Electronic Supplementary Material (ESI) for RSC Advances.


# Supplementary material

# for

# The eight structures of caffeic acid: pushing rotational spectroscopy to the limit

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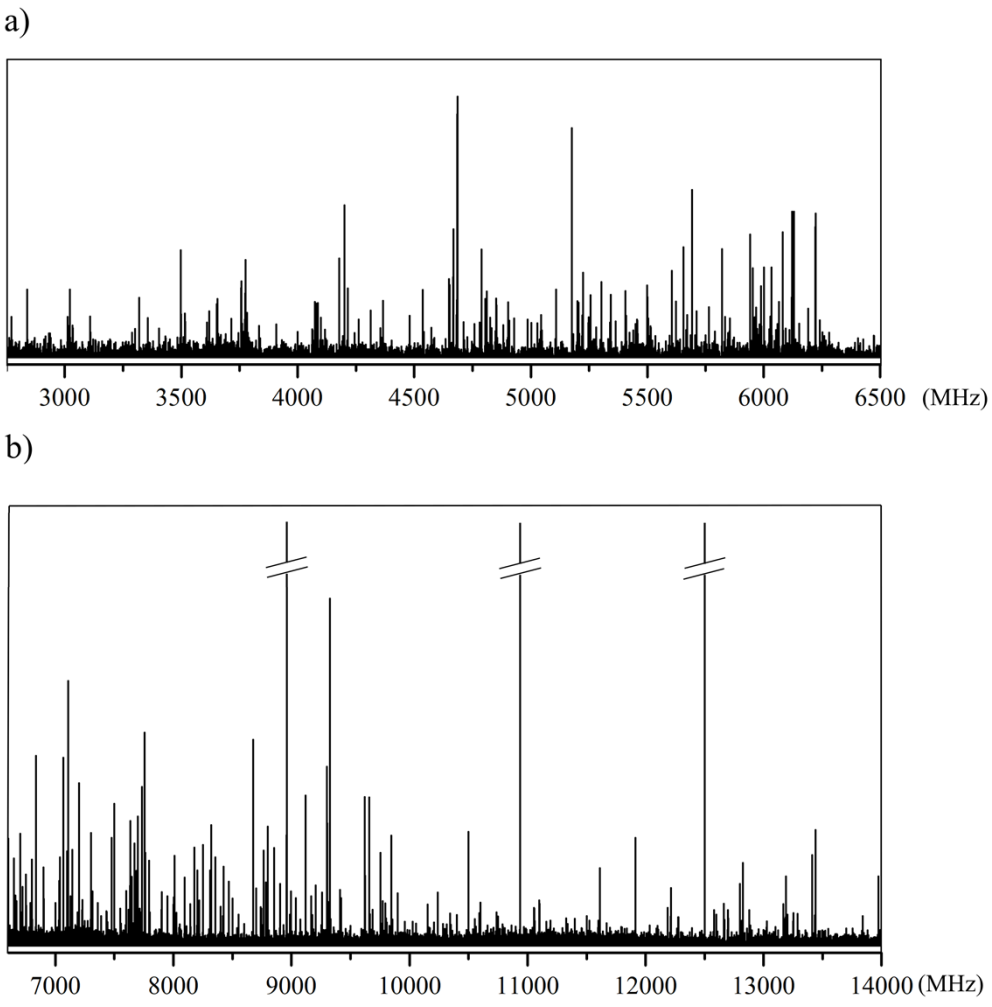
## 1-Broadband CP-FTMW rotational spectrum

