10 | 11 | 2 | 9 | 4035.465 | 4035.465 | 0.6 |
| 14 | 3 | 12 | 14 | 2 | 13 | 4040.400 | 4040.398 | 1.9 |
| 12 | 1 | 11 | 11 | 1 | 10 | 4048.669 | 4048.668 | 0.9 |
| 5 | 2 | 4 | 4 | 1 | 4 | 4071.548 | 4071.558 | -10.5 |
| 15 | 3 | 13 | 15 | 2 | 14 | 4087.779 | 4087.784 | -5.0 |
| 14 | 3 | 11 | 14 | 2 | 13 | 4092.111 | 4092.099 | 11.5 |
| 13 | 1 | 13 | 12 | 1 | 12 | 4138.653 | 4138.654 | -1.3 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4144.241 | 4144.240 | 0.9 |
| 6 | 2 | 5 | 5 | 1 | 4 | 4158.330 | 4158.330 | -0.1 |
| 6 | 2 | 4 | 5 | 1 | 4 | 4183.838 | 4183.840 | -1.6 |
| 17 | 3 | 15 | 17 | 2 | 16 | 4208.075 | 4208.063 | 11.8 |
| 9 | 1 | 8 | 8 | 0 | 8 | 4229.271 | 4229.269 | 1.1 |
| 14 | 0 | 14 | 13 | 1 | 13 | 4263.479 | 4263.482 | -3.7 |
| 13 | 2 | 12 | 12 | 2 | 11 | 4271.063 | 4271.070 | -7.2 |
| 18 | 3 | 16 | 18 | 2 | 17 | 4281.995 | 4281.992 | 2.5 |
| 13 | 6 | 8 | 12 | 6 | 7 | 4296.719 | 4296.726 | -6.9 |
| 13 | 6 | 7 | 12 | 6 | 6 | 4296.719 | 4296.726 | -7.0 |
| 13 | 5 | 9 | 12 | 5 | 8 | 4298.491 | 4298.488 | 3.3 |
| 13 | 5 | 8 | 12 | 5 | 7 | 4298.491 | 4298.497 | -5.8 |
| 13 | 4 | 10 | 12 | 4 | 9 | 4301.643 | 4301.644 | -1.0 |
| 13 | 4 | 9 | 12 | 4 | 8 | 4302.121 | 4302.122 | -1.8 |
| 13 | 3 | 11 | 12 | 3 | 10 | 4303.725 | 4303.721 | 3.6 |
| 13 | 3 | 10 | 12 | 3 | 9 | 4316.235 | 4316.229 | 5.7 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4411.184 | 4411.187 | -3.0 |
| 7 | 2 | 6 | 6 | 1 | 5 | 4430.272 | 4430.276 | -3.2 |
| 6 | 2 | 5 | 5 | 1 | 5 | 4450.324 | 4450.312 | 11.7 |
| 14 | 1 | 14 | 13 | 1 | 13 | 4453.330 | 4453.330 | -0.7 |
| 6 | 2 | 4 | 5 | 1 | 5 | 4475.835 | 4475.822 | 12.8 |
| 7 | 2 | 5 | 6 | 1 | 5 | 4475.928 | 4475.927 | 0.8 |
| 14 | 0 | 14 | 13 | 0 | 13 | 4492.208 | 4492.210 | -1.8 |
| 14 | 2 | 13 | 13 | 2 | 12 | 4595.885 | 4595.881 | 4.6 |
| 15 | 0 | 15 | 14 | 1 | 14 | 4611.477 | 4611.470 | 7.1 |
| 14 | 1 | 14 | 13 | 0 | 13 | 4682.046 | 4682.058 | -11.5 |

Table S7: Observed transitions for the *trans-gauche(+)* conformer (Conf1)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 8 | 2 | 7 | 7 | 1 | 6 | 4692.895 | 4692.892 | 3.3 |
| 14 | 1 | 13 | 13 | 1 | 12 | 4707.995 | 4708.000 | -4.6 |
| 15 | 1 | 15 | 14 | 1 | 14 | 4767.485 | 4767.480 | 4.9 |
| 8 | 2 | 6 | 7 | 1 | 6 | 4768.335 | 4768.332 | 2.5 |
| 7 | 2 | 6 | 6 | 1 | 6 | 4838.856 | 4838.857 | -1.3 |
| 3 | 3 | 1 | 2 | 2 | 0 | 4862.904 | 4862.905 | -1.4 |
| 3 | 3 | 0 | 2 | 2 | 0 | 4862.904 | 4862.909 | -5.7 |
| 3 | 3 | 1 | 2 | 2 | 1 | 4863.269 | 4863.272 | -3.2 |
| 3 | 3 | 0 | 2 | 2 | 1 | 4863.269 | 4863.277 | -7.5 |
| 7 | 2 | 5 | 6 | 1 | 6 | 4884.518 | 4884.509 | 9.6 |
| 9 | 2 | 8 | 8 | 1 | 7 | 4946.448 | 4946.460 | -12.5 |
| 16 | 0 | 16 | 15 | 1 | 15 | 4954.070 | 4954.078 | -8.0 |
| 15 | 1 | 15 | 14 | 0 | 14 | 4957.326 | 4957.328 | -2.6 |
| 9 | 2 | 7 | 8 | 1 | 7 | 5063.624 | 5063.623 | 1.3 |
| 16 | 1 | 16 | 15 | 1 | 15 | 5081.137 | 5081.143 | -6.4 |
| 16 | 0 | 16 | 15 | 0 | 15 | 5110.084 | 5110.088 | -4.6 |
| 10 | 2 | 9 | 9 | 1 | 8 | 5191.353 | 5191.358 | -4.6 |
| 4 | 3 | 2 | 3 | 2 | 1 | 5192.325 | 5192.319 | 5.7 |
| 4 | 3 | 2 | 3 | 2 | 2 | 5194.167 | 5194.154 | 12.8 |
| 16 | 1 | 16 | 15 | 0 | 15 | 5237.147 | 5237.154 | -6.7 |
| 8 | 2 | 7 | 7 | 1 | 7 | 5237.235 | 5237.245 | -9.9 |
| 16 | 2 | 15 | 15 | 2 | 14 | 5243.112 | 5243.118 | -6.0 |
| 17 | 4 | 14 | 17 | 3 | 14 | 5252.940 | 5252.922 | 18.7 |
| 17 | 4 | 13 | 17 | 3 | 14 | 5261.316 | 5261.321 | -4.5 |
| 17 | 0 | 17 | 16 | 1 | 16 | 5291.676 | 5291.687 | -10.8 |
| 16 | 4 | 12 | 16 | 3 | 13 | 5300.430 | 5300.415 | 15.1 |
| 8 | 2 | 6 | 7 | 1 | 7 | 5312.685 | 5312.685 | -0.1 |
| 15 | 4 | 12 | 15 | 3 | 12 | 5328.472 | 5328.455 | 17.5 |
| 16 | 3 | 13 | 15 | 3 | 12 | 5332.661 | 5332.654 | 7.4 |
| 14 | 4 | 11 | 14 | 3 | 11 | 5354.182 | 5354.184 | -2.5 |
| 14 | 4 | 10 | 14 | 3 | 11 | 5356.013 | 5356.015 | -1.9 |
| 10 | 2 | 8 | 9 | 1 | 8 | 5364.402 | 5364.399 | 2.4 |
| 13 | 4 | 10 | 13 | 3 | 10 | 5373.742 | 5373.735 | 7.7 |
| 13 | 4 | 9 | 13 | 3 | 10 | 5374.747 | 5374.755 | -7.9 |
| 19 | 1 | 18 | 18 | 2 | 17 | 5386.689 | 5386.706 | -17.0 |
| 12 | 4 | 9 | 12 | 3 | 9 | 5388.327 | 5388.320 | 7.3 |
| 12 | 4 | 8 | 12 | 3 | 9 | 5388.861 | 5388.861 | -0.2 |
| 17 | 1 | 17 | 16 | 1 | 16 | 5394.346 | 5394.362 | -15.7 |
| 11 | 4 | 8 | 11 | 3 | 8 | 5398.989 | 5398.991 | -2.1 |
| 11 | 4 | 7 | 11 | 3 | 8 | 5399.266 | 5399.263 | 3.1 |
| 15 | 4 | 12 | 15 | 3 | 13 | 5405.134 | 5405.132 | 2.6 |
| 14 | 4 | 11 | 14 | 3 | 12 | 5405.885 | 5405.885 | 0.2 |
| 10 | 4 | 7 | 10 | 3 | 7 | 5406.626 | 5406.634 | -8.5 |
| 10 | 4 | 6 | 10 | 3 | 7 | 5406.762 | 5406.761 | 0.7 |
| 13 | 4 | 10 | 13 | 3 | 11 | 5407.490 | 5407.493 | -2.7 |
| 14 | 4 | 10 | 14 | 3 | 12 | 5407.709 | 5407.716 | -6.3 |
| 15 | 4 | 11 | 15 | 3 | 13 | 5408.282 | 5408.282 | 0.4 |
| 13 | 4 | 9 | 13 | 3 | 11 | 5408.499 | 5408.513 | -14.4 |
| 12 | 4 | 9 | 12 | 3 | 10 | 5409.568 | 5409.571 | -2.7 |
| 11 | 4 | 8 | 11 | 3 | 9 | 5411.807 | 5411.813 | -5.5 |
| 10 | 4 | 6 | 10 | 3 | 8 | 5414.133 | 5414.119 | 13.9 |

