Supporting Information

for

# The conformational behaviour of free D-glucose -at last

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**Table S1.** Observed frequencies and residuals (in MHz) for the rotational transitions of conformers G-g+/cc/t, G+g-/cc/t, Tg+/cc/t and G-g+/cl/g- of α-D-glucose.

| | | | | | | **G-g+/cc/t** | | **G+g-/cc/t** | | **Tg+/cc/t** | | **G-g+/cl/g-** | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | Obs / MHz | Obs-cal/MHz | Obs / MHz | Obs-cal/MHz | Obs / MHz | Obs-cal/MHz | Obs / MHz | Obs-cal/MHz |
| 3 | 0 | 3 | 2 | 0 | 2 | 3884.7758 | 0.0027 | 3663.4837 | 0.0030 | 3669.27540 | 0.0035 | | |
| 3 | 1 | 2 | 2 | 1 | 1 | 437.18010 | 0.0024 | 4187.8717 | 0.0009 | 4101.15380 | 0.0021 | | |
| 3 | 1 | 3 | 2 | 1 | 2 | 3736.8509 | 0.0049 | 3500.1402 | 0.0018 | 3493.36650 | 0.0031 | | |
| 3 | 2 | 2 | 2 | 2 | 1 | 4075.9266 | 0.0025 | | | | | | |
| 4 | 0 | 4 | 3 | 0 | 3 | 5037.1523 | 0.0027 | 4723.4113 | 0.0013 | 4759.90680 | 0.0022 | | |
| 4 | 1 | 4 | 3 | 1 | 3 | 4937.7457 | 0.0033 | 4615.6187 | 0.0025 | 4620.56920 | 0.0014 | | |
| 4 | 1 | 3 | 3 | 1 | 2 | 5713.3028 | 0.0018 | 5487.5173 | 0.0020 | 5407.26840 | 0.0018 | | |
| 4 | 2 | 3 | 3 | 2 | 2 | 5393.0076 | 0.0021 | 5129.6020 | 0.0009 | 5065.63760 | 0.0008 | | |
| 4 | 2 | 2 | 3 | 2 | 1 | 5789.2298 | -0.0026 | 5582.3512 | 0.0004 | 5403.00440 | -0.0015 | | |
| 4 | 3 | 2 | 3 | 3 | 1 | 5518.6963 | 0.0014 | | | | | | |
| 5 | 0 | 5 | 4 | 0 | 4 | 6169.5517 | 0.0013 | 5762.6597 | 0.0006 | 5814.73760 | 0.0001 | | |
| 5 | 1 | 4 | 4 | 1 | 3 | 6992.4630 | -0.0006 | 6686.6256 | -0.0031 | 6648.35130 | -0.0009 | | |
| 5 | 1 | 5 | 4 | 1 | 4 | 6117.7711 | 0.0010 | 5707.5843 | 0.0015 | 5727.62850 | 0.0007 | | |