**Figure S1.** Broadband CP-FTMW rotational spectrums of caffeic acid from 2.75 to 6.5 and from 6.6 to 14 GHz



## 2-Line lists of measured transitions

**Table S1.** Measured rotational transitions and residuals (in MHz) of rotamer I.

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $\nu_{obs}$ | $\nu_{obs} - \nu_{cal}$ |
|---|---|---|---|---|---|---|---|
| 4 | 2 | 3 | 3 | 2 | 2 | 2414.907 | -0.016 |
| 5 | 2 | 4 | 4 | 2 | 3 | 3017.883 | -0.008 |
| 2 | 1 | 2 | 1 | 0 | 1 | 3108.121 | -0.001 |
| 8 | 0 | 8 | 7 | 1 | 7 | 3319.684 | 0.004 |
| 6 | 1 | 6 | 5 | 1 | 5 | 3498.642 | 0.013 |
| 6 | 2 | 5 | 5 | 2 | 4 | 3620.351 | -0.001 |
| 3 | 1 | 3 | 2 | 0 | 2 | 3652.310 | -0.018 |
| 4 | 1 | 4 | 3 | 0 | 3 | 4177.565 | -0.014 |
| 7 | 0 | 7 | 6 | 0 | 6 | 4193.245 | -0.021 |
| 7 | 1 | 6 | 6 | 1 | 5 | 4358.270 | -0.010 |
| 8 | 1 | 8 | 7 | 1 | 7 | 4659.631 | -0.022 |
| 5 | 1 | 5 | 4 | 0 | 4 | 4685.122 | 0.005 |
| 8 | 0 | 8 | 7 | 0 | 7 | 4780.744 | 0.001 |
| 13 | 2 | 11 | 13 | 1 | 12 | 4928.498 | -0.027 |
| 11 | 2 | 9 | 11 | 1 | 10 | 5028.626 | -0.019 |
| 10 | 2 | 8 | 10 | 1 | 9 | 5108.413 | -0.011 |
| 6 | 1 | 6 | 5 | 0 | 5 | 5176.645 | -0.004 |
| 9 | 2 | 7 | 9 | 1 | 8 | 5201.407 | -0.010 |
| 8 | 2 | 6 | 8 | 1 | 7 | 5302.479 | -0.026 |
| 9 | 0 | 9 | 8 | 0 | 8 | 5364.045 | -0.033 |
| 7 | 2 | 5 | 7 | 1 | 6 | 5406.638 | -0.009 |
| 9 | 2 | 8 | 8 | 2 | 7 | 5423.661 | -0.023 |
| 6 | 2 | 4 | 6 | 1 | 5 | 5509.051 | 0.000 |
| 9 | 1 | 8 | 8 | 1 | 7 | 5595.278 | -0.021 |
| 5 | 2 | 3 | 5 | 1 | 4 | 5605.322 | -0.003 |
| 7 | 1 | 7 | 6 | 0 | 6 | 5654.329 | 0.000 |
| 4 | 2 | 2 | 4 | 1 | 3 | 5691.579 | -0.015 |
| 3 | 2 | 1 | 3 | 1 | 2 | 5764.579 | 0.001 |
| 2 | 2 | 0 | 2 | 1 | 1 | 5821.615 | -0.017 |
| 2 | 2 | 1 | 2 | 1 | 2 | 5940.752 | -0.020 |
| 3 | 2 | 2 | 3 | 1 | 3 | 6001.010 | -0.015 |
| 10 | 2 | 9 | 9 | 2 | 8 | 6023.113 | -0.002 |
| 4 | 2 | 3 | 4 | 1 | 4 | 6081.564 | -0.021 |
| 8 | 1 | 8 | 7 | 0 | 7 | 6120.717 | 0.001 |
| 10 | 1 | 10 | 9 | 0 | 9 | 7031.401 | 0.034 |
| 2 | 2 | 1 | 1 | 1 | 0 | 7068.638 | 0.002 |
| 2 | 2 | 0 | 1 | 1 | 1 | 7109.173 | 0.011 |
| 3 | 2 | 2 | 2 | 1 | 1 | 7632.583 | 0.013 |
| 3 | 2 | 1 | 2 | 1 | 2 | 7755.377 | 0.011 |
| 4 | 2 | 3 | 3 | 1 | 2 | 8176.473 | 0.020 |
| 4 | 2 | 2 | 3 | 1 | 3 | 8425.095 | 0.015 |
| 5 | 2 | 4 | 4 | 1 | 3 | 8700.359 | 0.008 |
| 5 | 2 | 3 | 4 | 1 | 4 | 9120.772 | 0.015 |
| 6 | 2 | 5 | 5 | 1 | 4 | 9204.413 | 0.019 |
| 7 | 2 | 6 | 6 | 1 | 5 | 9688.804 | 0.008 |

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $\nu_{obs}$ | $\nu_{obs} - \nu_{cal}$ |
|---|---|---|---|---|---|---|---|
| 6 | 2 | 4 | 5 | 1 | 5 | 9845.451 | 0.012 |
| 8 | 2 | 7 | 7 | 1 | 6 | 10153.888 | 0.024 |
| 3 | 3 | 1 | 2 | 2 | 0 | 11612.819 | 0.008 |
| 3 | 3 | 0 | 2 | 2 | 1 | 11613.431 | 0.005 |
| 4 | 3 | 2 | 3 | 2 | 1 | 12215.420 | -0.004 |
| 4 | 3 | 1 | 3 | 2 | 2 | 12218.517 | 0.005 |
| 5 | 3 | 2 | 4 | 2 | 3 | 12824.992 | 0.000 |
| 6 | 3 | 4 | 5 | 2 | 3 | 13411.946 | 0.004 |
| 6 | 3 | 3 | 5 | 2 | 4 | 13433.713 | 0.000 |