Table S7: Observed transitions for the *trans-gauche(+)* conformer (Conf1)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 8 | 4 | 5 | 8 | 3 | 6 | 5417.597 | 5417.603 | -6.0 |
| 6 | 4 | 3 | 6 | 3 | 3 | 5419.496 | 5419.501 | -5.2 |
| 6 | 4 | 2 | 6 | 3 | 3 | 5419.496 | 5419.503 | -7.1 |
| 11 | 2 | 10 | 10 | 1 | 9 | 5428.078 | 5428.077 | 0.8 |
| 21 | 4 | 18 | 21 | 3 | 19 | 5449.390 | 5449.394 | -3.9 |
| 7 | 2 | 5 | 6 | 0 | 6 | 5474.744 | 5474.734 | 9.9 |
| 5 | 3 | 3 | 4 | 2 | 2 | 5520.317 | 5520.319 | -2.3 |
| 5 | 3 | 2 | 4 | 2 | 2 | 5520.439 | 5520.440 | -1.3 |
| 17 | 1 | 17 | 16 | 0 | 16 | 5521.426 | 5521.428 | -2.0 |
| 5 | 3 | 3 | 4 | 2 | 3 | 5525.814 | 5525.818 | -3.8 |
| 5 | 3 | 2 | 4 | 2 | 3 | 5525.940 | 5525.939 | 1.1 |
| 18 | 0 | 18 | 17 | 1 | 17 | 5624.782 | 5624.793 | -10.8 |
| 12 | 1 | 11 | 11 | 0 | 11 | 5641.912 | 5641.920 | -8.6 |
| 9 | 2 | 8 | 8 | 1 | 8 | 5645.526 | 5645.517 | 9.1 |
| 12 | 2 | 11 | 11 | 1 | 10 | 5657.242 | 5657.247 | -4.8 |
| 11 | 2 | 9 | 10 | 1 | 9 | 5673.183 | 5673.180 | 3.2 |
| 18 | 1 | 18 | 17 | 0 | 17 | 5809.851 | 5809.858 | -6.8 |
| 6 | 3 | 4 | 5 | 2 | 3 | 5845.885 | 5845.891 | -5.9 |
| 6 | 3 | 3 | 5 | 2 | 3 | 5846.255 | 5846.254 | 0.4 |
| 6 | 3 | 4 | 5 | 2 | 4 | 5858.687 | 5858.694 | -7.5 |
| 6 | 3 | 3 | 5 | 2 | 4 | 5859.052 | 5859.057 | -5.2 |
| 13 | 2 | 12 | 12 | 1 | 11 | 5879.649 | 5879.648 | 0.7 |
| 18 | 4 | 15 | 17 | 4 | 14 | 5965.816 | 5965.819 | -2.7 |
| 12 | 2 | 10 | 11 | 1 | 10 | 5992.302 | 5992.299 | 2.5 |
| 10 | 2 | 9 | 9 | 1 | 9 | 6063.691 | 6063.694 | -3.0 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6167.778 | 6167.781 | -2.7 |
| 7 | 3 | 4 | 6 | 2 | 4 | 6168.688 | 6168.688 | -0.3 |
| 7 | 3 | 5 | 6 | 2 | 5 | 6193.287 | 6193.291 | -4.2 |
| 7 | 3 | 4 | 6 | 2 | 5 | 6194.196 | 6194.198 | -2.5 |
| 15 | 2 | 14 | 14 | 1 | 13 | 6308.133 | 6308.144 | -11.0 |
| 13 | 2 | 11 | 12 | 1 | 11 | 6323.847 | 6323.849 | -2.1 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6484.527 | 6484.529 | -2.8 |
| 8 | 3 | 5 | 7 | 2 | 5 | 6486.520 | 6486.521 | -0.9 |
| 16 | 2 | 15 | 15 | 1 | 14 | 6516.680 | 6516.689 | -8.8 |
| 8 | 3 | 6 | 7 | 2 | 6 | 6530.184 | 6530.181 | 3.3 |
| 8 | 3 | 5 | 7 | 2 | 6 | 6532.174 | 6532.172 | 1.8 |
| 14 | 2 | 12 | 13 | 1 | 12 | 6669.666 | 6669.664 | 2.4 |
| 21 | 1 | 21 | 20 | 0 | 20 | 6695.814 | 6695.814 | -0.4 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6742.276 | 6742.277 | -1.1 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6742.276 | 6742.281 | -5.5 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6794.545 | 6794.545 | 0.6 |
| 9 | 3 | 6 | 8 | 2 | 6 | 6798.517 | 6798.519 | -2.0 |
| 9 | 3 | 7 | 8 | 2 | 7 | 6869.999 | 6869.985 | 13.8 |
| 9 | 3 | 6 | 8 | 2 | 7 | 6873.963 | 6873.959 | 3.3 |
| 7 | 5 | 3 | 7 | 4 | 3 | 6968.979 | 6968.974 | 4.5 |
| 7 | 5 | 3 | 7 | 4 | 4 | 6968.979 | 6968.981 | -2.4 |
| 7 | 5 | 2 | 7 | 4 | 4 | 6968.979 | 6968.981 | -2.5 |
| 7 | 5 | 2 | 7 | 4 | 3 | 6968.979 | 6968.974 | 4.5 |
| 15 | 2 | 13 | 14 | 1 | 13 | 7031.339 | 7031.342 | -2.3 |
| 5 | 4 | 1 | 4 | 3 | 1 | 7072.519 | 7072.506 | 13.0 |
| 10 | 3 | 8 | 9 | 2 | 7 | 7096.199 | 7096.201 | -2.0 |

Table S7: Observed transitions for the *trans-gauche(+)* conformer (Conf1)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 3 | 7 | 9 | 2 | 7 | 7103.561 | 7103.559 | 2.8 |
| 10 | 3 | 8 | 9 | 2 | 8 | 7213.361 | 7213.363 | -2.3 |
| 10 | 3 | 7 | 9 | 2 | 8 | 7220.716 | 7220.721 | -4.8 |
| 13 | 2 | 12 | 12 | 1 | 12 | 7377.325 | 7377.329 | -3.8 |
| 11 | 3 | 9 | 10 | 2 | 8 | 7387.949 | 7387.956 | -6.7 |
| 11 | 3 | 8 | 10 | 2 | 8 | 7400.777 | 7400.777 | -0.8 |
| 6 | 4 | 3 | 5 | 3 | 2 | 7402.622 | 7402.606 | 15.8 |
| 6 | 4 | 2 | 5 | 3 | 2 | 7402.622 | 7402.608 | 13.9 |
| 6 | 4 | 3 | 5 | 3 | 3 | 7402.716 | 7402.727 | -11.2 |
| 6 | 4 | 2 | 5 | 3 | 3 | 7402.716 | 7402.729 | -13.1 |
| 16 | 2 | 14 | 15 | 1 | 14 | 7410.271 | 7410.288 | -17.1 |
| 24 | 1 | 23 | 23 | 2 | 22 | 7418.363 | 7418.373 | -9.4 |
| 11 | 3 | 9 | 10 | 2 | 9 | 7561.000 | 7560.998 | 2.1 |
| 11 | 3 | 8 | 10 | 2 | 9 | 7573.824 | 7573.819 | 4.6 |
| 12 | 3 | 10 | 11 | 2 | 9 | 7668.472 | 7668.474 | -2.5 |
| 12 | 3 | 9 | 11 | 2 | 9 | 7689.717 | 7689.725 | -7.7 |
| 12 | 3 | 10 | 11 | 2 | 10 | 7913.574 | 7913.577 | -3.1 |
| 12 | 3 | 9 | 11 | 2 | 10 | 7934.832 | 7934.827 | 4.2 |
| 13 | 3 | 11 | 12 | 2 | 10 | 7936.737 | 7936.731 | 6.3 |

