# Synchrotron-based High Resolution Far-infrared Spectroscopy of *trans*-butadiene

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**ELECTRONIC SUPPORTING INFORMATION**

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## 1. SUPPLEMENTARY FIGURES

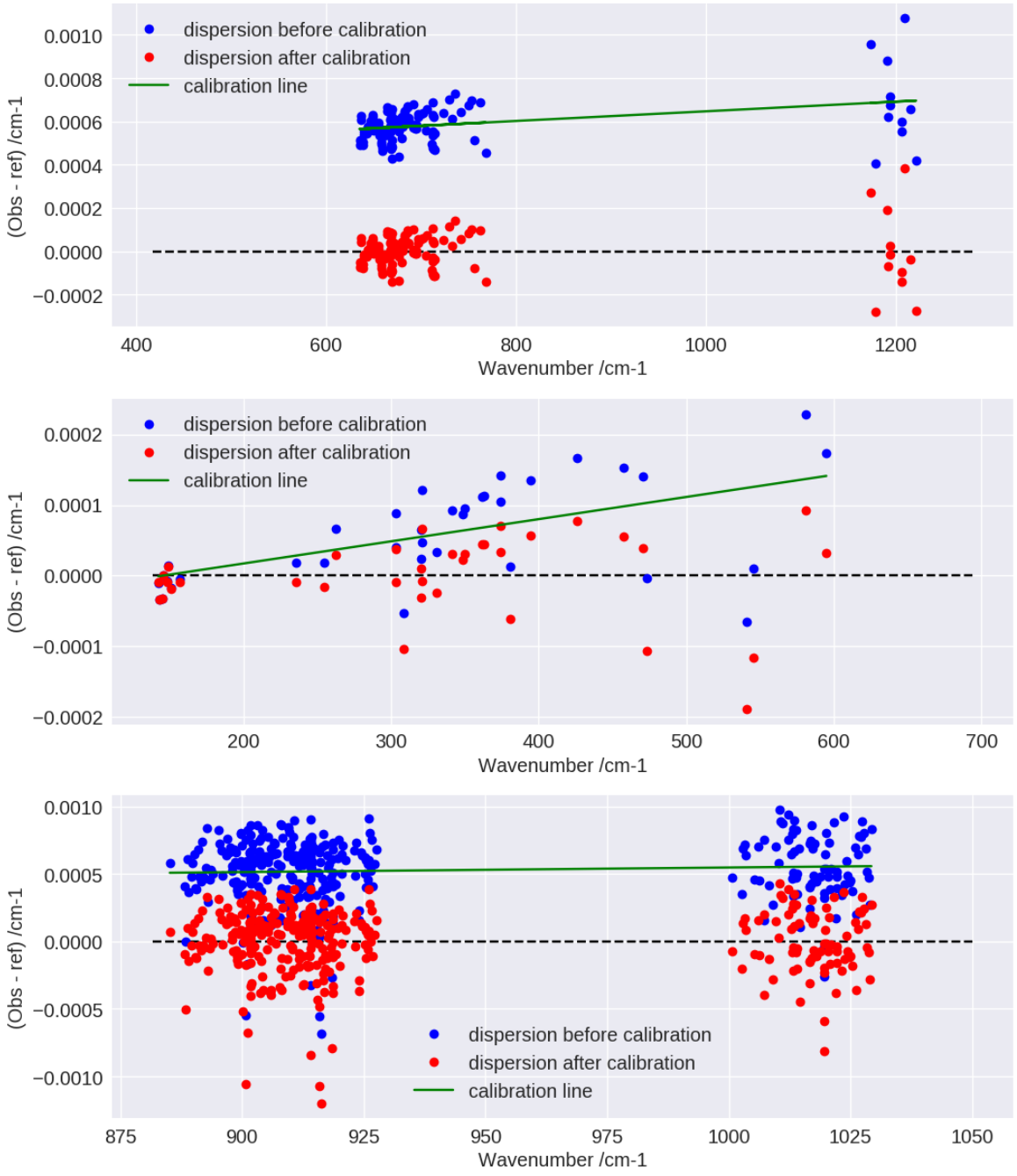


**Fig. S1.** Calibration plots for the warm spectrum recorded at CLS (top trace), the room temperature one recorded at SOLEIL (middle trace), and the cold spectrum recorded using the Jet-AILES apparatus at SOLEIL (bottom trace). Each dot represent the value of $\tilde{nu}_{exp} - \tilde{nu}_{ref}$, where exp refers to the experimental wavenumber and ref the accurate wavenumber used for calibration (see main text for information on reference molecules), before (in blue) and after (in red) calibration. The green lines are the calibration lines whose parameters were used to calibrate the experimental spectra. The residuals after calibration is an indication of the wavenumber accuracy one can expect from the experimental data.

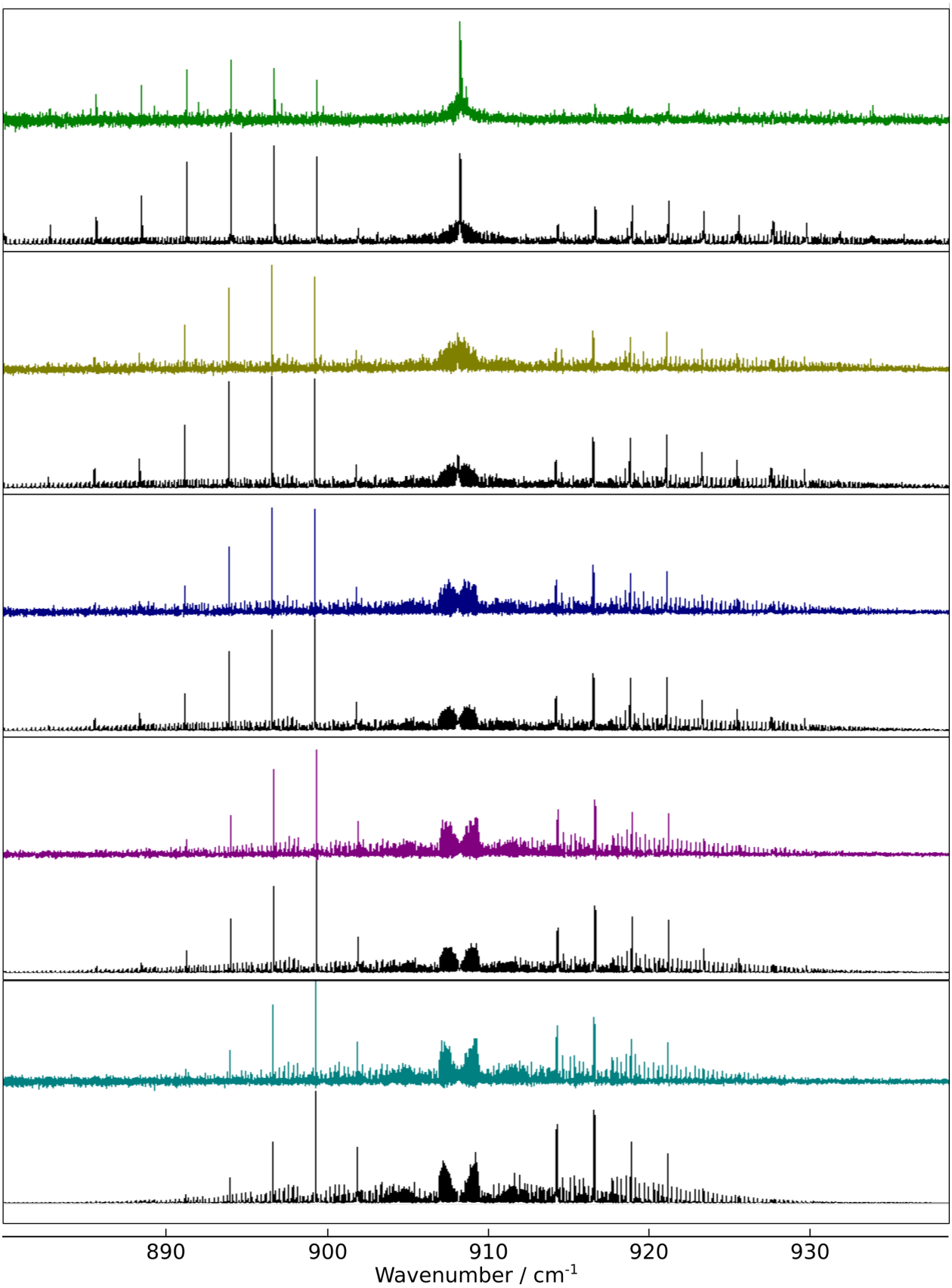


**Fig. S2.** Experimental Jet-AILES spectra recorded with 0, 5, 10, 20, and 30 slm of He seeded in 2 slm of butadiene (from top to bottom, colored traced) and comparison with PGOPHER [1] simulations at temperatures of 150, 100, 70, 50, and 40 K, respectively (black traces)