**Table S2.** Measured rotational transitions and residuals (in MHz) of rotamer II.

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $\nu_{obs}$ | $\nu_{obs} - \nu_{cal}$ |
|---|---|---|---|---|---|---|---|
| 5 | 0 | 5 | 4 | 0 | 4 | 3012.195 | -0.021 |
| 7 | 1 | 7 | 6 | 1 | 6 | 4086.434 | 0.013 |
| 7 | 0 | 7 | 6 | 0 | 6 | 4200.362 | 0.010 |
| 7 | 1 | 6 | 6 | 1 | 5 | 4365.874 | -0.003 |
| 8 | 1 | 8 | 7 | 1 | 7 | 4667.451 | 0.011 |
| 8 | 0 | 8 | 7 | 0 | 7 | 4788.789 | 0.001 |
| 8 | 2 | 7 | 7 | 2 | 6 | 4831.605 | 0.007 |
| 8 | 1 | 7 | 7 | 1 | 6 | 4986.196 | 0.007 |
| 9 | 1 | 9 | 8 | 1 | 8 | 5247.471 | 0.002 |
| 9 | 2 | 7 | 8 | 2 | 6 | 5503.807 | -0.011 |
| 9 | 1 | 8 | 8 | 1 | 7 | 5605.014 | -0.010 |
| 10 | 1 | 10 | 9 | 1 | 9 | 5826.421 | -0.028 |
| 10 | 0 | 10 | 9 | 0 | 9 | 5953.083 | 0.002 |
| 10 | 2 | 9 | 9 | 2 | 8 | 6033.408 | 0.011 |
| 10 | 2 | 8 | 9 | 2 | 7 | 6129.094 | 0.009 |
| 10 | 1 | 9 | 9 | 1 | 8 | 6222.120 | -0.002 |

**Table S3.** Measured rotational transitions and residuals (in MHz) of rotamer III.

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $\nu_{obs}$ | $\nu_{obs} - \nu_{cal}$ |
|---|---|---|---|---|---|---|---|
| 5 | 1 | 5 | 4 | 1 | 4 | 2931.355 | -0.009 |
| 5 | 0 | 5 | 4 | 0 | 4 | 3022.140 | 0.018 |
| 6 | 1 | 6 | 5 | 1 | 5 | 3516.024 | -0.013 |
| 6 | 0 | 6 | 5 | 0 | 5 | 3619.870 | -0.023 |
| 6 | 1 | 5 | 5 | 1 | 4 | 3756.577 | -0.031 |
| 7 | 1 | 7 | 6 | 1 | 6 | 4099.929 | 0.041 |
| 8 | 1 | 8 | 7 | 1 | 7 | 4682.827 | 0.005 |
| 8 | 0 | 8 | 7 | 0 | 7 | 4804.550 | 0.005 |
| 8 | 1 | 7 | 7 | 1 | 6 | 5002.565 | 0.018 |
| 9 | 0 | 9 | 8 | 0 | 8 | 5390.749 | 0.001 |
| 9 | 1 | 8 | 8 | 1 | 7 | 5623.425 | 0.011 |
| 10 | 1 | 10 | 9 | 1 | 9 | 5845.638 | -0.015 |
| 10 | 0 | 10 | 9 | 0 | 9 | 5972.679 | -0.002 |
| 10 | 2 | 9 | 9 | 2 | 8 | 6053.224 | -0.010 |

**Table S4.** Measured rotational transitions and residuals (in MHz) of rotamer IV.

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $\nu_{obs}$ | $\nu_{obs} - \nu_{cal}$ |
|---|---|---|---|---|---|---|---|
| 5 | 1 | 5 | 4 | 0 | 4 | 4711.237 | -0.010 |
| 6 | 1 | 6 | 5 | 0 | 5 | 5205.826 | -0.021 |
| 9 | 2 | 8 | 8 | 2 | 7 | 5458.911 | -0.017 |
| 2 | 2 | 0 | 2 | 1 | 1 | 5847.515 | -0.011 |
| 10 | 1 | 10 | 9 | 1 | 9 | 5854.232 | 0.003 |
| 2 | 2 | 1 | 2 | 1 | 2 | 5967.589 | -0.015 |
| 10 | 0 | 10 | 9 | 0 | 9 | 5981.419 | -0.006 |
| 3 | 2 | 2 | 3 | 1 | 3 | 6028.315 | -0.019 |
| 10 | 5 | 5 | 9 | 5 | 4 | 6083.089 | -0.009 |
| 10 | 3 | 7 | 9 | 3 | 6 | 6094.050 | 0.014 |
| 4 | 2 | 3 | 4 | 1 | 4 | 6109.487 | -0.046 |
| 10 | 1 | 9 | 9 | 1 | 8 | 6251.899 | -0.009 |
| 2 | 2 | 1 | 1 | 1 | 0 | 7102.698 | -0.001 |
| 2 | 2 | 0 | 1 | 1 | 1 | 7143.541 | -0.006 |
| 3 | 2 | 2 | 2 | 1 | 1 | 7670.259 | 0.013 |
| 3 | 2 | 1 | 2 | 1 | 2 | 7794.023 | 0.001 |
| 4 | 2 | 3 | 3 | 1 | 2 | 8217.607 | 0.021 |
| 4 | 2 | 2 | 3 | 1 | 3 | 8468.209 | 0.002 |
| 5 | 2 | 4 | 4 | 1 | 3 | 8744.797 | 0.015 |
| 5 | 2 | 3 | 4 | 1 | 4 | 9168.572 | -0.008 |
| 6 | 2 | 4 | 5 | 1 | 5 | 9898.238 | 0.023 |
| 7 | 2 | 5 | 6 | 1 | 6 | 10660.714 | 0.000 |
| 3 | 3 | 1 | 2 | 2 | 0 | 11668.531 | 0.000 |
| 4 | 3 | 2 | 3 | 2 | 1 | 12275.072 | 0.012 |
| 4 | 3 | 1 | 3 | 2 | 2 | 12278.185 | 0.002 |
| 5 | 3 | 3 | 4 | 2 | 2 | 12879.212 | -0.008 |
| 5 | 3 | 2 | 4 | 2 | 3 | 12888.638 | 0.016 |