Table S8: Observed transitions for the *cis-gauche(+)* conformer (Conf2)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 9 | 2 | 7 | 9 | 1 | 8 | 2015.424 | 2015.428 | -3.5 |
| 6 | 1 | 5 | 5 | 1 | 4 | 2035.965 | 2035.965 | 0.6 |
| 7 | 2 | 6 | 7 | 1 | 6 | 2055.348 | 2055.342 | 6.4 |
| 8 | 2 | 6 | 8 | 1 | 7 | 2056.298 | 2056.297 | 0.1 |
| 8 | 0 | 8 | 7 | 1 | 7 | 2073.582 | 2073.575 | 6.3 |
| 9 | 4 | 6 | 10 | 3 | 7 | 2098.908 | 2098.920 | -12.5 |
| 9 | 4 | 5 | 10 | 3 | 7 | 2098.984 | 2098.975 | 9.4 |
| 7 | 2 | 5 | 7 | 1 | 6 | 2100.970 | 2100.970 | -0.1 |
| 6 | 2 | 4 | 6 | 1 | 5 | 2146.728 | 2146.726 | 2.0 |
| 5 | 2 | 4 | 5 | 1 | 4 | 2178.212 | 2178.216 | -3.7 |
| 5 | 2 | 3 | 5 | 1 | 4 | 2191.010 | 2191.012 | -2.7 |
| 4 | 1 | 3 | 3 | 0 | 3 | 2192.831 | 2192.824 | 6.5 |
| 4 | 2 | 3 | 4 | 1 | 3 | 2226.046 | 2226.042 | 3.4 |
| 3 | 2 | 2 | 3 | 1 | 2 | 2264.508 | 2264.511 | -3.2 |
| 3 | 2 | 1 | 3 | 1 | 2 | 2266.346 | 2266.345 | 0.8 |
| 5 | 1 | 5 | 4 | 0 | 4 | 2281.741 | 2281.748 | -7.7 |
| 7 | 0 | 7 | 6 | 0 | 6 | 2290.605 | 2290.597 | 8.1 |
| 7 | 2 | 6 | 6 | 2 | 5 | 2307.902 | 2307.880 | 21.5 |
| 7 | 5 | 3 | 6 | 5 | 2 | 2312.050 | 2312.036 | 14.5 |
| 7 | 5 | 2 | 6 | 5 | 1 | 2312.050 | 2312.036 | 14.4 |
| 7 | 4 | 4 | 6 | 4 | 3 | 2312.568 | 2312.558 | 10.2 |
| 7 | 4 | 3 | 6 | 4 | 2 | 2312.568 | 2312.563 | 5.2 |
| 7 | 3 | 5 | 6 | 3 | 4 | 2313.518 | 2313.516 | 1.3 |
| 7 | 3 | 4 | 6 | 3 | 3 | 2314.066 | 2314.060 | 6.3 |
| 7 | 2 | 5 | 6 | 2 | 4 | 2328.007 | 2328.011 | -4.2 |
| 12 | 1 | 11 | 11 | 2 | 10 | 2336.831 | 2336.829 | 1.4 |
| 7 | 1 | 6 | 6 | 1 | 5 | 2373.776 | 2373.767 | 8.9 |

Table S8: Observed transitions for the *cis-gauche(+)* conformer (Conf2)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 4 | 2 | 3 | 4 | 1 | 4 | 2420.650 | 2420.662 | -11.7 |
| 9 | 0 | 9 | 8 | 1 | 8 | 2446.617 | 2446.615 | 2.1 |
| 5 | 2 | 3 | 5 | 1 | 5 | 2482.873 | 2482.866 | 7.7 |
| 6 | 2 | 5 | 6 | 1 | 6 | 2529.635 | 2529.630 | 5.1 |
| 6 | 1 | 6 | 5 | 0 | 5 | 2557.940 | 2557.942 | -1.5 |
| 5 | 1 | 4 | 4 | 0 | 4 | 2573.609 | 2573.602 | 7.4 |
| 7 | 2 | 6 | 7 | 1 | 7 | 2599.454 | 2599.455 | -0.9 |
| 8 | 0 | 8 | 7 | 0 | 7 | 2611.054 | 2611.050 | 3.7 |
| 8 | 2 | 7 | 7 | 2 | 6 | 2636.355 | 2636.358 | -2.7 |
| 8 | 3 | 5 | 7 | 3 | 4 | 2645.797 | 2645.795 | 2.2 |
| 8 | 2 | 7 | 8 | 1 | 8 | 2679.651 | 2679.644 | 6.7 |
| 8 | 1 | 7 | 7 | 1 | 6 | 2710.807 | 2710.804 | 3.1 |
| 9 | 2 | 8 | 9 | 1 | 9 | 2770.278 | 2770.276 | 1.8 |
| 13 | 1 | 12 | 12 | 2 | 11 | 2770.501 | 2770.508 | -7.1 |
| 10 | 0 | 10 | 9 | 1 | 9 | 2818.023 | 2818.020 | 2.1 |
| 7 | 1 | 7 | 6 | 0 | 6 | 2828.074 | 2828.072 | 1.8 |
| 10 | 2 | 9 | 10 | 1 | 10 | 2871.400 | 2871.396 | 3.8 |
| 9 | 1 | 9 | 8 | 1 | 8 | 2873.724 | 2873.718 | 5.8 |
| 9 | 2 | 8 | 8 | 2 | 7 | 2964.355 | 2964.350 | 5.3 |
| 6 | 1 | 5 | 5 | 0 | 5 | 2966.343 | 2966.343 | 0.2 |
| 2 | 2 | 1 | 1 | 1 | 0 | 2973.144 | 2973.151 | -6.9 |
| 2 | 2 | 0 | 1 | 1 | 0 | 2973.522 | 2973.518 | 4.1 |
| 9 | 3 | 7 | 8 | 3 | 6 | 2976.105 | 2976.101 | 4.1 |
| 9 | 3 | 6 | 8 | 3 | 5 | 2978.087 | 2978.083 | 4.1 |
| 2 | 2 | 1 | 1 | 1 | 1 | 2992.608 | 2992.616 | -7.5 |
| 2 | 2 | 0 | 1 | 1 | 1 | 2992.979 | 2992.983 | -4.0 |
| 9 | 2 | 7 | 8 | 2 | 6 | 3006.053 | 3006.051 | 1.6 |
| 9 | 1 | 8 | 8 | 1 | 7 | 3046.923 | 3046.921 | 2.4 |
| 15 | 1 | 14 | 14 | 2 | 12 | 3072.783 | 3072.786 | -2.8 |
| 8 | 1 | 8 | 7 | 0 | 7 | 3093.640 | 3093.643 | -3.3 |
| 17 | 3 | 15 | 17 | 2 | 15 | 3122.568 | 3122.577 | -9.3 |
| 19 | 3 | 16 | 19 | 2 | 17 | 3125.234 | 3125.223 | 10.2 |
| 11 | 0 | 11 | 10 | 1 | 10 | 3186.324 | 3186.323 | 0.7 |
| 10 | 1 | 10 | 9 | 1 | 9 | 3190.682 | 3190.680 | 2.5 |
| 18 | 3 | 15 | 18 | 2 | 16 | 3198.621 | 3198.611 | 10.1 |
| 14 | 1 | 13 | 13 | 2 | 12 | 3207.342 | 3207.337 | 4.8 |
| 13 | 2 | 12 | 13 | 1 | 13 | 3237.410 | 3237.404 | 6.1 |
| 17 | 3 | 14 | 17 | 2 | 15 | 3277.699 | 3277.689 | 9.9 |
| 3 | 2 | 2 | 2 | 1 | 1 | 3283.791 | 3283.791 | 0.4 |
| 3 | 2 | 1 | 2 | 1 | 1 | 3285.628 | 3285.625 | 3.5 |
| 10 | 2 | 9 | 9 | 2 | 8 | 3291.808 | 3291.800 | 7.9 |
| 10 | 3 | 7 | 9 | 3 | 6 | 3311.041 | 3311.047 | -6.2 |
| 3 | 2 | 1 | 2 | 1 | 2 | 3344.025 | 3344.020 | 5.1 |
| 10 | 2 | 8 | 9 | 2 | 7 | 3347.656 | 3347.651 | 4.8 |
| 9 | 1 | 9 | 8 | 0 | 8 | 3356.312 | 3356.311 | 1.5 |
| 16 | 3 | 13 | 16 | 2 | 14 | 3359.201 | 3359.193 | 8.7 |
| 16 | 1 | 15 | 15 | 2 | 13 | 3361.906 | 3361.906 | -0.2 |
| 7 | 1 | 6 | 6 | 0 | 6 | 3372.183 | 3372.185 | -1.5 |
| 10 | 1 | 9 | 9 | 1 | 8 | 3381.949 | 3381.947 | 1.9 |
| 14 | 3 | 12 | 14 | 2 | 12 | 3465.731 | 3465.727 | 3.1 |
| 11 | 1 | 11 | 10 | 1 | 10 | 3507.040 | 3507.044 | -4.0 |