## 2. SUPPLEMENTARY TABLES

**Table S1.** Calculated band centers determined at the CCSD(T)/ANO1 ("Harmonic"), hybrid harmonic/anharmonic CCSD(T)/ANO1//CCSD(T)/ANO0 ("Anharmonic"), and VPT2+K ("GUINEA") levels of theory [2]. Intensities calculated at the harmonic CCSD(T)/ANO1 level.

| $\nu$ | Symmetry | Frequency / $cm^{-1}$ | | | IR intensity / $km \cdot mol^{-1}$ | |
|---|---|---|---|---|---|---|
| | | Harmonic | Anharmonic | GUINEA | Harmonic | GUINEA |
| 13 | $a_u$ | 164.7543 | 158.1349 | | 0.47 | |
| 24 | $b_u$ | 289.6453 | 290.9936 | | 2.16 | |
| 9 | $a_g$ | 509.4167 | 504.6210 | | 0.00 | |
| 12 | $a_u$ | 533.9530 | 516.9960 | | 11.76 | |
| 16 | $b_g$ | 766.0941 | 738.7697 | | 0.00 | |
| 8 | $a_g$ | 895.6995 | 878.9920 | | 0.00 | |
| 11 | $a_u$ | 923.2770 | 884.8401 | | 72.09 | |
| 15 | $b_g$ | 925.1164 | 889.9208 | | 0.00 | |
| 14 | $b_g$ | 988.8452 | 956.5181 | | 0.00 | |
| 23 | $b_u$ | 994.7242 | 977.3987 | | 1.24 | |
| 10 | $a_u$ | 1042.5074 | 1014.1572 | 1012.2453 | 36.11 | 28.79 |
| 7 | $a_g$ | 1222.3291 | 1194.5204 | | 0.00 | |
| 6 | $a_g$ | 1307.8309 | 1285.3375 | | 0.00 | |
| 22 | $b_u$ | 1310.7191 | 1284.7354 | | 2.09 | |
| 21 | $b_u$ | 1408.7609 | 1369.7341 | | 4.00 | |
| 5 | $a_g$ | 1473.3658 | 1428.5660 | | 0.00 | |
| 20 | $b_u$ | 1633.5237 | 1586.8279 | | 14.39 | |
| 4 | $a_g$ | 1695.4519 | 1651.6894 | | 0.00 | |
| 3 | $a_g$ | 3144.9188 | 2941.0555 | | 0.00 | |
| 19 | $b_u$ | 3147.1063 | 3038.2044 | | 13.43 | |
| 2 | $a_g$ | 3156.4329 | 3041.4562 | | 0.00 | |
| 18 | $b_u$ | 3162.1996 | 3030.8058 | | 10.50 | |
| 1 | $a_g$ | 3241.3186 | 3105.6929 | | 0.00 | |
| 17 | $b_u$ | 3241.5700 | 3106.5926 | | 19.48 | |
| 9+12 | $a_u$ | | | 1034.4503 | | 0.22 |

**Table S2.** Predicted rotational constants (in $cm^{-1}$) in the vibrational states of interest for this study and comparison with experimental values. Predicted values for the $v_i = 1$ state have been obtained using the scaling formula $B_{i\,\mathrm{calc.}} = B_{i\,\mathrm{calc.}} \times B_{0\,\mathrm{exp.}} / B_{0\,\mathrm{calc.}}$

| $v_i = 1$ | Ab initio[a] | | | Scaled | | | Experimental | | | $\delta^b$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $i$ | $A$ | $B$ | $C$ | $A$ | $B$ | $C$ | $A$ | $B$ | $C$ | $\delta_A$ | $\delta_B$ | $\delta_C$ |
| 0 | 1.3674 | 0.1445 | 0.1307 | – | – | – | 1.3904 | 0.1479 | 0.1337 | | | |
| 10 | 1.3720 | 0.1435 | 0.1307 | 1.3950 | 0.1469 | 0.1337 | 1.3870 | 0.1495 | 0.1338 | 0.58 | -1.75 | -0.11 |
| 24 | 1.3233 | 0.1443 | 0.1307 | 1.3455 | 0.1478 | 0.1338 | 1.4316 | 0.1480 | 0.1336 | -6.02 | -0.13 | 0.11 |
| 9 + 12 | 1.3685 | 0.1446 | 0.1308 | 1.3915 | 0.1480 | 0.1338 | | | | | | |

[a] CCSD(T)/ANO0 VPT2 (harmonic)
[b] $\delta = \frac{B_{i\,\mathrm{exp.}} - B_{i\,\mathrm{scaled}}}{B_{i\,\mathrm{scaled}}} * 100$, in %

**Table S3.** Rotational constants and band centers (in $cm^{-1}$) of butadiene after the global fit performed in this work: refit in the *S* reduction of all the available literature data ($\nu_{13}$, $\nu_{12}$, $\nu_{11}$, $\nu_{20}$, and $\nu_{17}$ bands) and new assignments in $\nu_{10}$ and $\nu_{24}$. Brackets indicate parameters fixed to the GS values. Relevant parameters to the fit are also reported. Numbers in parenthesis are one standard deviation in units of the last quoted digit.

| Constant | $v=0$ | $v_{13}=1$ | $v_{24}=1$ | $v_{12}=1$ | $v_{11}=1$ | $v_{10}=1$ | $v_{20}=1$ | $v_{17}=1$ |
|---|---|---|---|---|---|---|---|---|
| $E$ | | 162.419463(12) | 297.0923451(62) | 524.5738512(91) | 908.071968(16) | 1013.368967(66) | 1596.44603(88) | 3100.63227(29) |
| $A$ | 1.39038236(43) | 1.34477745(77) | 1.43163076(55) | 1.38902369(45) | 1.36826885(95) | 1.386966(15) | 1.39260(12) | 1.387928(28) |
| $B$ | 0.147885699(62) | 0.147961986(77) | 0.147960763(63) | 0.147747042(66) | 0.147738901(80) | 0.14952571(74) | 0.1473896(45) | 0.1476913(82) |
| $C$ | 0.133694207(64) | 0.134118551(80) | 0.133616011(65) | 0.133708028(68) | 0.133725433(79) | 0.13382711(68) | 0.1333877(32) | 0.1335834(50) |
| $D_J\times10^6$ | 0.0287509(91) | 0.030249(11) | 0.0278283(90) | 0.0288470(96) | 0.029224(11) | 0.0470(12) | 0.0284(13) | [·] |
| $D_{JK}\times10^6$ | −0.23859(17) | −0.24946(27) | −0.24369(17) | −0.25072(18) | −0.20877(29) | −9.191(57) | −4.59(29) | [·] |
| $D_K\times10^6$ | 7.2913(12) | −5.4398(71) | 21.9587(59) | 7.1452(13) | 2.1983(98) | 53.51(82) | [·] | [·] |
| $d_1\times10^9$ | −3.5889(65) | −3.459(13) | −3.5927(71) | −3.5555(80) | −3.3252(96) | [·] | [·] | [·] |
| $d_2\times10^9$ | −0.1888(25) | 0.1844(60) | −0.5070(27) | [·] | [·] | [·] | [·] | [·] |
| $H_{JK}\times10^9$ | | | | | | −6.985(70) | | |
| $H_{KJ}\times10^6$ | | | | | | 0.3054(15) | | |
| $H_K\times10^9$ | | | 8.485(30) | | | 434.(13) | | |
| $L_K\times10^{12}$ | | | −4.010(49) | | | | | |