**Table S5.** Measured rotational transitions and residuals (in MHz) of rotamer V.

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $\nu_{obs}$ | $\nu_{obs} - \nu_{cal}$ |
|---|---|---|---|---|---|---|---|
| 4 | 1 | 4 | 3 | 1 | 3 | 2271.550 | 0.035 |
| 4 | 0 | 4 | 3 | 0 | 3 | 2336.888 | 0.029 |
| 4 | 1 | 3 | 3 | 1 | 2 | 2408.660 | -0.005 |
| 5 | 1 | 5 | 4 | 1 | 4 | 2838.663 | 0.008 |
| 6 | 0 | 6 | 5 | 0 | 5 | 3497.260 | 0.002 |
| 6 | 1 | 5 | 5 | 1 | 4 | 3610.897 | -0.007 |
| 7 | 0 | 7 | 6 | 0 | 6 | 4074.112 | -0.001 |
| 7 | 2 | 5 | 6 | 2 | 4 | 4115.885 | -0.001 |
| 8 | 1 | 8 | 7 | 1 | 7 | 4536.898 | -0.014 |
| 8 | 0 | 8 | 7 | 0 | 7 | 4648.296 | 0.000 |
| 8 | 1 | 7 | 7 | 1 | 6 | 4810.503 | 0.005 |
| 9 | 0 | 9 | 8 | 0 | 8 | 5219.552 | 0.004 |
| 9 | 1 | 8 | 8 | 1 | 7 | 5408.956 | -0.006 |
| 10 | 1 | 10 | 9 | 1 | 9 | 5665.749 | -0.014 |

**Table S6.** Measured rotational transitions and residuals (in MHz) of rotamer VI..

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $\nu_{obs}$ | $\nu_{obs} - \nu_{cal}$ |
|---|---|---|---|---|---|---|---|
| 5 | 1 | 4 | 4 | 1 | 3 | 3012.649 | -0.010 |
| 2 | 1 | 2 | 1 | 0 | 1 | 3301.486 | -0.003 |
| 7 | 0 | 7 | 6 | 0 | 6 | 4077.656 | 0.000 |
| 7 | 1 | 6 | 6 | 1 | 5 | 4214.761 | 0.017 |
| 4 | 1 | 4 | 3 | 0 | 3 | 4353.796 | -0.029 |
| 8 | 1 | 8 | 7 | 1 | 7 | 4540.888 | 0.000 |
| 8 | 0 | 8 | 7 | 0 | 7 | 4652.326 | -0.009 |
| 8 | 2 | 7 | 7 | 2 | 6 | 4680.928 | -0.003 |
| 8 | 2 | 6 | 7 | 2 | 5 | 4714.462 | -0.005 |
| 5 | 1 | 5 | 4 | 0 | 4 | 4856.054 | -0.021 |
| 9 | 1 | 9 | 8 | 1 | 8 | 5106.180 | 0.003 |
| 9 | 0 | 9 | 8 | 0 | 8 | 5224.071 | -0.009 |
| 6 | 1 | 6 | 5 | 0 | 5 | 5343.785 | -0.002 |
| 10 | 1 | 10 | 9 | 1 | 9 | 5670.721 | -0.006 |
| 7 | 1 | 7 | 6 | 0 | 6 | 5818.437 | 0.041 |
| 8 | 1 | 8 | 7 | 0 | 7 | 6281.615 | -0.014 |
| 3 | 2 | 2 | 3 | 1 | 3 | 6647.676 | -0.002 |
| 4 | 2 | 3 | 4 | 1 | 4 | 6716.768 | -0.027 |
| 5 | 2 | 4 | 5 | 1 | 5 | 6803.415 | -0.010 |
| 7 | 2 | 6 | 7 | 1 | 7 | 7029.784 | -0.006 |
| 2 | 2 | 1 | 1 | 1 | 0 | 7698.804 | 0.013 |
| 2 | 2 | 0 | 1 | 1 | 1 | 7733.516 | 0.005 |
| 3 | 2 | 2 | 2 | 1 | 1 | 8250.220 | 0.010 |
| 3 | 2 | 1 | 2 | 1 | 2 | 8355.193 | 0.012 |
| 4 | 2 | 3 | 3 | 1 | 2 | 8784.421 | 0.010 |
| 4 | 2 | 2 | 3 | 1 | 3 | 8996.366 | -0.004 |
| 5 | 2 | 4 | 4 | 1 | 3 | 9301.431 | -0.002 |
| 5 | 2 | 3 | 4 | 1 | 4 | 9658.723 | 0.006 |
| 6 | 2 | 5 | 5 | 1 | 4 | 9801.364 | 0.004 |
| 7 | 2 | 6 | 6 | 1 | 5 | 10284.318 | -0.005 |
| 6 | 2 | 4 | 5 | 1 | 5 | 10344.287 | 0.022 |
| 8 | 2 | 7 | 7 | 1 | 6 | 10750.517 | 0.006 |
| 7 | 2 | 5 | 6 | 1 | 6 | 11055.444 | 0.004 |
| 3 | 3 | 1 | 2 | 2 | 0 | 12664.505 | -0.012 |
| 3 | 3 | 1 | 2 | 2 | 1 | 12664.937 | 0.015 |
| 4 | 3 | 1 | 3 | 2 | 1 | 13249.436 | -0.018 |
| 4 | 3 | 2 | 3 | 2 | 2 | 13251.481 | 0.025 |
| 5 | 3 | 3 | 4 | 2 | 2 | 13832.768 | -0.030 |
| 5 | 3 | 2 | 4 | 2 | 3 | 13838.955 | 0.004 |