| 5 | 2 | 3 | 4 | 2 | 2 | 7291.4393 | -0.0030 | 7036.1037 | -0.0034 | 6834.69330 | -0.0028 | | |
| 5 | 3 | 2 | 4 | 3 | 1 | | | 6780.2790 | -0.0018 | | | | |
| 5 | 3 | 3 | 4 | 3 | 2 | 6902.0556 | -0.0033 | | | | | | |
| 5 | 4 | 2 | 4 | 4 | 1 | 6909.3900 | -0.0040 | | | | | | |
| 6 | 0 | 6 | 5 | 0 | 5 | 7306.9568 | -0.0020 | 6808.2194 | -0.0027 | 6865.47940 | -0.0024 | | |
| 6 | 1 | 6 | 5 | 1 | 5 | 7283.8750 | -0.0032 | 6784.1171 | -0.0019 | 6819.14580 | -0.0022 | | |
| 2 | 2 | 0 | 1 | 1 | 1 | 4655.5600 | 0.0034 | 4727.6291 | 0.0020 | | | | |
| 3 | 1 | 3 | 2 | 0 | 2 | 4074.0838 | 0.0029 | 3865.7365 | -0.0017 | 3981.75610 | 0.0010 | | |
| 3 | 2 | 2 | 2 | 1 | 1 | 5548.9227 | 0.0007 | 5495.9837 | 0.0001 | | | 5579.0913 | -0.0004 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 3 | 1 | 2 | 2 | 0 | 7023.7583 | -0.0047 | | | | | | |
| 4 | 0 | 4 | 3 | 1 | 3 | 4847.8454 | 0.0036 | 4521.1551 | 0.0026 | 4447.42390 | 0.0025 | 4821.3550 | 0.0022 |
| 4 | 1 | 4 | 3 | 0 | 3 | 5127.0522 | 0.0019 | 4817.8745 | 0.0008 | 4933.05130 | 0.0003 | 5106.5009 | 0.0041 |
| 5 | 0 | 5 | 4 | 1 | 4 | 6079.6521 | 0.0024 | 5668.1969 | 0.0015 | 5641.59250 | 0.0015 | 6046.3990 | -0.0022 |
| 5 | 1 | 4 | 4 | 2 | 3 | 6111.0161 | 0.0009 | 5736.4322 | 0.0021 | | | | |
| 5 | 1 | 5 | 4 | 0 | 4 | 6207.6713 | 0.0005 | 5802.0469 | 0.0004 | 5900.77470 | 0.0004 | 6176.8476 | -0.0026 |
| 6 | 0 | 6 | 5 | 1 | 5 | 7268.8326 | -0.0059 | 6768.8330 | -0.0017 | 6779.44340 | -0.0016 | | |
| 6 | 1 | 6 | 5 | 0 | 5 | 7321.9949 | -0.0037 | 6823.5047 | -0.0017 | 6905.18200 | -0.0028 | | |
| 3 | 2 | 1 | 2 | 1 | 1 | 5792.6573 | 0.0019 | | | | | | |
| 3 | 1 | 2 | 2 | 0 | 2 | 5303.4565 | 0.0035 | | | | | | |