| | Total | $\nu_{13}$ | $\nu_{24}$ | $\nu_{12}$ | $\nu_{11}$ | $\nu_{10}$ | $\nu_{20}$ | $\nu_{17}$ |
|---|---|---|---|---|---|---|---|---|
| $N(n)^a$ | 10619 (9444) | 1510 (1468) | 2840 (1953) | 2838 (2806) | 2081(2076) | 764 (562) | 311 (304) | 275 (275) |
| $J_{max}$, $K_{amax}$ [b] | 88, 18 | 70, 10 | 87, 18 | 72, 17 | 72, 10 | 26, 7 | 51, 4 | 17, 6 |
| rms /$cm^{-1}$ | 0.00140 | 0.00033 | 0.00011 | 0.00021 | 0.00032 | 0.00075 | 0.00070 | 0.00302 |
| $\sigma^c$ | 1.16 | 1.54 | 1.08 | 1.02 | 1.04 | 1.50 | 0.73 | 1.01 |

[a] Number of lines ($N$) and number of different frequencies ($n$) considered in the fit (this number may differ from the number of assigned transitions, see text)
[b] Upper state values except in the column “Total" where the ground state values are reported [c] Reduced standard deviation (unitless)

**Table S4.** Transitions from the literature for which the estimated uncertainty was increased. The value used in this work is reported in the "Unc." column. Reference to the experimental measurement is also indicated.

| Band | $J'$ | $K'_a$ | $K'_c$ | $J''$ | $K''_a$ | $K''_c$ | Freq. | Unc. | Ref. |
|---|---|---|---|---|---|---|---|---|---|
| $\nu_{13}$ | 48 | 6 | 42 | 49 | 7 | 42 | 131.502667 | 0.002 | [3] |
| $\nu_{13}$ | 35 | 3 | 32 | 35 | 2 | 34 | 171.462708 | 0.002 | [3] |
| $\nu_{13}$ | 7 | 6 | 1 | 6 | 5 | 1 | 176.513082 | 0.002 | [3] |
| $\nu_{13}$ | 29 | 5 | 25 | 28 | 4 | 25 | 180.853477 | 0.002 | [3] |
| $\nu_{13}$ | 30 | 5 | 26 | 29 | 4 | 26 | 181.143133 | 0.002 | [3] |
| $\nu_{13}$ | 63 | 9 | 54 | 62 | 8 | 54 | 198.520900 | 0.002 | [3] |
| $\nu_{12}$ | 30 | 0 | 30 | 31 | 1 | 30 | 509.759518 | 0.002 | [3] |
| $\nu_{12}$ | 33 | 3 | 31 | 32 | 2 | 31 | 541.217248 | 0.002 | [3] |
| $\nu_{12}$ | 58 | 5 | 53 | 57 | 4 | 53 | 549.323537 | 0.002 | [3] |
| $\nu_{12}$ | 56 | 12 | 44 | 55 | 11 | 44 | 568.615349 | 0.002 | [3] |
| $\nu_{11}$ | 65 | 4 | 62 | 66 | 5 | 62 | 876.337884 | 0.003 | [4] |
| $\nu_{11}$ | 48 | 0 | 48 | 47 | 1 | 46 | 909.847553 | 0.003 | [4] |
| $\nu_{11}$ | 44 | 0 | 44 | 43 | 1 | 42 | 909.920503 | 0.003 | [4] |
| $\nu_{20}$ | 37 | 3 | 35 | 36 | 3 | 34 | 1606.419508 | 0.07 | [4] |
| $\nu_{20}$ | 38 | 3 | 36 | 37 | 3 | 35 | 1606.679400 | 0.07 | [4] |
| $\nu_{20}$ | 39 | 3 | 37 | 38 | 3 | 36 | 1606.939468 | 0.07 | [4] |

## 3. LISTS OF ASSIGNED TRANSITIONS

All lists are reproduced in the following format:
$J'\ K_a'\ K_c'\ J''\ K_a''\ K_c''$ wavenumber uncertainty
(wavenumber and uncertainty in $cm^{-1}$)

Below are reported the first 100 lines of each list (by frequency order), the full lists are reported as electronic files.

### A. $\nu_{24}$ band

#### A.1. Assigned and fitted transitions on the room temperature spectrum

The full list can be found in the file `trans_butadiene_lin.txt` where $\nu_{24} = 1$ is coded at $v = 5$.