**Table S7.** Measured rotational transitions and residuals (in MHz) of rotamer VII..

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $\nu_{obs}$ | $\nu_{obs} - \nu_{cal}$ |
|---|---|---|---|---|---|---|---|
| 5 | 1 | 4 | 4 | 1 | 3 | 3033.537 | -0.005 |
| 2 | 1 | 2 | 1 | 0 | 1 | 3288.840 | 0.005 |
| 7 | 1 | 7 | 6 | 1 | 6 | 3999.145 | 0.024 |
| 8 | 1 | 7 | 7 | 1 | 6 | 4847.753 | -0.029 |
| 5 | 1 | 5 | 4 | 0 | 4 | 4850.921 | 0.000 |
| 9 | 0 | 9 | 8 | 0 | 8 | 5256.347 | 0.000 |
| 6 | 1 | 6 | 5 | 0 | 5 | 5340.612 | -0.016 |
| 10 | 1 | 10 | 9 | 1 | 9 | 5704.948 | -0.003 |
| 10 | 1 | 9 | 9 | 1 | 8 | 6052.548 | -0.016 |
| 6 | 2 | 4 | 6 | 1 | 5 | 6151.913 | -0.022 |
| 5 | 2 | 3 | 5 | 1 | 4 | 6240.572 | -0.015 |
| 2 | 2 | 1 | 1 | 1 | 0 | 7648.249 | 0.001 |
| 2 | 2 | 0 | 1 | 1 | 1 | 7683.684 | -0.005 |
| 3 | 2 | 2 | 2 | 1 | 1 | 8202.819 | 0.007 |
| 3 | 2 | 1 | 2 | 1 | 2 | 8310.001 | 0.016 |
| 4 | 2 | 3 | 3 | 1 | 2 | 8739.817 | 0.012 |
| 5 | 2 | 4 | 4 | 1 | 3 | 9259.283 | 0.014 |
| 5 | 2 | 3 | 4 | 1 | 4 | 9624.287 | 0.023 |
| 6 | 2 | 5 | 5 | 1 | 4 | 9761.320 | 0.030 |
| 3 | 3 | 0 | 2 | 2 | 0 | 12579.548 | -0.028 |
| 3 | 3 | 0 | 2 | 2 | 1 | 12580.009 | 0.008 |
| 4 | 3 | 2 | 3 | 2 | 1 | 13168.283 | -0.010 |
| 4 | 3 | 1 | 3 | 2 | 2 | 13170.437 | -0.004 |

**Table S8.** Measured rotational transitions and residuals (in MHz) of rotamer VIII.

| $J'$ | $K'_{-1}$ | $K'_{+1}$ | $J''$ | $K''_{-1}$ | $K''_{+1}$ | $\nu_{obs}$ | $\nu_{obs} - \nu_{cal}$ |
|---|---|---|---|---|---|---|---|
| 8 | 1 | 8 | 7 | 1 | 7 | 4573.206 | -0.019 |
| 8 | 0 | 8 | 7 | 0 | 7 | 4686.285 | -0.012 |
| 8 | 1 | 7 | 7 | 1 | 6 | 4852.838 | 0.002 |
| 9 | 1 | 8 | 8 | 1 | 7 | 5456.410 | -0.022 |
| 10 | 1 | 10 | 9 | 1 | 9 | 5710.907 | 0.019 |
| 10 | 0 | 10 | 9 | 0 | 9 | 5834.071 | 0.002 |
| 10 | 1 | 9 | 9 | 1 | 8 | 6058.893 | 0.022 |