**Table S2.** Observed frequencies and residuals (in MHz) for the rotational transitions of conformers G-g+/cc/t, G+g-/cc/t and Tg+/cc/t of β-D-glucose.

| | | | | | | **G-g+/cc/t** | | **G+g-/cc/t** | | **Tg+/cc/t** | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | Obs / MHz | Obs-cal/MHz | Obs / MHz | Obs-cal/MHz | Obs / MHz | Obs-cal/MHz |
| 3 | 0 | 3 | 2 | 0 | 2 | 3685.0790 | 0.0031 | | | | |
| 3 | 1 | 2 | 2 | 1 | 1 | 4385.9599 | 0.0043 | 4198.7199 | 0.0020 | 4001.6461 | 0.0022 |
| 3 | 1 | 3 | 2 | 1 | 2 | | | | | | |
| 3 | 2 | 1 | 2 | 2 | 0 | 4424.0597 | 0.0028 | 4229.7242 | 0.0018 | | |
| 3 | 2 | 2 | 2 | 2 | 1 | 4054.5620 | -0.0044 | 3848.8952 | -0.0008 | | |
| 4 | 0 | 4 | 3 | 0 | 3 | 4728.5695 | 0.0022 | 4428.8635 | 0.0007 | 4452.4104 | -0.0008 |
| 4 | 1 | 4 | 3 | 1 | 3 | 4678.6378 | 0.0018 | 4373.0777 | 0.0000 | 4333.7334 | 0.0003 |
| 4 | 1 | 3 | 3 | 1 | 2 | 5644.4721 | 0.0032 | 5391.3902 | 0.0012 | 5240.4088 | 0.0016 |
| 4 | 2 | 3 | 3 | 2 | 2 | 5314.1905 | 0.0017 | 5038.0093 | 0.0019 | 4864.6636 | 0.0023 |
| 4 | 2 | 2 | 3 | 2 | 1 | 5984.5922 | 0.0009 | 5734.1080 | 0.0001 | 5323.4008 | 0.0003 |
| 4 | 3 | 2 | 3 | 3 | 1 | 5568.3933 | -0.0032 | 5299.0298 | 0.0050 | 5009.5975 | 0.0056 |
| 5 | 0 | 5 | 4 | 0 | 4 | 5780.2646 | 0.0013 | 5397.0983 | -0.0001 | 5416.5576 | 0.0008 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 5 | 1 | 4 | 4 | 1 | 3 | 6740.6739 | -0.0007 | 6414.4703 | -0.0014 | 6379.1956 | -0.0012 |
| 5 | 1 | 5 | 4 | 1 | 4 | 5763.5250 | -0.0003 | 5377.9049 | 0.0004 | 5354.0355 | 0.0002 |
| 5 | 2 | 3 | 4 | 2 | 2 | 7434.0217 | -0.0034 | 7127.0757 | -0.0030 | 6720.5498 | -0.0008 |
| 5 | 3 | 2 | 4 | 3 | 1 | 7365.3088 | -0.0042 | 7036.8540 | -0.0026 | 6445.5458 | -0.0004 |
| 5 | 3 | 3 | 4 | 3 | 2 | 6931.0521 | -0.0010 | 6595.7418 | -0.0020 | 6266.7807 | -0.0048 |
| 5 | 4 | 2 | 4 | 4 | 1 | 7006.2557 | -0.0030 | | | | |
| 6 | 0 | 6 | 5 | 0 | 5 | 6842.6074 | -0.0024 | 6376.7815 | -0.0008 | 6386.1061 | -0.0006 |
| 6 | 1 | 6 | 5 | 1 | 5 | 6837.6916 | -0.0031 | 6371.0036 | -0.0010 | 6357.9364 | 0.0003 |
| 2 | 2 | 0 | 1 | 1 | 1 | 4455.3624 | 0.0027 | 4438.1043 | 0.0015 | | |
| 3 | 1 | 3 | 2 | 0 | 2 | 3758.4631 | 0.0070 | | | | |
| 3 | 2 | 2 | 2 | 1 | 1 | 5128.2229 | 0.0016 | 5013.3102 | 0.0014 | | |
| 3 | 3 | 1 | 2 | 2 | 0 | 6497.9817 | -0.0049 | 6475.6089 | -0.0017 | | |
| 4 | 0 | 4 | 3 | 1 | 3 | 4655.1904 | 0.0032 | 4345.9273 | 0.0017 | | |
| 4 | 1 | 4 | 3 | 0 | 3 | 4752.0174 | 0.0013 | 4456.0156 | 0.0007 | | |
| 4 | 1 | 3 | 3 | 2 | 2 | 4902.2080 | 0.0048 | 4576.7976 | -0.0005 | | |
| 5 | 0 | 5 | 4 | 1 | 4 | 5756.8146 | 0.0001 | 5369.9472 | 0.0009 | | |
| 5 | 1 | 4 | 4 | 2 | 3 | 6328.6887 | -0.0002 | 5953.2628 | 0.0004 | | |
| 5 | 1 | 5 | 4 | 0 | 4 | 5786.9752 | 0.0011 | 5405.0569 | 0.0002 | | |
| 6 | 0 | 6 | 5 | 1 | 5 | 6835.8966 | -0.0024 | 6368.8222 | -0.0019 | | |
| 6 | 1 | 6 | 5 | 0 | 5 | 6844.4032 | -0.0024 | 6378.9629 | 0.0000 | | |
| 3 | 2 | 1 | 2 | 1 | 1 | 5611.2286 | 0.0009 | | | | |
| 3 | 1 | 2 | 2 | 0 | 2 | 5422.5069 | 0.0058 | | | | |

**Table S3.** Cartesian coordinates for the four observed conformers of α-D-glucose. The geometries have been optimized *ab initio* at the MP2/6-311++G(d,p) level of theory.

