SUPPLEMENTARY MATERIAL

Vibrational spectroscopic investigation and molecular structure of a 5α-reductase inhibitor: finasteride

Lin-Jie Wang\textsuperscript{a,*,} \( ^{\ddagger} \), William B. Zeng\textsuperscript{b}, and Song Gao\textsuperscript{c}

\textsuperscript{a}School of Chemical Engineering, Shengli College, China University of Petroleum, 257000 Dongying, Shandong Province, China
\textsuperscript{b}School of Chemical Engineering, Xiangtan University, 411105 Xiangtan, Hunan Province, China
\textsuperscript{c}School of Optoelectronic Science and Engineering, University of Electronic Science and Technology of China, 610000 Chengdu, Sichuan Province, China

*\textit{e-mail: linjiewang1989@hotmail.com}
Figure 1S. The unit cell structure of finasteride
Table 1S. All of the calculated bond lengths and angles of Finasteride at different functionals in comparison with the XRD data

| Parameter       | Exp   | Calculated with GGA/ | PW91 | RPBE | HCTH | PBE  | BLYP |
|-----------------|-------|----------------------|------|------|------|------|------|
| Bond Length (Å) |       |                      |      |      |      |      |      |
| C₁⁻C₂          | 1.329 | 1.343                | 1.349| 1.338| 1.345| 1.346|
| C₁⁻C₉          | 1.508 | 1.514                | 1.525| 1.513| 1.516| 1.525|
| C₂⁻C₃          | 1.472 | 1.482                | 1.490| 1.475| 1.484| 1.489|
| C₃⁻O₁          | 1.230 | 1.234                | 1.240| 1.227| 1.236| 1.239|
| C₃⁻N₁          | 1.343 | 1.377                | 1.387| 1.367| 1.379| 1.387|
| N₁⁻H₅₆        | 0.983 | 1.017                | 1.019| 1.009| 1.018| 1.019|
| N₁⁻C₄         | 1.472 | 1.461                | 1.472| 1.451| 1.462| 1.476|
| C₄⁻C₉         | 1.541 | 1.551                | 1.563| 1.546| 1.552| 1.563|
| C₄⁻C₅         | 1.499 | 1.521                | 1.531| 1.515| 1.523| 1.531|
| C₅⁻C₆         | 1.531 | 1.529                | 1.539| 1.521| 1.530| 1.542|
| C₆⁻C₇         | 1.541 | 1.535                | 1.546| 1.528| 1.536| 1.547|
| C₇⁻C₈         | 1.541 | 1.555                | 1.568| 1.550| 1.556| 1.57 |
| C₇⁻C₁₃        | 1.527 | 1.530                | 1.544| 1.525| 1.531| 1.543|
| C₈⁻C₁₀        | 1.548 | 1.540                | 1.552| 1.533| 1.541| 1.552|
| C₈⁻C₉         | 1.562 | 1.561                | 1.577| 1.563| 1.562| 1.577|
| C₉⁻C₁₇        | 1.535 | 1.546                | 1.558| 1.541| 1.547| 1.559|
| C₁₀⁻C₁₁       | 1.532 | 1.538                | 1.548| 1.530| 1.539| 1.55 |
| C₁₁⁻C₁₂       | 1.522 | 1.532                | 1.544| 1.530| 1.533| 1.544|
| C₁₂⁻C₁₃       | 1.542 | 1.550                | 1.562| 1.545| 1.551| 1.563|
| C₁₂⁻C₁₆       | 1.555 | 1.564                | 1.577| 1.560| 1.565| 1.578|
| C₁₂⁻C₁₈       | 1.519 | 1.538                | 1.551| 1.534| 1.539| 1.551|
| C₁₃⁻C₁₄       | 1.532 | 1.533                | 1.543| 1.526| 1.534| 1.545|
| C₁₄⁻C₁₅       | 1.545 | 1.552                | 1.561| 1.539| 1.553| 1.564|
| C₁₅⁻C₁₆       | 1.548 | 1.549                | 1.559| 1.541| 1.550| 1.562|
| C₁₆⁻C₁₉       | 1.525 | 1.529                | 1.544| 1.530| 1.531| 1.541|
| C₁₉⁻O₂        | 1.219 | 1.235                | 1.239| 1.225| 1.237| 1.239|