## 3-Cartesian coordinates

**Table S9.** Cartesian coordinates of conformer *syn-cis-a* optimized at B3LYP-GD3BJ/6-311++G(d,p).

| Center Number | Atomic Number | X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.10397 | -0.48070 | 0.00018 |
| 2 | 6 | -0.88624 | -1.64440 | -0.00009 |
| 3 | 6 | -2.27513 | -1.58282 | -0.00034 |
| 4 | 6 | -2.91362 | -0.34981 | -0.00023 |
| 5 | 6 | -2.14074 | 0.82612 | 0.00022 |
| 6 | 6 | -0.76239 | 0.76441 | 0.00038 |
| 7 | 1 | -0.39535 | -2.61030 | -0.00013 |
| 8 | 1 | -2.87926 | -2.48118 | -0.00061 |
| 9 | 1 | -0.19100 | 1.68633 | 0.00085 |
| 10 | 8 | -2.87145 | 1.99096 | 0.00019 |
| 11 | 1 | -2.29081 | 2.75822 | 0.00163 |
| 12 | 8 | -4.26795 | -0.28278 | -0.00024 |
| 13 | 1 | -4.52986 | 0.64769 | -0.00067 |
| 14 | 6 | 1.34427 | -0.60539 | 0.00016 |
| 15 | 6 | 2.25530 | 0.38333 | -0.00014 |
| 16 | 1 | 1.99088 | 1.43299 | -0.00052 |
| 17 | 1 | 1.73193 | -1.62084 | 0.00041 |
| 18 | 6 | 3.68838 | 0.06774 | -0.00005 |
| 19 | 8 | 4.44489 | 1.20194 | -0.00086 |
| 20 | 1 | 5.37064 | 0.91812 | -0.00064 |
| 21 | 8 | 4.18921 | -1.03536 | 0.00080 |

**Table S10.** Cartesian coordinates of conformer *syn-cis-a* optimized at B3LYP-

| Center Number | Atomic Number | X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.10198 | -0.46882 | 0.00000 |
| 2 | 6 | -0.88182 | -1.63360 | 0.00041 |
| 3 | 6 | -2.27182 | -1.56181 | 0.00061 |
| 4 | 6 | -2.89625 | -0.32327 | 0.00035 |
| 5 | 6 | -2.13185 | 0.85678 | -0.00010 |
| 6 | 6 | -0.75175 | 0.77826 | -0.00036 |
| 7 | 1 | -0.39587 | -2.60166 | 0.00070 |
| 8 | 1 | -2.86869 | -2.46817 | 0.00123 |
| 9 | 1 | -0.19233 | 1.70460 | -0.00092 |
| 10 | 8 | -2.74240 | 2.07295 | -0.00013 |
| 11 | 1 | -3.69882 | 1.93793 | -0.00350 |
| 12 | 8 | -4.25494 | -0.13477 | 0.00080 |
| 13 | 1 | -4.71654 | -0.97918 | -0.00737 |
| 14 | 6 | 1.34827 | -0.60078 | -0.00018 |
| 15 | 6 | 2.26045 | 0.38530 | 0.00056 |
| 16 | 1 | 1.99735 | 1.43508 | 0.00154 |
| 17 | 1 | 1.73279 | -1.61745 | -0.00114 |
| 18 | 6 | 3.69340 | 0.06335 | -0.00005 |
| 19 | 8 | 4.45434 | 1.19315 | 0.00065 |
| 20 | 1 | 5.37904 | 0.90590 | 0.00023 |
| 21 | 8 | 4.18841 | -1.04252 | -0.00109 |

GD3BJ/6-311++G(d,p).

| Center Number | Atomic Number | X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.08724 | -0.44939 | 0.00002 |
| 2 | 6 | 0.84560 | -1.62865 | 0.00000 |
| 3 | 6 | 2.23549 | -1.59568 | -0.00003 |
| 4 | 6 | 2.89917 | -0.37603 | -0.00002 |
| 5 | 6 | 2.15034 | 0.81529 | 0.00002 |
| 6 | 6 | 0.77093 | 0.78178 | 0.00003 |
| 7 | 1 | 0.33550 | -2.58466 | 0.00000 |
| 8 | 1 | 2.82130 | -2.50610 | -0.00005 |
| 9 | 1 | 0.21936 | 1.71557 | 0.00003 |
| 10 | 8 | 2.90439 | 1.96481 | 0.00002 |
| 11 | 1 | 2.33974 | 2.74399 | 0.00011 |
| 12 | 8 | 4.25452 | -0.33676 | -0.00002 |
| 13 | 1 | 4.53557 | 0.58815 | -0.00005 |
| 14 | 6 | -1.36485 | -0.54474 | 0.00003 |
| 15 | 6 | -2.24748 | 0.47050 | -0.00008 |
| 16 | 1 | -1.94478 | 1.50991 | -0.00021 |
| 17 | 1 | -1.76357 | -1.55432 | 0.00014 |
| 18 | 6 | -3.70049 | 0.29013 | -0.00003 |
| 19 | 8 | -4.09827 | -1.01381 | 0.00003 |
| 20 | 1 | -5.06580 | -1.00357 | 0.00012 |
| 21 | 8 | -4.50227 | 1.19974 | -0.00001 |