Conformer **G-g+/cc/t:**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.495021 | -0.212021 | -0.633301 |
| 2 | 6 | 0 | 0.815267 | -1.500384 | -0.179731 |
| 3 | 8 | 0 | -0.586217 | -1.402596 | -0.249540 |
| 4 | 6 | 0 | -1.153019 | -0.308990 | 0.498344 |
| 5 | 6 | 0 | -0.562296 | 1.014351 | 0.029394 |
| 6 | 6 | 0 | 0.947511 | 0.968563 | 0.152742 |
| 7 | 8 | 0 | 1.278311 | -1.740253 | 1.135501 |
| 8 | 6 | 0 | -2.651986 | -0.399446 | 0.269526 |
| 9 | 8 | 0 | -2.979857 | -0.324578 | -1.108797 |
| 10 | 8 | 0 | -1.115160 | 2.030390 | 0.853565 |
| 11 | 8 | 0 | 1.451604 | 2.199735 | -0.352368 |
| 12 | 8 | 0 | 2.909027 | -0.299250 | -0.523144 |
| 13 | 1 | 0 | 1.077839 | -2.331318 | -0.841960 |
| 14 | 1 | 0 | -0.937408 | -0.434076 | 1.567529 |
| 15 | 1 | 0 | -0.833129 | 1.178070 | -1.022489 |
| 16 | 1 | 0 | 1.209222 | 0.859224 | 1.215368 |
| 17 | 1 | 0 | 1.278268 | -0.056911 | -1.694445 |
| 18 | 1 | 0 | 1.008191 | -2.630419 | 1.385218 |
| 19 | 1 | 0 | 3.080966 | -0.672857 | 0.350895 |
| 20 | 1 | 0 | 2.410606 | 2.106024 | -0.398194 |
| 21 | 1 | 0 | -0.637486 | 2.838918 | 0.633702 |
| 22 | 1 | 0 | -3.136961 | 0.445796 | 0.760357 |
| 23 | 1 | 0 | -3.019654 | -1.334476 | 0.712459 |
| 24 | 1 | 0 | -2.505115 | -1.047997 | -1.532024 |

Rotational constants (GHZ): 1.2799711 0.7849445 0.5795606

Conformer **G+g-/cc/t:**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.548374 | -0.486400 | -0.543951 |
| 2 | 6 | 0 | 0.491396 | -1.555342 | -0.279311 |
| 3 | 8 | 0 | -0.801053 | -1.084570 | -0.577883 |
| 4 | 6 | 0 | -1.182023 | 0.101164 | 0.148364 |
| 5 | 6 | 0 | -0.214224 | 1.230229 | -0.173779 |
| 6 | 6 | 0 | 1.191267 | 0.795791 | 0.193087 |
| 7 | 8 | 0 | 0.642931 | -1.920496 | 1.078226 |
| 8 | 6 | 0 | -2.606033 | 0.399932 | -0.277466 |
| 9 | 8 | 0 | -3.477569 | -0.671778 | 0.049238 |
| 10 | 8 | 0 | -0.616030 | 2.371205 | 0.567652 |
| 11 | 8 | 0 | 2.068934 | 1.856341 | -0.166922 |
| 12 | 8 | 0 | 2.850666 | -0.935738 | -0.197040 |
| 13 | 1 | 0 | 0.640712 | -2.418780 | -0.935160 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 1 | 0 | -1.159281 | -0.106346 | 1.224985 |
| 15 | 1 | 0 | -0.246491 | 1.437979 | -1.254864 |
| 16 | 1 | 0 | 1.229574 | 0.622209 | 1.278328 |
| 17 | 1 | 0 | 1.571092 | -0.277228 | -1.617629 |
| 18 | 1 | 0 | 0.097830 | -2.698137 | 1.239762 |
| 19 | 1 | 0 | 2.761777 | -1.354128 | 0.669155 |
| 20 | 1 | 0 | 2.966409 | 1.521753 | -0.051589 |
| 21 | 1 | 0 | 0.110399 | 3.002407 | 0.498344 |
| 22 | 1 | 0 | -2.962995 | 1.280699 | 0.257640 |
| 23 | 1 | 0 | -2.618862 | 0.607001 | -1.356844 |
| 24 | 1 | 0 | -3.105732 | -1.449393 | -0.379967 |