Table S8: Observed transitions for the *cis-gauche(+)* conformer (Conf2)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 14 | 3 | 11 | 14 | 2 | 12 | 3517.375 | 3517.399 | -23.7 |
| 12 | 0 | 12 | 11 | 1 | 11 | 3550.362 | 3550.360 | 1.9 |
| 13 | 3 | 11 | 13 | 2 | 11 | 3555.224 | 3555.227 | -2.7 |
| 11 | 0 | 11 | 10 | 0 | 10 | 3558.981 | 3558.982 | -1.7 |
| 4 | 2 | 3 | 3 | 1 | 2 | 3584.639 | 3584.644 | -4.7 |
| 13 | 3 | 10 | 13 | 2 | 11 | 3588.961 | 3588.966 | -4.4 |
| 4 | 2 | 2 | 3 | 1 | 2 | 3590.141 | 3590.140 | 0.9 |
| 10 | 1 | 10 | 9 | 0 | 9 | 3617.784 | 3617.783 | 0.9 |
| 11 | 2 | 10 | 10 | 2 | 9 | 3618.655 | 3618.652 | 2.7 |
| 12 | 3 | 10 | 12 | 2 | 10 | 3631.687 | 3631.687 | 0.2 |
| 11 | 5 | 7 | 10 | 5 | 6 | 3635.227 | 3635.218 | 8.8 |
| 11 | 5 | 6 | 10 | 5 | 5 | 3635.227 | 3635.220 | 6.9 |
| 11 | 4 | 8 | 10 | 4 | 7 | 3637.194 | 3637.191 | 2.3 |
| 11 | 3 | 9 | 10 | 3 | 8 | 3639.360 | 3639.370 | -9.6 |
| 11 | 3 | 8 | 10 | 3 | 7 | 3644.828 | 3644.830 | -2.3 |
| 15 | 1 | 14 | 14 | 2 | 13 | 3645.920 | 3645.930 | -9.6 |
| 12 | 3 | 9 | 12 | 2 | 10 | 3652.927 | 3652.925 | 1.6 |
| 11 | 2 | 9 | 10 | 2 | 8 | 3690.680 | 3690.677 | 2.7 |
| 11 | 3 | 9 | 11 | 2 | 9 | 3695.281 | 3695.282 | -0.7 |
| 4 | 2 | 3 | 3 | 1 | 3 | 3701.442 | 3701.430 | 12.4 |
| 4 | 2 | 2 | 3 | 1 | 3 | 3706.936 | 3706.926 | 10.2 |
| 11 | 1 | 10 | 10 | 1 | 9 | 3715.695 | 3715.696 | -0.5 |
| 10 | 3 | 8 | 10 | 2 | 8 | 3746.580 | 3746.589 | -9.6 |
| 10 | 3 | 7 | 10 | 2 | 8 | 3753.939 | 3753.943 | -3.8 |
| 9 | 3 | 7 | 9 | 2 | 7 | 3786.571 | 3786.575 | -3.9 |
| 9 | 3 | 6 | 9 | 2 | 7 | 3790.544 | 3790.547 | -2.8 |
| 8 | 1 | 7 | 7 | 0 | 7 | 3792.395 | 3792.391 | 3.7 |
| 8 | 3 | 6 | 8 | 2 | 6 | 3816.521 | 3816.524 | -3.9 |
| 8 | 3 | 5 | 8 | 2 | 6 | 3818.518 | 3818.515 | 3.3 |
| 12 | 1 | 12 | 11 | 1 | 11 | 3822.805 | 3822.812 | -6.8 |
| 7 | 3 | 5 | 7 | 2 | 5 | 3837.940 | 3837.945 | -5.6 |
| 7 | 3 | 4 | 7 | 2 | 5 | 3838.850 | 3838.851 | -1.1 |
| 6 | 3 | 4 | 6 | 2 | 4 | 3852.438 | 3852.440 | -2.5 |
| 6 | 3 | 3 | 6 | 2 | 4 | 3852.804 | 3852.803 | 1.1 |
| 5 | 3 | 3 | 5 | 2 | 3 | 3861.590 | 3861.591 | -1.4 |
| 5 | 3 | 2 | 5 | 2 | 3 | 3861.712 | 3861.712 | -0.4 |
| 4 | 3 | 1 | 4 | 2 | 2 | 3866.880 | 3866.889 | -9.2 |
| 12 | 0 | 12 | 11 | 0 | 11 | 3871.083 | 3871.081 | 2.1 |
| 4 | 3 | 2 | 4 | 2 | 3 | 3872.355 | 3872.355 | -0.4 |
| 5 | 3 | 3 | 5 | 2 | 4 | 3874.382 | 3874.387 | -5.7 |
| 5 | 3 | 2 | 5 | 2 | 4 | 3874.510 | 3874.508 | 1.9 |
| 5 | 2 | 4 | 4 | 1 | 3 | 3875.759 | 3875.751 | 8.2 |
| 5 | 2 | 4 | 4 | 1 | 3 | 3875.760 | 3875.751 | 9.6 |
| 6 | 3 | 4 | 6 | 2 | 5 | 3877.937 | 3877.937 | -0.8 |
| 6 | 3 | 3 | 6 | 2 | 5 | 3878.298 | 3878.300 | -2.1 |
| 11 | 1 | 11 | 10 | 0 | 10 | 3879.713 | 3879.703 | 10.3 |
| 7 | 3 | 5 | 7 | 2 | 6 | 3883.565 | 3883.573 | -7.9 |
| 7 | 3 | 4 | 7 | 2 | 6 | 3884.472 | 3884.479 | -7.8 |
| 5 | 2 | 3 | 4 | 1 | 3 | 3888.542 | 3888.547 | -4.7 |
| 8 | 3 | 6 | 8 | 2 | 7 | 3891.924 | 3891.926 | -2.7 |
| 8 | 3 | 5 | 8 | 2 | 7 | 3893.914 | 3893.917 | -3.1 |