| | | | |
|---|---|---|---|
| 87 1 86 | 88 1 87 | 273.381097 | 0.0001 |
| 87 3 84 | 88 3 85 | 273.587850 | 0.0001 |
| 86 1 85 | 87 1 86 | 273.649241 | 0.0001 |
| 86 3 83 | 87 3 84 | 273.840097 | 0.0001 |
| 85 1 84 | 86 1 85 | 273.917131 | 0.0001 |
| 85 3 82 | 86 3 83 | 274.091812 | 0.0001 |
| 84 1 83 | 85 1 84 | 274.185065 | 0.0001 |
| 84 3 81 | 85 3 82 | 274.343286 | 0.0001 |
| 83 1 82 | 84 1 83 | 274.453095 | 0.0001 |
| 83 3 80 | 84 3 81 | 274.594412 | 0.0001 |
| 82 1 81 | 83 1 82 | 274.720822 | 0.0001 |
| 82 2 80 | 83 2 81 | 274.836181 | 0.0001 |
| 82 3 79 | 83 3 80 | 274.844949 | 0.0001 |
| 81 1 80 | 82 1 81 | 274.988684 | 0.0001 |
| 81 3 78 | 82 3 79 | 275.095212 | 0.0001 |
| 81 2 79 | 82 2 80 | 275.096833 | 0.0001 |
| 80 1 79 | 81 1 80 | 275.256329 | 0.0001 |
| 80 3 77 | 81 3 78 | 275.344857 | 0.0001 |
| 80 2 78 | 81 2 79 | 275.357385 | 0.0001 |
| 79 1 78 | 80 1 79 | 275.524066 | 0.0001 |
| 79 3 76 | 80 3 77 | 275.593907 | 0.0001 |
| 79 2 77 | 80 2 78 | 275.618045 | 0.0001 |
| 78 1 77 | 79 1 78 | 275.791637 | 0.0001 |
| 78 3 75 | 79 3 76 | 275.842199 | 0.0001 |
| 78 2 76 | 79 2 77 | 275.878435 | 0.0001 |
| 77 1 76 | 78 1 77 | 276.059155 | 0.0001 |
| 77 3 74 | 78 3 75 | 276.090261 | 0.0001 |
| 77 2 75 | 78 2 76 | 276.138788 | 0.0001 |
| 76 1 75 | 77 1 76 | 276.326538 | 0.0001 |
| 76 3 73 | 77 3 74 | 276.337707 | 0.0001 |
| 76 2 74 | 77 2 75 | 276.398775 | 0.0001 |
| 75 3 72 | 76 3 73 | 276.584181 | 0.0001 |
| 75 2 73 | 76 2 74 | 276.658563 | 0.0001 |
| 74 3 71 | 75 3 72 | 276.830003 | 0.0001 |
| 74 2 72 | 75 2 73 | 276.918388 | 0.0001 |
| 73 3 70 | 74 3 71 | 277.075368 | 0.0001 |
| 73 2 71 | 74 2 72 | 277.177864 | 0.0001 |
| 72 3 69 | 73 3 70 | 277.319876 | 0.0001 |
| 72 2 70 | 73 2 71 | 277.437073 | 0.0001 |
| 71 3 68 | 72 3 69 | 277.564034 | 0.0001 |
| 71 1 70 | 72 1 71 | 277.662227 | 0.0001 |
| 71 2 69 | 72 2 70 | 277.696161 | 0.0001 |
| 70 3 67 | 71 3 68 | 277.807638 | 0.0001 |
| 84 11 73 | 85 11 74 | 277.922049 | 0.0001 |
| 70 1 69 | 71 1 70 | 277.929348 | 0.0001 |
| 70 2 68 | 71 2 69 | 277.954923 | 0.0001 |
| 69 3 66 | 70 3 67 | 278.050611 | 0.0001 |
| 69 1 68 | 70 1 69 | 278.196057 | 0.0001 |
| 83 11 72 | 84 11 73 | 278.204331 | 0.0001 |
| 69 2 67 | 70 2 68 | 278.213303 | 0.0001 |
| 68 3 65 | 69 3 66 | 278.293448 | 0.0001 |
| 68 1 67 | 69 1 68 | 278.462838 | 0.0001 |
| 68 2 66 | 69 2 67 | 278.471504 | 0.0001 |
| 82 11 71 | 83 11 72 | 278.486327 | 0.0001 |
| 67 3 64 | 68 3 65 | 278.536039 | 0.0001 |
| 67 1 66 | 68 1 67 | 278.729378 | 0.0001 |
| 67 2 65 | 68 2 66 | 278.729378 | 0.0001 |
| 81 11 70 | 82 11 71 | 278.768557 | 0.0001 |
| 66 3 63 | 67 3 64 | 278.778484 | 0.0001 |
| 66 2 64 | 67 2 65 | 278.986606 | 0.0001 |
| 66 1 65 | 67 1 66 | 278.995958 | 0.0001 |
| 65 3 62 | 66 3 63 | 279.021110 | 0.0001 |
| 80 11 69 | 81 11 70 | 279.050755 | 0.0001 |
| 65 2 63 | 66 2 64 | 279.243568 | 0.0001 |
| 65 1 64 | 66 1 65 | 279.262310 | 0.0001 |
| 79 11 68 | 80 11 69 | 279.332789 | 0.0001 |
| 64 2 62 | 65 2 63 | 279.500145 | 0.0001 |
| 63 3 60 | 64 3 61 | 279.508204 | 0.0001 |
| 64 1 63 | 65 1 64 | 279.528605 | 0.0001 |
| 78 11 67 | 79 11 68 | 279.614955 | 0.0001 |
| 62 3 59 | 63 3 60 | 279.752810 | 0.0001 |
| 63 2 61 | 64 2 62 | 279.756200 | 0.0001 |
| 63 1 62 | 64 1 63 | 279.794717 | 0.0001 |
| 77 11 66 | 78 11 67 | 279.896906 | 0.0001 |
| 61 3 58 | 62 3 59 | 279.998654 | 0.0001 |
| 62 2 60 | 63 2 61 | 280.011813 | 0.0001 |
| 62 1 61 | 63 1 62 | 280.060712 | 0.0001 |
| 76 11 65 | 77 11 66 | 280.179226 | 0.0001 |
| 60 3 57 | 61 3 58 | 280.245841 | 0.0001 |
| 61 2 59 | 62 2 60 | 280.266794 | 0.0001 |
| 61 1 60 | 62 1 61 | 280.326592 | 0.0001 |
| 59 3 56 | 60 3 57 | 280.494620 | 0.0001 |
| 60 2 58 | 61 2 59 | 280.521376 | 0.0001 |
| 60 1 59 | 61 1 60 | 280.592208 | 0.0001 |
| 74 11 63 | 75 11 64 | 280.743499 | 0.0001 |
| 58 3 55 | 59 3 56 | 280.745272 | 0.0001 |
| 59 2 57 | 60 2 58 | 280.775360 | 0.0001 |
| 59 1 58 | 60 1 59 | 280.857797 | 0.0001 |
| 57 3 54 | 58 3 55 | 280.997871 | 0.0001 |
| 73 11 62 | 74 11 63 | 281.025208 | 0.0001 |
| 58 2 56 | 59 2 57 | 281.028820 | 0.0001 |
| 58 1 57 | 59 1 58 | 281.123188 | 0.0001 |
| 56 3 53 | 57 3 54 | 281.252655 | 0.0001 |
| 57 2 55 | 58 2 56 | 281.281772 | 0.0001 |
| 72 11 61 | 73 11 62 | 281.307384 | 0.0001 |
| 57 1 56 | 58 1 57 | 281.388315 | 0.0001 |
| 55 3 52 | 56 3 53 | 281.509816 | 0.0001 |
| 56 2 54 | 57 2 55 | 281.534267 | 0.0001 |
| 71 11 60 | 72 11 61 | 281.589284 | 0.0001 |
| 56 1 55 | 57 1 56 | 281.653146 | 0.0001 |

### B. $\nu_{10}$ band

#### B.1. Assigned and fitted transitions from the Jet-AILES spectrum

The full list can be found in the file `trans_butadiene_lin.txt` where $\nu_{10} = 1$ is coded at $v = 6$.

| | | | |
|---|---|---|---|
| 11 7 4 | 12 8 4 | 991.253455 | 0.0005 |
| 11 7 5 | 12 8 5 | 991.253455 | 0.0005 |
| 18 6 12 | 19 7 12 | 992.110766 | 0.0005 |
| 18 6 13 | 19 7 13 | 992.110766 | 0.0005 |
| 17 6 11 | 18 7 11 | 992.339372 | 0.0005 |
| 17 6 12 | 18 7 12 | 992.339372 | 0.0005 |
| 15 6 9 | 16 7 9 | 992.804081 | 0.0005 |
| 15 6 10 | 16 7 10 | 992.804081 | 0.0005 |
| 14 6 8 | 15 7 8 | 993.041078 | 0.0005 |
| 14 6 9 | 15 7 9 | 993.041078 | 0.0005 |
| 13 6 7 | 14 7 7 | 993.279740 | 0.0005 |
| 13 6 8 | 14 7 8 | 993.279740 | 0.0005 |
| 12 6 6 | 13 7 6 | 993.521450 | 0.0005 |
| 12 6 7 | 13 7 7 | 993.521450 | 0.0005 |
| 11 6 5 | 12 7 5 | 993.765834 | 0.0005 |
| 11 6 6 | 12 7 6 | 993.765834 | 0.0005 |
| 21 5 16 | 22 6 16 | 993.882154 | 0.0005 |
| 21 5 17 | 22 6 17 | 993.882154 | 0.0005 |
| 10 6 4 | 11 7 4 | 994.013307 | 0.0005 |
| 10 6 5 | 11 7 5 | 994.013307 | 0.0005 |
| 20 5 15 | 21 6 15 | 994.111527 | 0.0005 |
| 20 5 16 | 21 6 16 | 994.111527 | 0.0005 |
| 9 6 3 | 10 7 3 | 994.263384 | 0.0005 |
| 9 6 4 | 10 7 4 | 994.263384 | 0.0005 |
| 19 5 14 | 20 6 14 | 994.344398 | 0.0005 |
| 19 5 15 | 20 6 15 | 994.344398 | 0.0005 |
| 8 6 2 | 9 7 2 | 994.516495 | 0.0005 |
| 8 6 3 | 9 7 3 | 994.516495 | 0.0005 |
| 18 5 13 | 19 6 13 | 994.579972 | 0.0005 |
| 18 5 14 | 19 6 14 | 994.579972 | 0.0005 |
| 7 6 1 | 8 7 1 | 994.772359 | 0.0005 |
| 7 6 2 | 8 7 2 | 994.772359 | 0.0005 |
| 17 5 12 | 18 6 12 | 994.816881 | 0.0005 |