Rotational constants (GHZ): 1.3085944 0.7663058 0.5335425

Conformer **Tg+/cc/t:**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.086801 | -0.538760 | 0.029295 |
| 2 | 1 | 0 | -1.052457 | -0.720414 | 1.110634 |
| 3 | 6 | 0 | -2.511466 | -0.771811 | -0.461266 |
| 4 | 1 | 0 | -2.602293 | -0.411234 | -1.495899 |
| 5 | 1 | 0 | -2.708222 | -1.846227 | -0.452183 |
| 6 | 8 | 0 | -3.468687 | -0.167318 | 0.390170 |
| 7 | 1 | 0 | -3.207396 | 0.757833 | 0.475516 |
| 8 | 8 | 0 | -0.253895 | -1.483211 | -0.662265 |
| 9 | 6 | 0 | 1.100970 | -1.434712 | -0.286224 |
| 10 | 1 | 0 | 1.600007 | -2.171095 | -0.923599 |
| 11 | 6 | 0 | 1.703243 | -0.046555 | -0.493921 |
| 12 | 8 | 0 | 1.299753 | -1.735852 | 1.082140 |
| 13 | 1 | 0 | 1.074559 | -2.662969 | 1.215548 |
| 14 | 8 | 0 | 3.054267 | 0.013407 | -0.060091 |
| 15 | 1 | 0 | 1.714584 | 0.171188 | -1.566149 |
| 16 | 6 | 0 | 0.849989 | 1.003231 | 0.202443 |
| 17 | 1 | 0 | 3.073123 | -0.426491 | 0.799818 |
| 18 | 8 | 0 | 1.280993 | 2.319352 | -0.125042 |
| 19 | 6 | 0 | -0.583159 | 0.869062 | -0.265149 |
| 20 | 1 | 0 | 0.883535 | 0.850684 | 1.290692 |
| 21 | 1 | 0 | 2.229975 | 2.348964 | 0.046079 |
| 22 | 8 | 0 | -1.438375 | 1.795235 | 0.398037 |
| 23 | 1 | 0 | -0.616587 | 1.033963 | -1.353082 |
| 24 | 1 | 0 | -1.017936 | 2.660170 | 0.317967 |

Rotational constants (GHZ): 1.3996560 0.7409966 0.5379605

Conformer **G-g+/cl/g-:**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.576186 | 0.971338 | 0.005363 |
| 2 | 6 | 0 | -1.113621 | -0.377427 | 0.482154 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 8 | 0 | -0.538942 | -1.414423 | -0.327691 |
| 4 | 6 | 0 | 0.858200 | -1.505682 | -0.223577 |
| 5 | 6 | 0 | 1.522090 | -0.185567 | -0.620620 |
| 6 | 6 | 0 | 0.929923 | 0.970711 | 0.161799 |
| 7 | 6 | 0 | -2.615350 | -0.515572 | 0.325614 |
| 8 | 8 | 0 | -3.037155 | -0.258991 | -1.007254 |
| 9 | 8 | 0 | 1.198213 | -1.855469 | 1.098181 |
| 10 | 8 | 0 | 2.913343 | -0.330344 | -0.359414 |
| 11 | 8 | 0 | 1.533848 | 2.155366 | -0.345570 |
| 12 | 8 | 0 | -1.072168 | 2.054934 | 0.791804 |
| 13 | 1 | 0 | -0.841811 | -0.528209 | 1.534519 |
| 14 | 1 | 0 | -3.119819 | 0.215203 | 0.962109 |
| 15 | 1 | 0 | -2.909386 | -1.520843 | 0.650821 |
| 16 | 1 | 0 | -2.595615 | -0.915433 | -1.557262 |
| 17 | 1 | 0 | 1.146821 | -2.298665 | -0.921953 |
| 18 | 1 | 0 | 2.135093 | -1.635288 | 1.192226 |
| 19 | 1 | 0 | 1.345367 | -0.013906 | -1.690915 |
| 20 | 1 | 0 | 3.297472 | 0.550723 | -0.443958 |
| 21 | 1 | 0 | 1.170599 | 0.851699 | 1.227780 |
| 22 | 1 | 0 | 1.103840 | 2.890334 | 0.107439 |
| 23 | 1 | 0 | -0.832188 | 1.113976 | -1.051039 |
| 24 | 1 | 0 | -1.907821 | 2.335020 | 0.405381 |