Table S8: Observed transitions for the *cis-gauche(+)* conformer (Conf2)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 9 | 3 | 7 | 9 | 2 | 8 | 3903.673 | 3903.678 | -4.2 |
| 9 | 3 | 6 | 9 | 2 | 8 | 3907.641 | 3907.650 | -8.3 |
| 13 | 0 | 13 | 12 | 1 | 12 | 3909.341 | 3909.337 | 4.4 |
| 10 | 3 | 8 | 10 | 2 | 9 | 3919.544 | 3919.544 | 0.2 |
| 10 | 3 | 7 | 10 | 2 | 9 | 3926.915 | 3926.897 | 18.0 |
| 11 | 3 | 9 | 11 | 2 | 10 | 3940.264 | 3940.261 | 2.4 |
| 11 | 3 | 8 | 11 | 2 | 10 | 3953.082 | 3953.075 | 6.8 |
| 12 | 3 | 10 | 12 | 2 | 11 | 3966.569 | 3966.572 | -3.1 |
| 12 | 4 | 9 | 11 | 4 | 8 | 3968.932 | 3968.923 | 8.6 |
| 12 | 3 | 10 | 11 | 3 | 9 | 3971.161 | 3971.164 | -2.9 |
| 12 | 3 | 9 | 11 | 3 | 8 | 3979.588 | 3979.589 | -0.7 |
| 12 | 3 | 9 | 12 | 2 | 11 | 3987.812 | 3987.810 | 2.0 |
| 8 | 5 | 4 | 9 | 4 | 6 | 3991.180 | 3991.167 | 13.3 |
| 8 | 5 | 3 | 9 | 4 | 6 | 3991.180 | 3991.167 | 13.2 |
| 13 | 3 | 11 | 13 | 2 | 12 | 3999.212 | 3999.207 | 5.4 |
| 13 | 3 | 10 | 13 | 2 | 12 | 4032.948 | 4032.946 | 1.9 |
| 12 | 2 | 10 | 11 | 2 | 9 | 4034.768 | 4034.759 | 9.4 |
| 14 | 3 | 12 | 14 | 2 | 13 | 4038.869 | 4038.872 | -2.7 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4143.535 | 4143.533 | 2.4 |
| 6 | 2 | 4 | 5 | 1 | 4 | 4182.688 | 4182.691 | -2.7 |
| 14 | 0 | 14 | 13 | 1 | 13 | 4262.833 | 4262.830 | 3.2 |
| 13 | 3 | 11 | 12 | 3 | 10 | 4302.974 | 4302.990 | -16.3 |
| 13 | 3 | 10 | 12 | 3 | 9 | 4315.497 | 4315.491 | 6.2 |
| 13 | 1 | 12 | 12 | 1 | 11 | 4378.544 | 4378.533 | 11.5 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4410.449 | 4410.449 | -0.6 |
| 7 | 2 | 6 | 6 | 1 | 5 | 4429.111 | 4429.109 | 2.1 |
| 6 | 2 | 4 | 5 | 1 | 5 | 4474.558 | 4474.544 | 14.5 |
| 7 | 2 | 5 | 6 | 1 | 5 | 4474.744 | 4474.737 | 7.0 |
| 15 | 0 | 15 | 14 | 1 | 14 | 4610.758 | 4610.758 | -0.1 |
| 14 | 1 | 14 | 13 | 0 | 13 | 4681.288 | 4681.287 | 1.5 |
| 8 | 2 | 6 | 7 | 1 | 6 | 4767.103 | 4767.101 | 1.4 |
| 7 | 2 | 6 | 6 | 1 | 6 | 4837.513 | 4837.511 | 2.1 |
| 16 | 0 | 16 | 15 | 1 | 15 | 4953.309 | 4953.308 | 0.8 |
| 15 | 1 | 15 | 14 | 0 | 14 | 4956.524 | 4956.522 | 1.5 |
| 9 | 2 | 7 | 8 | 1 | 7 | 5062.350 | 5062.349 | 1.8 |
| 10 | 2 | 9 | 9 | 1 | 8 | 5190.117 | 5190.125 | -8.0 |
| 4 | 3 | 2 | 3 | 2 | 1 | 5190.657 | 5190.654 | 2.5 |
| 4 | 3 | 1 | 3 | 2 | 2 | 5192.508 | 5192.519 | -10.3 |
| 8 | 2 | 7 | 7 | 1 | 7 | 5235.811 | 5235.812 | -1.3 |
| 16 | 1 | 16 | 15 | 0 | 15 | 5236.301 | 5236.311 | -9.5 |
| 17 | 0 | 17 | 16 | 1 | 16 | 5290.842 | 5290.862 | -19.8 |
| 14 | 4 | 10 | 14 | 3 | 11 | 5354.049 | 5354.034 | 15.2 |
| 10 | 2 | 8 | 9 | 1 | 8 | 5363.077 | 5363.079 | -2.6 |
| 12 | 4 | 8 | 12 | 3 | 9 | 5386.868 | 5386.863 | 4.6 |
| 11 | 4 | 8 | 11 | 3 | 8 | 5396.987 | 5396.988 | -0.8 |
| 11 | 4 | 7 | 11 | 3 | 8 | 5397.256 | 5397.259 | -2.2 |
| 15 | 4 | 12 | 15 | 3 | 13 | 5403.121 | 5403.122 | -0.9 |
| 16 | 4 | 13 | 16 | 3 | 14 | 5403.686 | 5403.686 | -0.1 |
| 14 | 4 | 11 | 14 | 3 | 12 | 5403.875 | 5403.876 | -0.9 |
| 10 | 4 | 7 | 10 | 3 | 7 | 5404.622 | 5404.627 | -4.3 |
| 10 | 4 | 6 | 10 | 3 | 7 | 5404.744 | 5404.753 | -9.3 |

Table S8: Observed transitions for the *cis-gauche(+)* conformer (Conf2)

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 13 | 4 | 10 | 13 | 3 | 11 | 5405.482 | 5405.484 | -1.6 |
| 14 | 4 | 10 | 14 | 3 | 12 | 5405.701 | 5405.705 | -4.4 |
| 17 | 4 | 14 | 17 | 3 | 15 | 5406.109 | 5406.109 | 0.2 |
| 13 | 4 | 9 | 13 | 3 | 11 | 5406.494 | 5406.503 | -9.2 |
| 12 | 4 | 9 | 12 | 3 | 10 | 5407.564 | 5407.560 | 3.4 |
| 12 | 4 | 8 | 12 | 3 | 10 | 5408.109 | 5408.101 | 7.9 |
| 11 | 4 | 8 | 11 | 3 | 9 | 5409.791 | 5409.802 | -10.9 |
| 9 | 4 | 5 | 9 | 3 | 6 | 5410.020 | 5410.022 | -2.1 |
| 8 | 4 | 4 | 8 | 3 | 5 | 5413.623 | 5413.619 | 3.4 |
| 11 | 2 | 10 | 10 | 1 | 9 | 5426.829 | 5426.830 | -0.1 |
| 5 | 3 | 3 | 4 | 2 | 2 | 5518.598 | 5518.599 | -1.5 |
| 5 | 3 | 2 | 4 | 2 | 2 | 5518.719 | 5518.720 | -0.9 |
| 17 | 1 | 17 | 16 | 0 | 16 | 5520.545 | 5520.546 | -1.0 |
| 5 | 3 | 3 | 4 | 2 | 3 | 5524.095 | 5524.095 | -0.7 |
| 5 | 3 | 2 | 4 | 2 | 3 | 5524.215 | 5524.216 | -1.1 |
| 18 | 0 | 18 | 17 | 1 | 17 | 5623.897 | 5623.915 | -17.3 |
| 9 | 2 | 8 | 8 | 1 | 8 | 5644.002 | 5643.994 | 8.1 |
| 12 | 2 | 11 | 11 | 1 | 10 | 5655.993 | 5655.987 | 6.1 |
| 18 | 1 | 18 | 17 | 0 | 17 | 5808.926 | 5808.935 | -9.2 |
| 6 | 3 | 4 | 5 | 2 | 3 | 5844.116 | 5844.118 | -2.6 |
| 6 | 3 | 3 | 5 | 2 | 3 | 5844.476 | 5844.481 | -4.9 |
| 6 | 3 | 4 | 5 | 2 | 4 | 5856.917 | 5856.915 | 2.8 |
| 6 | 3 | 3 | 5 | 2 | 4 | 5857.274 | 5857.277 | -3.4 |
| 13 | 2 | 12 | 12 | 1 | 11 | 5878.385 | 5878.380 | 5.7 |
| 19 | 0 | 19 | 18 | 1 | 18 | 5953.001 | 5953.015 | -14.0 |
| 12 | 2 | 10 | 11 | 1 | 10 | 5990.874 | 5990.872 | 1.9 |
| 14 | 2 | 13 | 13 | 1 | 12 | 6094.979 | 6094.960 | 19.0 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6165.954 | 6165.956 | -2.2 |
| 7 | 3 | 4 | 6 | 2 | 4 | 6166.864 | 6166.863 | 1.2 |
| 7 | 3 | 5 | 6 | 2 | 5 | 6191.455 | 6191.454 | 1.4 |
| 7 | 3 | 4 | 6 | 2 | 5 | 6192.361 | 6192.360 | 0.6 |
| 20 | 0 | 20 | 19 | 1 | 19 | 6278.709 | 6278.716 | -6.1 |
| 15 | 2 | 14 | 14 | 1 | 13 | 6306.867 | 6306.863 | 3.7 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6482.652 | 6482.656 | -3.6 |
| 8 | 3 | 5 | 7 | 2 | 5 | 6484.644 | 6484.646 | -2.1 |
| 8 | 3 | 6 | 7 | 2 | 6 | 6528.280 | 6528.284 | -3.5 |
| 8 | 3 | 5 | 7 | 2 | 6 | 6530.277 | 6530.274 | 2.5 |
| 14 | 2 | 12 | 13 | 1 | 12 | 6668.095 | 6668.105 | -9.5 |
| 21 | 1 | 21 | 20 | 0 | 20 | 6694.753 | 6694.763 | -9.8 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6740.034 | 6740.038 | -4.2 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6740.034 | 6740.042 | -8.6 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6792.628 | 6792.626 | 2.7 |
| 9 | 3 | 6 | 8 | 2 | 6 | 6796.604 | 6796.598 | 6.8 |
| 9 | 3 | 6 | 8 | 2 | 7 | 6872.009 | 6871.999 | 9.4 |
| 7 | 5 | 2 | 7 | 4 | 3 | 6966.377 | 6966.388 | -10.9 |
| 15 | 2 | 13 | 14 | 1 | 13 | 7029.689 | 7029.705 | -16.6 |
| 5 | 4 | 2 | 4 | 3 | 1 | 7070.219 | 7070.211 | 8.0 |
| 10 | 3 | 8 | 9 | 2 | 7 | 7094.243 | 7094.241 | 2.9 |
| 10 | 3 | 7 | 9 | 2 | 7 | 7101.588 | 7101.594 | -5.9 |
| 10 | 3 | 8 | 9 | 2 | 8 | 7211.339 | 7211.343 | -4.6 |
| 10 | 3 | 7 | 9 | 2 | 8 | 7218.694 | 7218.697 | -2.7 |