| C₁₉⁻N₂        | 1.349 | 1.368                | 1.377| 1.362| 1.369| 1.377|
| N₂⁻C₂₀       | 1.478 | 1.483                | 1.495| 1.478| 1.484| 1.499|
| N₂⁻H₅₅       | 0.952 | 1.014                | 1.015| 1.004| 1.016| 1.015|
| C₂₀⁻C₂₁       | 1.530 | 1.535                | 1.547| 1.531| 1.537| 1.547|
| C₂₀⁻C₂₂       | 1.535 | 1.535                | 1.548| 1.531| 1.536| 1.546|
| C₂₀⁻C₂₃       | 1.521 | 1.531                | 1.544| 1.527| 1.532| 1.544|
| Bond angle (°) |       |                      |      |      |      |      |      |
| C₂⁻C₁⁻C₉     | 121.519| 122.131              | 122.312| 121.816| 122.147| 122.317 |
| Bond | Distance (Å) |
|------|--------------|
| C1-C2-C3 | 121.756 |
| C2-C3-O1 | 121.457 |
| O1-C3-N1 | 123.201 |
| C2-C3-N1 | 115.312 |
| C3-N1-H36 | 113.171 |
| C3-N1-C4 | 120.898 |
| H36-N1-C4 | 125.791 |
| N1-C4-C9 | 109.732 |
| N1-C4-C5 | 110.910 |
| C5-C4-C9 | 114.197 |
| C4-C5-C6 | 109.568 |
| C5-C6-C7 | 111.067 |
| C6-C7-C8 | 111.262 |
| C6-C7-H8 | 107.527 |
| C8-C7-C13 | 108.806 |
| C7-C8-C9 | 110.445 |
| C7-C8-C10 | 112.350 |
| C9-C8-C10 | 113.168 |
| C1-C9-C4 | 105.079 |
| C1-C9-C8 | 113.289 |
| C1-C9-C17 | 106.638 |
| C4-C9-C8 | 107.200 |
| C4-C9-C17 | 112.686 |
| C8-C9-C17 | 111.847 |
| C8-C10-C11 | 113.222 |
| C10-C11-C12 | 111.152 |
| C11-C12-C13 | 107.825 |
| C11-C12-C16 | 116.225 |
| C11-C12-C18 | 110.008 |
| C13-C12-C16 | 100.112 |
| C13-C12-C18 | 113.046 |
| C16-C12-C18 | 109.381 |
| C12-C13-C14 | 103.642 |
| C12-C13-C7 | 112.861 |
| C14-C13-C7 | 118.550 |
| C13-C14-C15 | 104.203 |
| C14-C15-C16 | 106.500 |
| C15-C16-C12 | 104.056 |
| Bond              | 1st Value  | 2nd Value  | 3rd Value  | 4th Value  | 5th Value  | 6th Value  |
|-------------------|------------|------------|------------|------------|------------|------------|
| C_{15}-C_{16}-C_{19} | 112.109    | 112.947    | 112.918    | 112.962    | 112.944    | 112.967    |
| C_{12}-C_{16}-C_{19} | 112.932    | 114.748    | 115.818    | 116.501    | 114.856    | 115.796    |
| C_{16}-C_{19}-O_{2} | 122.433    | 122.734    | 122.766    | 122.505    | 122.756    | 122.705    |
| N_{2}-C_{19}-C_{16} | 114.222    | 114.063    | 113.900    | 114.162    | 114.072    | 114.210    |
| N_{2}-C_{19}-O_{2} | 123.264    | 123.180    | 123.325    | 123.330    | 123.147    | 123.078    |
| C_{19}-N_{2}-C_{20} | 126.172    | 126.320    | 127.192    | 127.779    | 126.304    | 126.915    |
| C_{19}-N_{2}-H_{35} | 117.067    | 117.000    | 116.703    | 116.486    | 117.007    | 116.795    |
| C_{20}-N_{2}-H_{35} | 116.748    | 116.673    | 116.075    | 115.734    | 116.687    | 116.243    |
| N_{2}-C_{20}-C_{21} | 109.896    | 109.788    | 110.002    | 110.365    | 109.846    | 109.965    |
| N_{2}-C_{20}-C_{22} | 108.796    | 109.981    | 110.245    | 109.766    | 109.952    | 110.040    |
| N_{2}-C_{20}-C_{23} | 105.495    | 106.318    | 106.131    | 106.288    | 106.332    | 106.198    |
| C_{21}-C_{20}-C_{22} | 110.150    | 110.649    | 110.784    | 110.520    | 110.617    | 110.685    |
| C_{21}-C_{20}-C_{23} | 110.145    | 110.082    | 110.006    | 109.969    | 110.045    | 109.966    |
| C_{22}-C_{20}-C_{23} | 112.241    | 109.932    | 109.567    | 109.846    | 109.958    | 109.890    |