**Table S11.** Cartesian coordinates of conformer *syn-trans-a* optimized at B3LYP-GD3BJ/6-311++G(d,p).

| Center Number | Atomic Number | X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.08545 | -0.43652 | 0.00030 |
| 2 | 6 | 0.84103 | -1.61706 | 0.00016 |
| 3 | 6 | 2.23230 | -1.57443 | 0.00010 |
| 4 | 6 | 2.88239 | -0.34922 | 0.00005 |
| 5 | 6 | 2.14242 | 0.84626 | 0.00021 |
| 6 | 6 | 0.76086 | 0.79658 | 0.00026 |
| 7 | 1 | 0.33565 | -2.57522 | 0.00026 |
| 8 | 1 | 2.81009 | -2.49306 | 0.00029 |
| 9 | 1 | 0.22165 | 1.73477 | 0.00035 |
| 10 | 8 | 2.77759 | 2.04943 | 0.00049 |
| 11 | 1 | 3.73109 | 1.89522 | -0.00282 |
| 12 | 8 | 4.24467 | -0.18881 | 0.00015 |
| 13 | 1 | 4.68893 | -1.04245 | -0.00708 |
| 14 | 6 | -1.36879 | -0.53906 | 0.00019 |
| 15 | 6 | -2.25306 | 0.47329 | 0.00028 |
| 16 | 1 | -1.95225 | 1.51306 | 0.00044 |
| 17 | 1 | -1.76401 | -1.55001 | -0.00013 |
| 18 | 6 | -3.70625 | 0.28493 | -0.00018 |
| 19 | 8 | -4.09714 | -1.02169 | 0.00023 |
| 20 | 1 | -5.06470 | -1.01588 | -0.00036 |
| 21 | 8 | -4.51319 | 1.18919 | -0.00076 |

**Table S12.** Cartesian coordinates of conformer *syn-trans-b* optimized at B3LYP-GD3BJ/6-311++G(d,p).

| Center Number | Atomic Number | X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.08781 | 0.02137 | 0.00014 |
| 2 | 6 | 0.53886 | -1.30837 | 0.00018 |
| 3 | 6 | 1.89376 | -1.60264 | 0.00005 |
| 4 | 6 | 2.83613 | -0.57676 | -0.00006 |
| 5 | 6 | 2.40049 | 0.75537 | 0.00008 |
| 6 | 6 | 1.04849 | 1.04888 | 0.00011 |
| 7 | 1 | -0.17452 | -2.12210 | 0.00029 |
| 8 | 1 | 2.24633 | -2.62642 | 0.00000 |
| 9 | 1 | 0.72305 | 2.08483 | 0.00025 |
| 10 | 8 | 3.40544 | 1.69473 | 0.00010 |
| 11 | 1 | 3.04018 | 2.58482 | -0.00150 |
| 12 | 8 | 4.15989 | -0.87364 | -0.00016 |
| 13 | 1 | 4.66032 | -0.04667 | -0.00078 |
| 14 | 6 | -1.31946 | 0.38935 | 0.00010 |
| 15 | 6 | -2.38346 | -0.43179 | 0.00018 |
| 16 | 1 | -2.29916 | -1.51066 | 0.00028 |
| 17 | 1 | -1.53524 | 1.45503 | -0.00015 |
| 18 | 6 | -3.74142 | 0.12548 | -0.00006 |
| 19 | 8 | -4.68156 | -0.86042 | -0.00030 |
| 20 | 1 | -5.54478 | -0.42178 | -0.00034 |
| 21 | 8 | -4.04419 | 1.29903 | 0.00007 |