Table S8: Observed transitions for the *cis-gauche(+)* conformer (Conf2)

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 12 | 2 | 10 | 11 | 1 | 11 | 7262.738 | 7262.743 | -5.0 |
| 11 | 3 | 9 | 10 | 2 | 8 | 7385.964 | 7385.959 | 4.8 |
| 11 | 3 | 9 | 10 | 2 | 9 | 7558.913 | 7558.913 | 0.2 |
| 11 | 3 | 8 | 10 | 2 | 9 | 7571.729 | 7571.727 | 1.8 |
| 12 | 3 | 10 | 11 | 2 | 9 | 7666.441 | 7666.446 | -5.1 |
| 12 | 3 | 9 | 11 | 2 | 10 | 7932.672 | 7932.664 | 7.8 |
| 13 | 3 | 11 | 12 | 2 | 10 | 7934.678 | 7934.677 | 1.1 |

Table S9: Observed transitions for *cis-anti* conformer (Conf3)

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 5 | 1 | 5 | 4 | 0 | 4 | 2279.664 | 2279.663 | 1.0 |
| 9 | 0 | 9 | 8 | 1 | 8 | 2451.438 | 2451.436 | 1.5 |
| 6 | 2 | 5 | 6 | 1 | 6 | 2521.923 | 2521.916 | 6.3 |
| 6 | 1 | 6 | 5 | 0 | 5 | 2555.950 | 2555.948 | 2.3 |
| 10 | 0 | 10 | 9 | 1 | 9 | 2822.932 | 2822.923 | 8.4 |
| 7 | 1 | 7 | 6 | 0 | 6 | 2826.178 | 2826.175 | 2.9 |
| 8 | 1 | 8 | 7 | 0 | 7 | 3091.868 | 3091.862 | 6.2 |
| 11 | 0 | 11 | 10 | 1 | 10 | 3191.260 | 3191.251 | 9.1 |
| 9 | 1 | 9 | 8 | 0 | 8 | 3354.680 | 3354.676 | 4.4 |
| 13 | 3 | 10 | 13 | 2 | 11 | 3573.153 | 3573.157 | -4.4 |
| 10 | 1 | 10 | 9 | 0 | 9 | 3616.338 | 3616.336 | 2.5 |
| 10 | 3 | 7 | 10 | 2 | 8 | 3739.109 | 3739.106 | 2.7 |
| 9 | 3 | 6 | 9 | 2 | 7 | 3775.987 | 3775.987 | -0.1 |
| 8 | 3 | 5 | 8 | 2 | 6 | 3804.173 | 3804.183 | -9.2 |
| 5 | 3 | 2 | 5 | 2 | 3 | 3847.754 | 3847.757 | -3.1 |
| 4 | 3 | 1 | 4 | 2 | 2 | 3852.989 | 3852.982 | 7.6 |
| 5 | 3 | 3 | 5 | 2 | 4 | 3860.550 | 3860.549 | 0.7 |
| 6 | 3 | 4 | 6 | 2 | 5 | 3864.137 | 3864.132 | 5.3 |
| 7 | 3 | 4 | 7 | 2 | 6 | 3870.749 | 3870.739 | 9.9 |
| 8 | 3 | 6 | 8 | 2 | 7 | 3878.250 | 3878.246 | 3.9 |
| 11 | 1 | 11 | 10 | 0 | 10 | 3878.494 | 3878.491 | 2.4 |
| 9 | 3 | 7 | 9 | 2 | 8 | 3890.096 | 3890.101 | -5.3 |
| 9 | 3 | 6 | 9 | 2 | 8 | 3894.131 | 3894.136 | -5.0 |
| 10 | 3 | 8 | 10 | 2 | 9 | 3906.108 | 3906.105 | 2.5 |
| 13 | 0 | 13 | 12 | 1 | 12 | 3914.182 | 3914.174 | 8.0 |
| 13 | 3 | 11 | 13 | 2 | 12 | 3986.427 | 3986.433 | -6.6 |
| 14 | 3 | 12 | 14 | 2 | 13 | 4026.420 | 4026.416 | 3.6 |
| 16 | 3 | 14 | 16 | 2 | 15 | 4130.249 | 4130.249 | -0.1 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4142.603 | 4142.605 | -1.9 |
| 17 | 3 | 15 | 17 | 2 | 16 | 4195.267 | 4195.270 | -2.7 |
| 14 | 0 | 14 | 13 | 1 | 13 | 4267.574 | 4267.575 | -0.2 |
| 19 | 3 | 17 | 19 | 2 | 18 | 4353.906 | 4353.914 | -8.0 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4409.847 | 4409.850 | -2.7 |
| 7 | 2 | 6 | 6 | 1 | 5 | 4421.712 | 4421.715 | -2.8 |
| 11 | 6 | 6 | 12 | 5 | 7 | 4512.850 | 4512.867 | -16.4 |
| 23 | 1 | 22 | 23 | 0 | 23 | 4633.787 | 4633.789 | -1.5 |
| 14 | 1 | 14 | 13 | 0 | 13 | 4681.041 | 4681.050 | -9.1 |
| 8 | 2 | 7 | 7 | 1 | 6 | 4684.333 | 4684.334 | -0.4 |
| 3 | 3 | 0 | 2 | 2 | 1 | 4848.439 | 4848.448 | -9.6 |