| | | | | | |
|---|---|---|---|---|---|
| 17 | 5 13 | 18 | 6 13 | 994.816881 | 0.0005 |
| 6 | 6 0 | 7 | 7 0 | 995.031393 | 0.0005 |
| 6 | 6 1 | 7 | 7 1 | 995.031393 | 0.0005 |
| 16 | 5 11 | 17 | 6 11 | 995.056420 | 0.0005 |
| 16 | 5 12 | 17 | 6 12 | 995.056420 | 0.0005 |
| 15 | 5 10 | 16 | 6 10 | 995.298486 | 0.0005 |
| 15 | 5 11 | 16 | 6 11 | 995.298486 | 0.0005 |
| 14 | 5 9 | 15 | 6 9 | 995.542415 | 0.0005 |
| 14 | 5 10 | 15 | 6 10 | 995.542415 | 0.0005 |
| 13 | 5 8 | 14 | 6 8 | 995.789088 | 0.0005 |
| 13 | 5 9 | 14 | 6 9 | 995.789088 | 0.0005 |
| 12 | 5 7 | 13 | 6 7 | 996.038005 | 0.0005 |
| 12 | 5 8 | 13 | 6 8 | 996.038005 | 0.0005 |
| 11 | 5 6 | 12 | 6 6 | 996.289015 | 0.0005 |
| 11 | 5 7 | 12 | 6 7 | 996.289015 | 0.0005 |
| 10 | 5 5 | 11 | 6 5 | 996.543367 | 0.0005 |
| 10 | 5 6 | 11 | 6 6 | 996.543367 | 0.0005 |
| 9 | 5 4 | 10 | 6 4 | 996.799269 | 0.0005 |
| 9 | 5 5 | 10 | 6 5 | 996.799269 | 0.0005 |
| 8 | 5 3 | 9 | 6 3 | 997.058117 | 0.0005 |
| 8 | 5 4 | 9 | 6 4 | 997.058117 | 0.0005 |
| 7 | 5 2 | 8 | 6 2 | 997.319480 | 0.0005 |
| 7 | 5 3 | 8 | 6 3 | 997.319480 | 0.0005 |
| 6 | 5 1 | 7 | 6 1 | 997.583082 | 0.0005 |
| 6 | 5 2 | 7 | 6 2 | 997.583082 | 0.0005 |
| 5 | 5 0 | 6 | 6 0 | 997.849521 | 0.0005 |
| 5 | 5 1 | 6 | 6 1 | 997.849521 | 0.0005 |
| 11 | 4 7 | 12 | 5 7 | 998.811822 | 0.0005 |
| 11 | 4 8 | 12 | 5 8 | 998.811822 | 0.0005 |
| 10 | 4 6 | 11 | 5 6 | 999.069676 | 0.0005 |
| 10 | 4 7 | 11 | 5 7 | 999.069676 | 0.0005 |
| 9 | 4 5 | 10 | 5 5 | 999.329570 | 0.0005 |
| 9 | 4 6 | 10 | 5 6 | 999.329570 | 0.0005 |
| 8 | 4 4 | 9 | 5 4 | 999.591535 | 0.0005 |
| 8 | 4 5 | 9 | 5 5 | 999.591535 | 0.0005 |
| 9 | 5 4 | 9 | 6 4 | 999.616063 | 0.0005 |
| 9 | 5 5 | 9 | 6 3 | 999.616063 | 0.0005 |
| 18 | 3 15 | 19 | 4 15 | 999.628566 | 0.0005 |
| 10 | 5 5 | 10 | 6 5 | 999.641418 | 0.0005 |
| 10 | 5 6 | 10 | 6 4 | 999.641418 | 0.0005 |
| 11 | 5 6 | 11 | 6 6 | 999.669757 | 0.0005 |
| 11 | 5 7 | 11 | 6 5 | 999.669757 | 0.0005 |
| 12 | 5 7 | 12 | 6 7 | 999.699703 | 0.0005 |
| 12 | 5 8 | 12 | 6 6 | 999.699703 | 0.0005 |
| 13 | 5 8 | 13 | 6 8 | 999.732478 | 0.0005 |
| 13 | 5 9 | 13 | 6 7 | 999.732478 | 0.0005 |
| 15 | 5 10 | 15 | 6 10 | 999.806160 | 0.0005 |
| 15 | 5 11 | 15 | 6 9 | 999.806160 | 0.0005 |
| 16 | 5 11 | 16 | 6 11 | 999.846246 | 0.0005 |
| 16 | 5 12 | 16 | 6 10 | 999.846246 | 0.0005 |
| 7 | 4 3 | 8 | 5 3 | 999.855708 | 0.0005 |
| 7 | 4 4 | 8 | 5 4 | 999.855708 | 0.0005 |
| 17 | 3 14 | 18 | 4 14 | 999.860482 | 0.0005 |
| 17 | 5 12 | 17 | 6 12 | 999.888650 | 0.0005 |
| 17 | 5 13 | 17 | 6 11 | 999.888650 | 0.0005 |
| 18 | 5 13 | 18 | 6 13 | 999.934058 | 0.0005 |
| 18 | 5 14 | 18 | 6 12 | 999.934058 | 0.0005 |
| 19 | 5 14 | 19 | 6 14 | 999.980921 | 0.0005 |
| 19 | 5 15 | 19 | 6 13 | 999.980921 | 0.0005 |
| 20 | 5 15 | 20 | 6 15 | 1000.030720 | 0.0005 |
| 20 | 5 16 | 20 | 6 14 | 1000.030720 | 0.0005 |
| 16 | 3 13 | 17 | 4 13 | 1000.097790 | 0.0005 |
| 6 | 4 2 | 7 | 5 2 | 1000.121710 | 0.0005 |
| 6 | 4 3 | 7 | 5 3 | 1000.121710 | 0.0005 |
| 15 | 3 13 | 16 | 4 13 | 1000.322940 | 0.0005 |
| 5 | 4 1 | 6 | 5 1 | 1000.390280 | 0.0005 |
| 5 | 4 2 | 6 | 5 2 | 1000.390280 | 0.0005 |

### *B.2. Additional lines assigned in the Jet-AILES spectrum (unfitted)*

The full list of transitions excluded from the fit is reported here in the following format:
$J'\ K'_a\ K'_c\ J''\ K''_a\ K''_c$ wavenumber uncertainty
(wavenumber and uncertainty in $cm^{-1}$)