Rotational constants (GHZ): 1.2965965 0.7877045 0.5736370

**Table S4.** Cartesian coordinates for the three observed conformers of β-D-glucose. The geometries have been optimized *ab initio* at the MP2/6-311++G(d,p) level of theory.

Conformer **G-g+/cc/t:**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 0.427818 | -1.383267 | -0.124444 |
| 2 | 6 | 0 | -0.956564 | -1.268191 | -0.400736 |
| 3 | 6 | 0 | 1.177592 | -0.262663 | -0.612099 |
| 4 | 8 | 0 | -1.610640 | -2.390309 | 0.107521 |
| 5 | 6 | 0 | 2.632835 | -0.572230 | -0.303302 |
| 6 | 1 | 0 | 1.048634 | -0.165595 | -1.702390 |
| 7 | 6 | 0 | 0.693999 | 1.021717 | 0.055128 |
| 8 | 8 | 0 | 1.412287 | 2.094313 | -0.536928 |
| 9 | 6 | 0 | -0.798615 | 1.184958 | -0.160223 |
| 10 | 1 | 0 | 0.899615 | 0.963155 | 1.131932 |
| 11 | 8 | 0 | -1.204412 | 2.345568 | 0.553252 |
| 12 | 1 | 0 | -0.984490 | 1.321767 | -1.237298 |
| 13 | 6 | 0 | -1.535455 | -0.053322 | 0.305247 |
| 14 | 8 | 0 | -2.907904 | 0.134016 | -0.009835 |
| 15 | 1 | 0 | -1.389768 | -0.187888 | 1.385970 |
| 16 | 1 | 0 | -3.370306 | -0.662910 | 0.273517 |
| 17 | 1 | 0 | -2.163099 | 2.402338 | 0.465304 |
| 18 | 1 | 0 | 1.015639 | 2.902288 | -0.190308 |
| 19 | 1 | 0 | 3.248203 | 0.281435 | -0.591871 |
| 20 | 8 | 0 | 2.837740 | -0.784111 | 1.083825 |
| 21 | 1 | 0 | 2.936254 | -1.451362 | -0.886966 |
| 22 | 1 | 0 | 2.240508 | -1.497907 | 1.333692 |
| 23 | 1 | 0 | -1.300078 | -3.159213 | -0.382336 |

| | | | | | |
|---|---|---|---|---|---|
| 24 | 1 | 0 | -1.102985 | -1.177393 | -1.490471 |