**Table S13.** Cartesian coordinates of conformer *anti-cis-b* optimized at B3LYP-GD3BJ/6-311++G(d,p).

| Center Number | Atomic Number | X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.08746 | 0.03748 | -0.00010 |
| 2 | 6 | 0.53533 | -1.29292 | -0.00014 |
| 3 | 6 | 1.89366 | -1.57866 | -0.00008 |
| 4 | 6 | 2.82504 | -0.54492 | 0.00001 |
| 5 | 6 | 2.39881 | 0.78929 | 0.00002 |
| 6 | 6 | 1.04100 | 1.06860 | -0.00003 |
| 7 | 1 | -0.17404 | -2.10972 | -0.00025 |
| 8 | 1 | 2.23586 | -2.60877 | -0.00011 |
| 9 | 1 | 0.72881 | 2.10605 | -0.00001 |
| 10 | 8 | 3.30061 | 1.80844 | 0.00006 |
| 11 | 1 | 4.19034 | 1.43254 | 0.00020 |
| 12 | 8 | 4.18537 | -0.72586 | 0.00008 |
| 13 | 1 | 4.40480 | -1.66279 | 0.00006 |
| 14 | 6 | -1.32382 | 0.40070 | -0.00012 |
| 15 | 6 | -2.38146 | -0.42741 | 0.00020 |
| 16 | 1 | -2.28919 | -1.50572 | 0.00054 |
| 17 | 1 | -1.54223 | 1.46549 | -0.00040 |
| 18 | 6 | -3.74546 | 0.11698 | 0.00005 |
| 19 | 8 | -4.67506 | -0.87944 | 0.00006 |
| 20 | 1 | -5.54287 | -0.44988 | -0.00001 |
| 21 | 8 | -4.06027 | 1.28660 | -0.00006 |

**Table S14.** Cartesian coordinates of conformer *anti-cis-a* optimized at B3LYP-GD3BJ/6-311++G(d,p).

| Center Number | Atomic Number | X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.07490 | -0.00853 | 0.00005 |
| 2 | 6 | 0.54999 | -1.32971 | 0.00010 |
| 3 | 6 | 1.91006 | -1.59936 | 0.00008 |
| 4 | 6 | 2.83403 | -0.55699 | 0.00000 |
| 5 | 6 | 2.37428 | 0.76697 | -0.00002 |
| 6 | 6 | 1.01708 | 1.03587 | 0.00001 |
| 7 | 1 | -0.14775 | -2.15676 | 0.00017 |
| 8 | 1 | 2.28078 | -2.61670 | 0.00011 |
| 9 | 1 | 0.67385 | 2.06616 | -0.00001 |
| 10 | 8 | 3.36202 | 1.72453 | -0.00006 |
| 11 | 1 | 2.98077 | 2.60785 | -0.00019 |
| 12 | 8 | 4.16282 | -0.83011 | -0.00005 |
| 13 | 1 | 4.64862 | 0.00551 | -0.00004 |
| 14 | 6 | -1.34036 | 0.33472 | 0.00006 |
| 15 | 6 | -2.38289 | -0.51492 | -0.00010 |
| 16 | 1 | -2.26142 | -1.59040 | -0.00026 |
| 17 | 1 | -1.56515 | 1.39698 | 0.00018 |
| 18 | 6 | -3.78271 | -0.08451 | -0.00005 |
| 19 | 8 | -3.94795 | 1.26990 | 0.00011 |
| 20 | 1 | -4.90275 | 1.42664 | 0.00012 |
| 21 | 8 | -4.73104 | -0.83937 | -0.00012 |

**Table S15.** Cartesian coordinates of conformer *anti-trans-b* optimized at B3LYP-GD3BJ/6-311++G(d,p).

| Center Number | Atomic Number | X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.07438 | 0.00580 | 0.00012 |
| 2 | 6 | 0.54718 | -1.31569 | 0.00020 |
| 3 | 6 | 1.91076 | -1.57567 | 0.00014 |
| 4 | 6 | 2.82272 | -0.52493 | 0.00001 |
| 5 | 6 | 2.37133 | 0.80095 | -0.00006 |
| 6 | 6 | 1.00852 | 1.05445 | 0.00001 |
| 7 | 1 | -0.14593 | -2.14624 | 0.00034 |
| 8 | 1 | 2.27191 | -2.59928 | 0.00024 |
| 9 | 1 | 0.67754 | 2.08613 | -0.00003 |
| 10 | 8 | 3.25366 | 1.83720 | -0.00022 |
| 11 | 1 | 4.15032 | 1.47810 | -0.00022 |
| 12 | 8 | 4.18620 | -0.68006 | -0.00002 |
| 13 | 1 | 4.42342 | -1.61266 | -0.00006 |
| 14 | 6 | -1.34476 | 0.34365 | 0.00013 |
| 15 | 6 | -2.38108 | -0.51232 | -0.00018 |
| 16 | 1 | -2.25288 | -1.58711 | -0.00052 |
| 17 | 1 | -1.57247 | 1.40498 | 0.00042 |
| 18 | 6 | -3.78517 | -0.09302 | -0.00010 |
| 19 | 8 | -3.96108 | 1.25856 | 0.00029 |
| 20 | 1 | -4.91685 | 1.40937 | 0.00041 |
| 21 | 8 | -4.72608 | -0.85728 | -0.00032 |

**Table S16.** Cartesian coordinates of conformer *anti-trans-a* optimized at B3LYP-GD3BJ/6-311++G(d,p).