| | | | | | |
|---|---|---|---|---|---|
| 14 | 7 7 | 15 | 8 7 | 990.574036 | 0.0005 |
| 14 | 7 8 | 15 | 8 8 | 990.574036 | 0.0005 |
| 12 | 7 5 | 13 | 8 5 | 991.023893 | 0.0005 |
| 12 | 7 6 | 13 | 8 6 | 991.023893 | 0.0005 |
| 10 | 7 3 | 11 | 8 3 | 991.486854 | 0.0005 |
| 10 | 7 4 | 11 | 8 4 | 991.486854 | 0.0005 |
| 9 | 7 2 | 10 | 8 2 | 991.723093 | 0.0005 |
| 9 | 7 3 | 10 | 8 3 | 991.723093 | 0.0005 |
| 7 | 7 0 | 8 | 8 0 | 992.207873 | 0.0005 |
| 7 | 7 1 | 8 | 8 1 | 992.207873 | 0.0005 |
| 18 | 4 14 | 19 | 5 14 | 997.020643 | 0.0005 |
| 17 | 4 13 | 18 | 5 13 | 997.287492 | 0.0005 |
| 17 | 4 14 | 18 | 5 14 | 997.287492 | 0.0005 |
| 16 | 4 12 | 17 | 5 12 | 997.543715 | 0.0005 |
| 16 | 4 13 | 17 | 5 13 | 997.543715 | 0.0005 |
| 15 | 4 11 | 16 | 5 11 | 997.797170 | 0.0005 |
| 15 | 4 12 | 16 | 5 12 | 997.797170 | 0.0005 |
| 14 | 4 10 | 15 | 5 10 | 998.049117 | 0.0005 |
| 14 | 4 11 | 15 | 5 11 | 998.049117 | 0.0005 |
| 13 | 4 9 | 14 | 5 9 | 998.301750 | 0.0005 |
| 13 | 4 10 | 14 | 5 10 | 998.301750 | 0.0005 |
| 12 | 4 8 | 13 | 5 8 | 998.555949 | 0.0005 |
| 12 | 4 9 | 13 | 5 9 | 998.555949 | 0.0005 |
| 12 | 4 8 | 12 | 5 8 | 1002.218440 | 0.0005 |
| 12 | 4 9 | 12 | 5 7 | 1002.218440 | 0.0005 |
| 13 | 4 9 | 13 | 5 9 | 1002.246310 | 0.0005 |
| 13 | 4 10 | 13 | 5 8 | 1002.246310 | 0.0005 |
| 14 | 4 10 | 14 | 5 10 | 1002.275860 | 0.0005 |
| 14 | 4 11 | 14 | 5 9 | 1002.275860 | 0.0005 |
| 19 | 2 17 | 20 | 3 17 | 1002.297620 | 0.0005 |
| 15 | 4 11 | 15 | 5 11 | 1002.305550 | 0.0005 |
| 15 | 4 12 | 15 | 5 10 | 1002.305550 | 0.0005 |
| 16 | 4 12 | 16 | 5 12 | 1002.334540 | 0.0005 |
| 16 | 4 13 | 16 | 5 11 | 1002.334540 | 0.0005 |
| 17 | 4 13 | 17 | 5 13 | 1002.360690 | 0.0005 |
| 17 | 4 14 | 17 | 5 12 | 1002.360690 | 0.0005 |
| 18 | 2 16 | 19 | 3 16 | 1002.470700 | 0.0005 |
| 17 | 3 15 | 17 | 4 13 | 1004.904400 | 0.0005 |
| 18 | 3 16 | 18 | 4 14 | 1004.942270 | 0.0005 |
| 19 | 3 17 | 19 | 4 15 | 1004.982560 | 0.0005 |
| 18 | 3 15 | 18 | 4 15 | 1004.989480 | 0.0005 |
| 20 | 3 18 | 20 | 4 16 | 1005.024230 | 0.0005 |
| 19 | 3 16 | 19 | 4 16 | 1005.046270 | 0.0005 |
| 13 | 1 13 | 14 | 2 13 | 1005.109580 | 0.0005 |
| 22 | 3 20 | 22 | 4 18 | 1005.109580 | 0.0005 |
| 23 | 3 21 | 23 | 4 19 | 1005.152320 | 0.0005 |
| 17 | 2 15 | 17 | 3 15 | 1007.763860 | 0.0005 |
| 18 | 2 16 | 18 | 3 16 | 1007.879120 | 0.0005 |
| 19 | 2 17 | 19 | 3 17 | 1008.004010 | 0.0005 |
| 20 | 2 18 | 20 | 3 18 | 1008.136370 | 0.0005 |
| 19 | 2 17 | 20 | 1 19 | 1011.203580 | 0.0005 |
| 18 | 2 16 | 19 | 1 18 | 1011.441510 | 0.0005 |
| 17 | 2 15 | 18 | 1 17 | 1011.691360 | 0.0005 |
| 24 | 0 24 | 24 | 1 24 | 1013.426480 | 0.0005 |
| 25 | 0 25 | 25 | 1 25 | 1013.466850 | 0.0005 |
| 26 | 0 26 | 26 | 1 26 | 1013.504110 | 0.0005 |
| 27 | 0 27 | 27 | 1 27 | 1013.539230 | 0.0005 |
| 28 | 0 28 | 28 | 1 28 | 1013.572300 | 0.0005 |
| 29 | 0 29 | 29 | 1 29 | 1013.603200 | 0.0005 |
| 24 | 1 24 | 24 | 0 24 | 1013.809240 | 0.0005 |
| 23 | 1 23 | 23 | 0 23 | 1013.823930 | 0.0005 |
| 22 | 1 22 | 22 | 0 22 | 1013.842510 | 0.0005 |
| 13 | 3 10 | 14 | 2 12 | 1015.666260 | 0.0005 |
| 22 | 2 21 | 22 | 1 21 | 1015.882610 | 0.0005 |
| 17 | 2 15 | 17 | 1 17 | 1018.998880 | 0.0005 |
| 25 | 3 23 | 25 | 2 23 | 1019.087220 | 0.0005 |
| 24 | 3 22 | 24 | 2 22 | 1019.174020 | 0.0005 |
| 21 | 3 19 | 21 | 2 19 | 1019.391020 | 0.0005 |
| 20 | 3 18 | 20 | 2 18 | 1019.447710 | 0.0005 |
| 19 | 3 17 | 19 | 2 17 | 1019.496920 | 0.0005 |
| 18 | 3 16 | 18 | 2 16 | 1019.538420 | 0.0005 |
| 17 | 3 15 | 17 | 2 15 | 1019.572640 | 0.0005 |
| 8 | 4 4 | 9 | 3 6 | 1019.577070 | 0.0005 |
| 19 | 2 17 | 19 | 1 19 | 1019.577070 | 0.0005 |
| 16 | 3 14 | 16 | 2 14 | 1019.599950 | 0.0005 |
| 18 | 3 15 | 18 | 2 17 | 1020.118440 | 0.0005 |
| 19 | 3 16 | 19 | 2 18 | 1020.206640 | 0.0005 |
| 20 | 3 17 | 20 | 2 19 | 1020.307140 | 0.0005 |
| 22 | 3 19 | 22 | 2 21 | 1020.546500 | 0.0005 |
| 23 | 3 20 | 23 | 2 22 | 1020.686240 | 0.0005 |
| 17 | 2 15 | 16 | 1 15 | 1021.731470 | 0.0005 |
| 18 | 2 16 | 17 | 1 16 | 1022.046060 | 0.0005 |
| 12 | 4 9 | 12 | 3 9 | 1022.196510 | 0.0005 |
| 13 | 4 10 | 13 | 3 10 | 1022.220000 | 0.0005 |