Table S9: Observed transitions for *cis-anti* conformer (Conf3)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 22 | 4 | 18 | 22 | 3 | 19 | 4892.865 | 4892.873 | -7.1 |
| 15 | 1 | 15 | 14 | 0 | 14 | 4956.661 | 4956.674 | -12.8 |
| 16 | 0 | 16 | 15 | 1 | 15 | 4957.843 | 4957.836 | 7.1 |
| 4 | 3 | 2 | 3 | 2 | 1 | 5177.632 | 5177.641 | -8.9 |
| 4 | 3 | 1 | 3 | 2 | 2 | 5179.521 | 5179.523 | -2.1 |
| 16 | 1 | 16 | 15 | 0 | 15 | 5236.871 | 5236.862 | 9.1 |
| 17 | 0 | 17 | 16 | 1 | 16 | 5295.277 | 5295.288 | -10.7 |
| 15 | 4 | 11 | 15 | 3 | 12 | 5309.177 | 5309.167 | 10.4 |
| 14 | 4 | 10 | 14 | 3 | 11 | 5333.860 | 5333.855 | 5.2 |
| 13 | 4 | 9 | 13 | 3 | 10 | 5352.813 | 5352.810 | 3.1 |
| 11 | 4 | 7 | 11 | 3 | 8 | 5377.594 | 5377.596 | -2.3 |
| 15 | 4 | 12 | 15 | 3 | 13 | 5383.745 | 5383.749 | -4.6 |
| 14 | 4 | 11 | 14 | 3 | 12 | 5384.446 | 5384.452 | -5.6 |
| 10 | 4 | 6 | 10 | 3 | 7 | 5385.171 | 5385.178 | -6.3 |
| 13 | 4 | 10 | 13 | 3 | 11 | 5386.042 | 5386.030 | 12.2 |
| 12 | 4 | 9 | 12 | 3 | 10 | 5388.085 | 5388.094 | -8.9 |
| 11 | 4 | 8 | 11 | 3 | 9 | 5390.324 | 5390.334 | -10.2 |
| 9 | 4 | 5 | 9 | 3 | 6 | 5390.502 | 5390.506 | -4.5 |
| 10 | 4 | 7 | 10 | 3 | 8 | 5392.521 | 5392.517 | 4.1 |
| 8 | 4 | 5 | 8 | 3 | 6 | 5396.135 | 5396.145 | -10.1 |
| 7 | 4 | 3 | 7 | 3 | 4 | 5396.541 | 5396.542 | -0.5 |
| 7 | 4 | 4 | 7 | 3 | 5 | 5397.450 | 5397.455 | -5.1 |
| 5 | 3 | 3 | 4 | 2 | 2 | 5505.786 | 5505.781 | 4.9 |
| 5 | 3 | 2 | 4 | 2 | 3 | 5511.451 | 5511.451 | -0.8 |
| 18 | 0 | 18 | 17 | 1 | 17 | 5628.248 | 5628.256 | -7.1 |
| 12 | 1 | 11 | 11 | 0 | 11 | 5643.634 | 5643.640 | -6.0 |
| 12 | 2 | 11 | 11 | 1 | 10 | 5648.600 | 5648.597 | 3.3 |
| 18 | 1 | 18 | 17 | 0 | 17 | 5810.278 | 5810.277 | 0.7 |
| 6 | 3 | 4 | 5 | 2 | 3 | 5831.474 | 5831.473 | 0.8 |
| 6 | 3 | 3 | 5 | 2 | 4 | 5844.760 | 5844.757 | 3.1 |
| 13 | 2 | 12 | 12 | 1 | 11 | 5870.992 | 5870.986 | 5.9 |
| 19 | 0 | 19 | 18 | 1 | 18 | 5957.278 | 5957.292 | -13.5 |
| 14 | 2 | 13 | 13 | 1 | 12 | 6087.590 | 6087.587 | 2.8 |
| 19 | 1 | 19 | 18 | 0 | 18 | 6102.798 | 6102.792 | 6.7 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6153.458 | 6153.450 | 8.3 |
| 7 | 3 | 4 | 6 | 2 | 5 | 6180.111 | 6180.103 | 7.3 |
| 15 | 2 | 14 | 14 | 1 | 13 | 6299.543 | 6299.547 | -4.2 |
| 20 | 1 | 20 | 19 | 0 | 19 | 6398.590 | 6398.579 | 11.5 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6470.238 | 6470.242 | -3.9 |
| 8 | 3 | 5 | 7 | 2 | 6 | 6518.310 | 6518.310 | -0.4 |
| 21 | 1 | 21 | 20 | 0 | 20 | 6697.164 | 6697.172 | -7.8 |
| 17 | 2 | 16 | 16 | 1 | 15 | 6715.041 | 6715.035 | 6.6 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6721.491 | 6721.488 | 2.9 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6721.491 | 6721.492 | -1.5 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6780.246 | 6780.246 | 0.0 |
| 9 | 3 | 6 | 8 | 2 | 6 | 6784.283 | 6784.281 | 2.4 |
| 22 | 5 | 17 | 22 | 4 | 18 | 6809.684 | 6809.674 | 9.9 |
| 9 | 3 | 6 | 8 | 2 | 7 | 6860.374 | 6860.366 | 7.2 |
| 17 | 5 | 12 | 17 | 4 | 13 | 6901.787 | 6901.782 | 5.4 |
| 18 | 5 | 14 | 18 | 4 | 15 | 6903.118 | 6903.107 | 11.4 |
| 17 | 5 | 13 | 17 | 4 | 14 | 6910.118 | 6910.115 | 2.8 |

Table S9: Observed transitions for *cis-anti* conformer (Conf3)

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 16 | 5 | 11 | 16 | 4 | 12 | 6911.150 | 6911.141 | 8.9 |
| 16 | 5 | 12 | 16 | 4 | 13 | 6916.347 | 6916.346 | 0.1 |
| 18 | 2 | 17 | 17 | 1 | 16 | 6921.670 | 6921.678 | -8.1 |
| 15 | 5 | 11 | 15 | 4 | 12 | 6921.775 | 6921.777 | -1.6 |
| 14 | 5 | 9 | 14 | 4 | 10 | 6924.589 | 6924.580 | 8.9 |
| 12 | 5 | 7 | 12 | 4 | 8 | 6932.946 | 6932.934 | 12.6 |
| 11 | 5 | 6 | 11 | 4 | 7 | 6935.762 | 6935.754 | 7.8 |
| 11 | 5 | 7 | 11 | 4 | 8 | 6936.026 | 6936.028 | -1.2 |
| 10 | 5 | 6 | 10 | 4 | 7 | 6938.011 | 6938.018 | -6.8 |
| 8 | 5 | 4 | 8 | 4 | 5 | 6940.624 | 6940.640 | -15.6 |
| 8 | 5 | 3 | 8 | 4 | 4 | 6940.624 | 6940.619 | 5.7 |
| 7 | 5 | 3 | 7 | 4 | 4 | 6941.419 | 6941.424 | -4.8 |
| 7 | 5 | 2 | 7 | 4 | 3 | 6941.419 | 6941.417 | 2.3 |
| 6 | 5 | 2 | 6 | 4 | 3 | 6941.947 | 6941.951 | -4.3 |
| 6 | 5 | 1 | 6 | 4 | 2 | 6941.947 | 6941.949 | -2.4 |
| 5 | 5 | 1 | 5 | 4 | 2 | 6942.288 | 6942.284 | 4.5 |
| 5 | 5 | 0 | 5 | 4 | 1 | 6942.288 | 6942.284 | 4.9 |
| 15 | 2 | 13 | 14 | 1 | 13 | 7027.755 | 7027.758 | -3.6 |
| 5 | 4 | 2 | 4 | 3 | 1 | 7051.861 | 7051.877 | -16.2 |
| 10 | 3 | 8 | 9 | 2 | 7 | 7081.837 | 7081.828 | 9.4 |
| 19 | 2 | 18 | 18 | 1 | 17 | 7129.805 | 7129.813 | -8.3 |
| 10 | 3 | 8 | 9 | 2 | 8 | 7199.988 | 7199.977 | 11.4 |
| 10 | 3 | 7 | 9 | 2 | 8 | 7207.445 | 7207.446 | -0.8 |
| 20 | 2 | 19 | 19 | 1 | 18 | 7341.098 | 7341.106 | -8.2 |
| 13 | 2 | 12 | 12 | 1 | 12 | 7372.022 | 7372.022 | -0.1 |
| 11 | 3 | 9 | 10 | 2 | 8 | 7373.446 | 7373.441 | 4.3 |
| 6 | 4 | 3 | 5 | 3 | 2 | 7382.137 | 7382.137 | -0.1 |
| 6 | 4 | 2 | 5 | 3 | 2 | 7382.137 | 7382.139 | -2.0 |
| 6 | 4 | 2 | 5 | 3 | 3 | 7382.259 | 7382.262 | -3.2 |
| 6 | 4 | 3 | 5 | 3 | 3 | 7382.260 | 7382.260 | -0.1 |
| 11 | 3 | 9 | 10 | 2 | 9 | 7547.904 | 7547.909 | -4.6 |
| 11 | 3 | 8 | 10 | 2 | 9 | 7560.917 | 7560.924 | -6.8 |
| 12 | 3 | 10 | 11 | 2 | 9 | 7653.755 | 7653.751 | 3.8 |
| 7 | 4 | 4 | 6 | 3 | 3 | 7712.135 | 7712.138 | -2.5 |
| 7 | 4 | 3 | 6 | 3 | 4 | 7712.522 | 7712.513 | 9.1 |
| 13 | 3 | 11 | 12 | 2 | 10 | 7921.736 | 7921.739 | -3.4 |
| 12 | 3 | 9 | 11 | 2 | 10 | 7922.393 | 7922.392 | 1.8 |

Table S10: Observed transitions for the C1-$^{13}$C-substituted species of conformer 1

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3606.4049 | 3606.4023 | 2.6 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4130.8452 | 4130.8364 | 8.8 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4397.1334 | 4397.1453 | 11.9 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6143.0978 | 6143.1042 | - 6.4 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6712.7888 | 6712.7873 | 1.5 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6712.7888 | 6712.7917 | -2.9 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6767.9930 | 6767.9847 | 8.3 |