Rotational constants (GHZ): 1.1803008 0.8197394 0.5361228

Conformer **G+g-/cc/t:**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 0.712414 | -1.132496 | 0.258378 |
| 2 | 6 | 0 | -0.576682 | -1.415215 | -0.257950 |
| 3 | 6 | 0 | 1.215653 | 0.116407 | -0.236558 |
| 4 | 8 | 0 | -1.006012 | -2.646144 | 0.237044 |
| 5 | 6 | 0 | 2.641175 | 0.229287 | 0.268095 |
| 6 | 1 | 0 | 1.222121 | 0.100789 | -1.337744 |
| 7 | 6 | 0 | 0.321230 | 1.250963 | 0.250452 |
| 8 | 8 | 0 | 0.828895 | 2.464912 | -0.279583 |
| 9 | 6 | 0 | -1.102264 | 1.002906 | -0.213485 |
| 10 | 1 | 0 | 0.334611 | 1.269524 | 1.350731 |
| 11 | 8 | 0 | -1.909285 | 2.039440 | 0.329755 |
| 12 | 1 | 0 | -1.122169 | 1.047021 | -1.313622 |
| 13 | 6 | 0 | -1.568927 | -0.369746 | 0.226486 |
| 14 | 8 | 0 | -2.860106 | -0.566954 | -0.331804 |
| 15 | 1 | 0 | -1.598581 | -0.417073 | 1.323815 |
| 16 | 1 | 0 | -3.148750 | -1.446254 | -0.061972 |
| 17 | 1 | 0 | -2.819423 | 1.840507 | 0.080328 |
| 18 | 1 | 0 | 0.154633 | 3.133062 | -0.106517 |
| 19 | 1 | 0 | 3.081267 | 1.156402 | -0.101062 |
| 20 | 1 | 0 | 2.625681 | 0.252390 | 1.366720 |
| 21 | 8 | 0 | 3.443173 | -0.837729 | -0.212163 |
| 22 | 1 | 0 | 2.997968 | -1.644408 | 0.067916 |
| 23 | 1 | 0 | -0.535140 | -1.417036 | -1.360207 |
| 24 | 1 | 0 | -0.445962 | -3.330775 | -0.143636 |

Rotational constants (GHZ): 1.1802622 0.7933139 0.4954657

Conformer **Tg+/cc/t:**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.074981 | -0.597383 | -0.195879 |
| 2 | 1 | 0 | 1.100472 | -0.593124 | -1.297238 |
| 3 | 6 | 0 | 2.425310 | -1.087308 | 0.315669 |
| 4 | 1 | 0 | 2.482251 | -0.919359 | 1.400448 |
| 5 | 1 | 0 | 2.496160 | -2.160919 | 0.127930 |
| 6 | 8 | 0 | 3.503541 | -0.474319 | -0.368379 |
| 7 | 1 | 0 | 3.361930 | 0.477732 | -0.298108 |
| 8 | 8 | 0 | 0.081543 | -1.511170 | 0.274961 |
| 9 | 6 | 0 | -1.190877 | -1.213303 | -0.272444 |
| 10 | 8 | 0 | -2.114248 | -2.146105 | 0.197612 |
| 11 | 6 | 0 | -1.665433 | 0.154341 | 0.195810 |
| 12 | 8 | 0 | -2.897719 | 0.522398 | -0.407074 |

| | | | | | |
|---|---|---|---|---|---|
| 13 | 1 | 0 | -1.752632 | 0.123028 | 1.290640 |
| 14 | 6 | 0 | -0.645857 | 1.201956 | -0.202323 |
| 15 | 1 | 0 | -3.539794 | -0.154278 | -0.163582 |
| 16 | 8 | 0 | -0.944862 | 2.477266 | 0.350638 |
| 17 | 6 | 0 | 0.723013 | 0.800382 | 0.308804 |
| 18 | 1 | 0 | -0.609012 | 1.265504 | -1.300709 |
| 19 | 1 | 0 | -1.843902 | 2.693993 | 0.077079 |
| 20 | 8 | 0 | 1.725857 | 1.706444 | -0.139305 |
| 21 | 1 | 0 | 0.696866 | 0.773730 | 1.408229 |
| 22 | 1 | 0 | 1.410256 | 2.592052 | 0.078672 |
| 23 | 1 | 0 | -1.124468 | -1.232257 | -1.373783 |
| 24 | 1 | 0 | -1.837856 | -3.014328 | -0.115027 |

Rotational constants (GHZ): 1.3223546 0.7359715 0.4957015

**Reference 27**:

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