| 13 | 4 9 | 13 | 3 11 | 1022.225020 | 0.0005 |
| 14 | 4 11 | 14 | 3 11 | 1022.243210 | 0.0005 |
| 14 | 4 10 | 14 | 3 12 | 1022.251390 | 0.0005 |
| 15 | 4 12 | 15 | 3 12 | 1022.265620 | 0.0005 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 17 | 4 | 14 | 17 | 3 | 14 | 1022.298830 | 0.0005 |
| 19 | 2 | 17 | 18 | 1 | 17 | 1022.370900 | 0.0005 |
| 20 | 2 | 18 | 19 | 1 | 18 | 1022.703510 | 0.0005 |
| 17 | 3 | 14 | 16 | 2 | 14 | 1024.462370 | 0.0005 |
| 18 | 3 | 15 | 17 | 2 | 15 | 1024.732760 | 0.0005 |
| 19 | 3 | 16 | 18 | 2 | 16 | 1024.999570 | 0.0005 |
| 18 | 3 | 16 | 17 | 2 | 16 | 1025.122720 | 0.0005 |
| 20 | 3 | 17 | 19 | 2 | 17 | 1025.263080 | 0.0005 |
| 22 | 2 | 21 | 21 | 1 | 21 | 1025.359170 | 0.0005 |
| 19 | 3 | 17 | 18 | 2 | 17 | 1025.472060 | 0.0005 |
| 21 | 3 | 18 | 20 | 2 | 18 | 1025.526020 | 0.0005 |
| 13 | 4 | 9 | 12 | 3 | 9 | 1025.887130 | 0.0005 |
| 13 | 4 | 10 | 12 | 3 | 10 | 1025.887130 | 0.0005 |
| 14 | 4 | 10 | 13 | 3 | 10 | 1026.194060 | 0.0005 |
| 14 | 4 | 11 | 13 | 3 | 11 | 1026.198880 | 0.0005 |
| 24 | 2 | 23 | 23 | 1 | 23 | 1026.306700 | 0.0005 |
| 15 | 4 | 11 | 14 | 3 | 11 | 1026.499950 | 0.0005 |
| 15 | 4 | 12 | 14 | 3 | 12 | 1026.507500 | 0.0005 |
| 22 | 3 | 20 | 21 | 2 | 20 | 1026.562000 | 0.0005 |
| 23 | 3 | 21 | 22 | 2 | 21 | 1026.938090 | 0.0005 |
| 17 | 4 | 13 | 16 | 3 | 13 | 1027.101830 | 0.0005 |
| 18 | 4 | 14 | 17 | 3 | 14 | 1027.388220 | 0.0005 |
| 7 | 7 | 0 | 7 | 6 | 2 | 1029.429890 | 0.0005 |
| 7 | 7 | 1 | 7 | 6 | 1 | 1029.429890 | 0.0005 |
| 8 | 7 | 1 | 8 | 6 | 3 | 1029.466880 | 0.0005 |
| 8 | 7 | 2 | 8 | 6 | 2 | 1029.466880 | 0.0005 |
| 9 | 7 | 2 | 9 | 6 | 4 | 1029.507230 | 0.0005 |
| 9 | 7 | 3 | 9 | 6 | 3 | 1029.507230 | 0.0005 |
| 10 | 7 | 3 | 10 | 6 | 5 | 1029.552100 | 0.0005 |
| 10 | 7 | 4 | 10 | 6 | 4 | 1029.552100 | 0.0005 |
| 13 | 7 | 6 | 13 | 6 | 8 | 1029.708350 | 0.0005 |
| 13 | 7 | 7 | 13 | 6 | 7 | 1029.708350 | 0.0005 |
| 14 | 7 | 7 | 14 | 6 | 9 | 1029.766060 | 0.0005 |
| 14 | 7 | 8 | 14 | 6 | 8 | 1029.766060 | 0.0005 |
| 15 | 7 | 8 | 15 | 6 | 10 | 1029.826540 | 0.0005 |
| 15 | 7 | 9 | 15 | 6 | 9 | 1029.826540 | 0.0005 |
| 16 | 7 | 9 | 16 | 6 | 11 | 1029.889820 | 0.0005 |
| 16 | 7 | 10 | 16 | 6 | 10 | 1029.889820 | 0.0005 |
| 17 | 7 | 10 | 17 | 6 | 12 | 1029.954640 | 0.0005 |
| 17 | 7 | 11 | 17 | 6 | 11 | 1029.954640 | 0.0005 |
| 18 | 7 | 11 | 18 | 6 | 13 | 1030.021240 | 0.0005 |
| 18 | 7 | 12 | 18 | 6 | 12 | 1030.021240 | 0.0005 |
| 19 | 7 | 12 | 19 | 6 | 14 | 1030.091550 | 0.0005 |
| 19 | 7 | 13 | 19 | 6 | 13 | 1030.091550 | 0.0005 |
| 20 | 7 | 13 | 20 | 6 | 15 | 1030.162590 | 0.0005 |
| 20 | 7 | 14 | 20 | 6 | 14 | 1030.162590 | 0.0005 |
| 22 | 5 | 17 | 21 | 4 | 17 | 1031.283970 | 0.0005 |
| 7 | 7 | 0 | 6 | 6 | 0 | 1031.400880 | 0.0005 |
| 7 | 7 | 1 | 6 | 6 | 1 | 1031.400880 | 0.0005 |
| 8 | 7 | 1 | 7 | 6 | 1 | 1031.719890 | 0.0005 |
| 8 | 7 | 2 | 7 | 6 | 2 | 1031.719890 | 0.0005 |
| 9 | 7 | 2 | 8 | 6 | 2 | 1032.042970 | 0.0005 |
| 9 | 7 | 3 | 8 | 6 | 3 | 1032.042970 | 0.0005 |
| 10 | 7 | 3 | 9 | 6 | 3 | 1032.369460 | 0.0005 |
| 10 | 7 | 4 | 9 | 6 | 4 | 1032.369460 | 0.0005 |
| 12 | 7 | 5 | 11 | 6 | 5 | 1033.032860 | 0.0005 |
| 12 | 7 | 6 | 11 | 6 | 6 | 1033.032860 | 0.0005 |
| 13 | 7 | 6 | 12 | 6 | 6 | 1033.369770 | 0.0005 |
| 13 | 7 | 7 | 12 | 6 | 7 | 1033.369770 | 0.0005 |
| 14 | 7 | 7 | 13 | 6 | 7 | 1033.709920 | 0.0005 |
| 14 | 7 | 8 | 13 | 6 | 8 | 1033.709920 | 0.0005 |
| 15 | 7 | 8 | 14 | 6 | 8 | 1034.052200 | 0.0005 |
| 15 | 7 | 9 | 14 | 6 | 9 | 1034.052200 | 0.0005 |
| 16 | 7 | 9 | 15 | 6 | 9 | 1034.397040 | 0.0005 |
| 16 | 7 | 10 | 15 | 6 | 10 | 1034.397040 | 0.0005 |
| 17 | 7 | 10 | 16 | 6 | 10 | 1034.744360 | 0.0005 |
| 17 | 7 | 11 | 16 | 6 | 11 | 1034.744360 | 0.0005 |
| 19 | 7 | 12 | 18 | 6 | 12 | 1035.444720 | 0.0005 |
| 19 | 7 | 13 | 18 | 6 | 13 | 1035.444720 | 0.0005 |
| 20 | 7 | 13 | 19 | 6 | 13 | 1035.799460 | 0.0005 |
| 20 | 7 | 14 | 19 | 6 | 14 | 1035.799460 | 0.0005 |
| 21 | 7 | 14 | 20 | 6 | 14 | 1036.153760 | 0.0005 |
| 21 | 7 | 15 | 20 | 6 | 15 | 1036.153760 | 0.0005 |
| 22 | 7 | 15 | 21 | 6 | 15 | 1036.510630 | 0.0005 |
| 22 | 7 | 16 | 21 | 6 | 16 | 1036.510630 | 0.0005 |