Table S11: Observed transitions for the C2-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3599.8323 | 3599.8359 | -3.6 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4122.6464 | 4122.6411 | 5.3 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4388.0565 | 4388.0571 | -0.6 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6140.9526 | 6140.9597 | -7.1 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6477.8527 | 6477.8500 | 2.7 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6714.9668 | 6714.9668 | 0.0 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6714.9668 | 6714.9624 | 4.4 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6764.3489 | 6764.3511 | -2.2 |
| 10 | 3 | 7 | 9 | 2 | 8 | 7188.1491 | 7188.1460 | 3.1 |

Table S12: Observed transitions for the C3-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 12 | 1 | 12 | 11 | 0 | 11 | 4124.0799 | 4124.0790 | 0.9 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6157.3443 | 6157.3414 | 2.9 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6472.2379 | 6472.2320 | 5.9 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6739.8120 | 6739.8142 | -2.2 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6739.8120 | 6739.8100 | 2.0 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6780.5411 | 6780.5497 | -8.6 |

Table S13: Observed transitions for the C4-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3604.7558 | 3604.7652 | -9.4 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4393.4551 | 4393.4477 | 7.4 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6153.3333 | 6153.3362 | -2.9 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6730.9915 | 6730.9929 | -1.4 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6730.9915 | 6730.9887 | 2.8 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6777.3807 | 6777.3785 | 2.2 |
| 10 | 3 | 7 | 9 | 2 | 8 | 7200.5738 | 7200.5745 | -0.7 |

Table S14: Observed transitions for the C5-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3611.6710 | 3611.6592 | 11.8 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4136.3727 | 4136.3814 | -8.7 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6158.4528 | 6158.4612 | -8.4 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6474.6001 | 6474.5997 | 0.4 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6732.7630 | 6732.7635 | -0.5 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6732.7630 | 6732.7591 | 3.9 |
| 11 | 3 | 8 | 10 | 2 | 9 | 7562.0864 | 7562.0838 | 2.6 |

Table S15: Observed transitions for the C6-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3611.6710 | 3611.6592 | 11.8 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4136.3727 | 4136.3814 | -8.7 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6158.4528 | 6158.4612 | -8.4 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6474.6001 | 6474.5997 | 0.4 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6732.7630 | 6732.7635 | -0.5 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6732.7630 | 6732.7591 | 3.9 |
| 11 | 3 | 8 | 10 | 2 | 9 | 7562.0864 | 7562.0838 | 2.6 |

Table S16: Observed transitions for the C7-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3605.3173 | 3605.3278 | -10.5 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4397.8338 | 4397.8246 | 9.2 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6127.0664 | 6127.0652 | 1.2 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6443.1820 | 6443.1861 | -4.1 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6687.2387 | 6687.2398 | -1.1 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6687.2387 | 6687.2352 | 3.5 |

Table S17: Observed transitions for the C8-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3616.4759 | 3616.4697 | 6.2 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4142.2055 | 4142.2027 | 2.8 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4409.1306 | 4409.1386 | -8.0 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6161.8092 | 6161.8069 | 2.3 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6734.3316 | 6734.3347 | -3.1 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6734.3316 | 6734.3303 | 1.3 |

Table S18: Observed transitions for the C9-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3617.5981 | 3617.5880 | 10.1 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4410.4493 | 4410.4551 | -5.8 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6162.9402 | 6162.9557 | -15.5 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6735.6908 | 6735.6895 | 1.3 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6735.6908 | 6735.6851 | 5.7 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6787.2667 | 6787.2669 | -0.2 |
| 11 | 3 | 8 | 10 | 2 | 9 | 7568.8586 | 7568.8537 | 4.9 |

Table S19: Observed transitions for the C10-$^{13}$C-substituted species of conformer 1

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3615.5261 | 3615.5373 | -11.2 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4140.7897 | 4140.7827 | 7.0 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4407.4276 | 4407.4238 | 3.8 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6153.3322 | 6153.3362 | -4.0 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6480.9060 | 6480.8954 | 10.6 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6739.5869 | 6739.5882 | -1.3 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6739.5869 | 6739.5838 | 3.1 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6790.6223 | 6790.6350 | -12.7 |

Table S20: Observed transitions for the C11-$^{13}$C-substituted species of conformer 1

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3609.3502 | 3609.3471 | 3.1 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4401.8625 | 4401.8681 | -5.6 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6140.1802 | 6140.1697 | 10.5 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6505.1473 | 6505.1562 | -8.9 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6705.0115 | 6705.0168 | -5.3 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6705.0115 | 6705.0123 | -0.8 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6765.9246 | 6765.9175 | 7.1 |

Table S21: Observed transitions for the C12-$^{13}$C-substituted species of conformer 1

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3606.2154 | 3606.2181 | -2.7 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4397.8342 | 4397.8358 | -1.6 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6136.0723 | 6136.0670 | 5.3 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6452.0574 | 6452.0549 | 2.5 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6701.3738 | 6701.3799 | -6.1 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6701.3738 | 6701.3754 | -1.6 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6761.2131 | 6761.2059 | 7.2 |
| 10 | 3 | 7 | 9 | 2 | 8 | 7188.4947 | 7188.4914 | 3.3 |

Table S22: Observed transitions for the C13-$^{13}$C-substituted species of conformer 1

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3612.2815 | 3612.2755 | 6.0 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4136.8708 | 4136.8641 | 6.7 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4403.1503 | 4403.1639 | -13.6 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6161.7520 | 6161.7390 | 13.0 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6477.8527 | 6477.8500 | 2.7 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6737.8444 | 6737.8466 | -2.2 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6737.8444 | 6737.8509 | -6.5 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6787.2667 | 6787.2669 | -0.2 |
| 11 | 3 | 8 | 10 | 2 | 9 | 7564.3631 | 7564.3665 | -3.4 |

Table S23: Observed transitions for the C14-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3609.347 | 3609.334 | 12.4 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4139.128 | 4139.133 | -4.6 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4405.741 | 4405.737 | 4.4 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6734.006 | 6734.008 | -2.1 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6734.006 | 6734.008 | -2.3 |
| 10 | 3 | 7 | 9 | 2 | 8 | 7211.604 | 7211.604 | 0.1 |

Table S24: Observed transitions for the C15-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3602.0201 | 3602.0162 | 3.9 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6448.9804 | 6448.9830 | -2.6 |
| 8 | 3 | 5 | 7 | 2 | 6 | 6497.2190 | 6497.2270 | -8.0 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6700.6111 | 6700.6102 | 0.9 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6700.6111 | 6700.6057 | 5.4 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6757.6968 | 6757.7046 | -7.8 |

Table S25: Observed transitions for the C16-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3600.0991 | 3600.1037 | -4.6 |
| 12 | 1 | 12 | 11 | 0 | 11 | 4122.4901 | 4122.4964 | -6.3 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4387.6504 | 4387.6402 | 10.2 |
| 6 | 3 | 4 | 5 | 2 | 3 | 5826.8193 | 5826.8125 | 6.8 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6146.7810 | 6146.7890 | -8.0 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6724.3853 | 6724.3869 | -1.6 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6724.3853 | 6724.3826 | 2.7 |

Table S26: Observed transitions for the C17-$^{13}$C-substituted species of conformer 1

| $J'$ | $K_a'$ | $K_c'$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3605.1856 | 3605.1912 | -5.6 |
| 13 | 1 | 13 | 12 | 0 | 12 | 4393.4469 | 4393.4439 | 3.0 |
| 7 | 3 | 5 | 6 | 2 | 4 | 6158.1704 | 6158.1787 | -8.3 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6473.4438 | 6473.4534 | -9.6 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6738.4644 | 6738.4657 | -1.3 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6738.4644 | 6738.4615 | 2.9 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6782.1371 | 6782.1209 | 16.2 |

Table S27: Observed transitions for the C18-$^{13}$C-substituted species of conformer 1

| $J'$ | $K'_a$ | $K'_c$ | $J$ | $K_a$ | $K_c$ | $\nu_{obs}$[MHz] | $\nu_{calc}$[MHz] | $\nu_{obs}$-$\nu_{calc}$ [kHz] |
|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 10 | 9 | 0 | 9 | 3609.0907 | 3609.0913 | -0.6 |
| 8 | 3 | 6 | 7 | 2 | 5 | 6452.1668 | 6452.1733 | -6.5 |
| 4 | 4 | 0 | 3 | 3 | 1 | 6702.6193 | 6702.6214 | -2.1 |
| 4 | 4 | 1 | 3 | 3 | 0 | 6702.6193 | 6702.6171 | 2.2 |
| 9 | 3 | 7 | 8 | 2 | 6 | 6761.6099 | 6761.6035 | 6.4 |