### *B.3. Assigned transitions in the warm CLS spectrum (unfitted)*

The full list can be found in the file:
`trans_butadiene_nu10_AssignedCLS_lin.txt`

where $v_{10} = 1$ is coded at $v = 6$.

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 7 | 0 | 7 | 8 | 1 | 7 | 1009.648040 | 0.0002 |
| 8 | 0 | 8 | 9 | 1 | 8 | 1009.308150 | 0.0002 |
| 9 | 0 | 9 | 10 | 1 | 9 | 1008.959280 | 0.0002 |
| 11 | 0 | 11 | 12 | 1 | 11 | 1008.229940 | 0.0002 |
| 12 | 0 | 12 | 13 | 1 | 12 | 1007.848580 | 0.0002 |
| 13 | 0 | 13 | 14 | 1 | 13 | 1007.454390 | 0.0002 |
| 14 | 0 | 14 | 15 | 1 | 14 | 1007.047010 | 0.0002 |
| 15 | 0 | 15 | 16 | 1 | 15 | 1006.626690 | 0.0002 |
| 16 | 0 | 16 | 17 | 1 | 16 | 1006.191460 | 0.0002 |
| 17 | 0 | 17 | 18 | 1 | 17 | 1005.742730 | 0.0002 |
| 18 | 0 | 18 | 19 | 1 | 18 | 1005.279640 | 0.0002 |
| 19 | 0 | 19 | 20 | 1 | 19 | 1004.803090 | 0.0002 |
| 20 | 0 | 20 | 21 | 1 | 20 | 1004.312970 | 0.0002 |
| 21 | 0 | 21 | 22 | 1 | 21 | 1003.810180 | 0.0002 |
| 24 | 0 | 24 | 25 | 1 | 24 | 1002.237610 | 0.0002 |
| 25 | 0 | 25 | 26 | 1 | 25 | 1001.696170 | 0.0002 |
| 26 | 0 | 26 | 27 | 1 | 26 | 1001.147820 | 0.0002 |
| 27 | 0 | 27 | 28 | 1 | 27 | 1000.593550 | 0.0002 |
| 6 | 0 | 6 | 6 | 1 | 6 | 1012.296550 | 0.0002 |
| 7 | 0 | 7 | 7 | 1 | 7 | 1012.352500 | 0.0002 |
| 8 | 0 | 8 | 8 | 1 | 8 | 1012.413040 | 0.0002 |
| 9 | 0 | 9 | 9 | 1 | 9 | 1012.478440 | 0.0002 |
| 10 | 0 | 10 | 10 | 1 | 10 | 1012.547490 | 0.0002 |
| 11 | 0 | 11 | 11 | 1 | 11 | 1012.619370 | 0.0002 |
| 12 | 0 | 12 | 12 | 1 | 12 | 1012.692660 | 0.0002 |
| 13 | 0 | 13 | 13 | 1 | 13 | 1012.766540 | 0.0002 |
| 14 | 0 | 14 | 14 | 1 | 14 | 1012.840110 | 0.0002 |
| 15 | 0 | 15 | 15 | 1 | 15 | 1012.912380 | 0.0002 |
| 16 | 0 | 16 | 16 | 1 | 16 | 1012.982450 | 0.0002 |
| 17 | 0 | 17 | 17 | 1 | 17 | 1013.050560 | 0.0002 |
| 18 | 0 | 18 | 18 | 1 | 18 | 1013.114750 | 0.0002 |
| 19 | 0 | 19 | 19 | 1 | 19 | 1013.175330 | 0.0002 |
| 20 | 0 | 20 | 20 | 1 | 20 | 1013.233010 | 0.0002 |
| 21 | 0 | 21 | 21 | 1 | 21 | 1013.286840 | 0.0002 |
| 22 | 0 | 22 | 22 | 1 | 22 | 1013.336430 | 0.0002 |
| 23 | 0 | 23 | 23 | 1 | 23 | 1013.382570 | 0.0002 |
| 24 | 0 | 24 | 24 | 1 | 24 | 1013.426390 | 0.0002 |
| 25 | 0 | 25 | 25 | 1 | 25 | 1013.466570 | 0.0002 |
| 26 | 0 | 26 | 26 | 1 | 26 | 1013.503690 | 0.0002 |
| 27 | 0 | 27 | 27 | 1 | 27 | 1013.538760 | 0.0002 |
| 28 | 0 | 28 | 28 | 1 | 28 | 1013.571370 | 0.0002 |
| 29 | 0 | 29 | 29 | 1 | 29 | 1013.602480 | 0.0002 |
| 30 | 0 | 30 | 30 | 1 | 30 | 1013.631980 | 0.0002 |
| 32 | 0 | 32 | 32 | 1 | 32 | 1013.687460 | 0.0002 |
| 33 | 0 | 33 | 33 | 1 | 33 | 1013.713990 | 0.0002 |
| 34 | 0 | 34 | 34 | 1 | 34 | 1013.739170 | 0.0002 |
| 35 | 0 | 35 | 35 | 1 | 35 | 1013.764050 | 0.0002 |
| 37 | 0 | 37 | 37 | 1 | 37 | 1013.813410 | 0.0002 |
| 38 | 0 | 38 | 38 | 1 | 38 | 1013.837460 | 0.0002 |
| 39 | 0 | 39 | 39 | 1 | 39 | 1013.862020 | 0.0002 |
| 9 | 1 | 8 | 10 | 2 | 8 | 1007.171500 | 0.0002 |
| 10 | 1 | 9 | 11 | 2 | 9 | 1006.958730 | 0.0002 |
| 12 | 1 | 11 | 13 | 2 | 11 | 1006.533940 | 0.0002 |
| 13 | 1 | 12 | 14 | 2 | 12 | 1006.319790 | 0.0002 |
| 14 | 1 | 13 | 15 | 2 | 13 | 1006.102940 | 0.0002 |
| 15 | 1 | 14 | 16 | 2 | 14 | 1005.881660 | 0.0002 |
| 17 | 1 | 16 | 18 | 2 | 16 | 1005.419750 | 0.0002 |
| 18 | 1 | 17 | 19 | 2 | 17 | 1005.177550 | 0.0002 |
| 19 | 1 | 18 | 20 | 2 | 18 | 1004.925550 | 0.0002 |
| 20 | 1 | 19 | 21 | 2 | 19 | 1004.663100 | 0.0002 |
| 21 | 1 | 20 | 22 | 2 | 20 | 1004.388500 | 0.0002 |
| 22 | 1 | 21 | 23 | 2 | 21 | 1004.101340 | 0.0002 |
| 23 | 1 | 22 | 24 | 2 | 22 | 1003.800600 | 0.0002 |
| 24 | 1 | 23 | 25 | 2 | 23 | 1003.486330 | 0.0002 |
| 25 | 1 | 24 | 26 | 2 | 24 | 1003.155700 | 0.0002 |
| 26 | 1 | 25 | 27 | 2 | 25 | 1002.810550 | 0.0002 |
| 27 | 1 | 26 | 28 | 2 | 26 | 1002.448500 | 0.0002 |
| 28 | 1 | 27 | 29 | 2 | 27 | 1002.069920 | 0.0002 |
| 29 | 1 | 28 | 30 | 2 | 28 | 1001.673920 | 0.0002 |
| 30 | 1 | 29 | 31 | 2 | 29 | 1001.260740 | 0.0002 |
| 31 | 1 | 30 | 32 | 2 | 30 | 1000.830730 | 0.0002 |
| 32 | 1 | 31 | 33 | 2 | 31 | 1000.383800 | 0.0002 |
| 34 | 1 | 33 | 35 | 2 | 33 | 999.440171 | 0.0002 |
| 36 | 1 | 35 | 37 | 2 | 35 | 998.436977 | 0.0002 |
| 37 | 1 | 36 | 38 | 2 | 36 | 997.914997 | 0.0002 |
| 38 | 1 | 37 | 39 | 2 | 37 | 997.381285 | 0.0002 |
| 39 | 1 | 38 | 40 | 2 | 38 | 996.836785 | 0.0002 |
| 40 | 1 | 39 | 41 | 2 | 39 | 996.282122 | 0.0002 |
| 41 | 1 | 40 | 42 | 2 | 40 | 995.719652 | 0.0002 |
| 9 | 1 | 8 | 9 | 2 | 8 | 1010.043290 | 0.0002 |
| 10 | 1 | 9 | 10 | 2 | 9 | 1010.136520 | 0.0002 |
| 11 | 1 | 10 | 11 | 2 | 10 | 1010.237740 | 0.0002 |
| 12 | 1 | 11 | 12 | 2 | 11 | 1010.347330 | 0.0002 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 13 | 1 | 12 | 13 | 2 | 12 | 1010.464750 | 0.0002 |
| 14 | 1 | 13 | 14 | 2 | 13 | 1010.589600 | 0.0002 |
| 15 | 1 | 14 | 15 | 2 | 14 | 1010.721510 | 0.0002 |
| 16 | 1 | 15 | 16 | 2 | 15 | 1010.859340 | 0.0002 |
| 18 | 1 | 17 | 18 | 2 | 17 | 1011.152460 | 0.0002 |
| 19 | 1 | 18 | 19 | 2 | 18 | 1011.306260 | 0.0002 |
| 20 | 1 | 19 | 20 | 2 | 19 | 1011.463830 | 0.0002 |
| 21 | 1 | 20 | 21 | 2 | 20 | 1011.624100 | 0.0002 |
| 22 | 1 | 21 | 22 | 2 | 21 | 1011.786340 | 0.0002 |
| 23 | 1 | 22 | 23 | 2 | 22 | 1011.949560 | 0.0002 |
| 24 | 1 | 23 | 24 | 2 | 23 | 1012.113400 | 0.0002 |
| 25 | 1 | 24 | 25 | 2 | 24 | 1012.275910 | 0.0002 |
| 26 | 1 | 25 | 26 | 2 | 25 | 1012.436770 | 0.0002 |
| 27 | 1 | 26 | 27 | 2 | 26 | 1012.594730 | 0.0002 |
| 28 | 1 | 27 | 28 | 2 | 27 | 1012.748300 | 0.0002 |
| 29 | 1 | 28 | 29 | 2 | 28 | 1012.897940 | 0.0002 |
| 30 | 1 | 29 | 30 | 2 | 29 | 1013.041970 | 0.0002 |

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