mean absolute deviation: 0.457 0.543 0.557 0.458 0.522
Table 2S. Dihedral angles of Finasteride at different functionals in comparison with the XRD data

| Dihedral angle(º)          | Exp | Calculated with GGA/ |       |       |       |       |
|---------------------------|-----|----------------------|-------|-------|-------|-------|
|                           |     | PW91                 | RPBE  | HCTH  | PBE   | BLYP  |
| C1-C2-C3-O1               | 162.724 | 167.854  | 169.211 | 167.290 | 167.889 | 169.57 |
| C1-C2-C3-N1               | -15.337 | -9.756   | -8.195   | -10.962  | -9.730   | -8.155  |
| C1-C9-C4-N1               | -55.112 | -53.545  | -53.155  | -54.066  | -53.571  | -52.945  |
| C1-C9-C4-C3               | 179.658 | -179.555  | -179.437  | 179.338  | -179.550  | -179.290  |
| C1-C9-C8-C7               | -171.891 | -171.865  | -171.736  | -171.768  | -171.871  | -171.984  |
| C1-C9-C8-C10              | 61.170  | 60.715  | 60.371   | 59.287   | 60.666   | 60.163  |
| C2-C3-N1-C4               | -10.612 | -18.570  | -20.527  | -16.388  | -18.685  | -19.759  |
| C13-C12-C16-C19           | -161.489 | -164.157  | -164.977  | -165.140  | -164.376  | -164.947  |
| C2-C1-C9-C4               | 34.582  | 30.637  | 29.754   | 32.078   | 30.563   | 30.473  |
| C2-C1-C9-C8               | 151.286 | 147.198  | 145.888  | 148.491  | 147.089  | 146.710  |
| C2-C1-C9-C17              | -85.246 | -89.267  | -90.320  | -87.809  | -89.310  | -89.596  |
| C3-N1-C4-C5               | 174.566 | 178.416  | 179.944  | 178.071  | 178.527  | 178.889  |
| C3-N1-C4-C9               | 47.467  | 52.044  | 53.174   | 50.831   | 52.181   | 52.147  |
| C3-C2-C1-C9               | 0.050  | 1.109   | 0.994    | 0.309    | 1.172    | 0.219  |
| N1-C4-C5-C6               | 176.785 | 175.218  | 174.853  | 176.512  | 175.190  | 175.037  |
| N1-C4-C9-C17              | 60.611  | 62.915  | 63.088   | 61.830   | 62.795   | 63.554  |
| N1-C4-C9-C8               | -175.912 | -173.747  | -173.324  | -174.573  | -173.797  | -173.059  |
| C4-N1-C3-O1               | 171.365 | 163.819  | 162.056  | 165.359  | 163.695  | 162.514  |
| C4-C5-C6-C7               | 55.174  | 54.816  | 54.419   | 53.480   | 54.927   | 53.997  |
| C4-C9-C8-C10              | 176.621 | 176.547  | 175.916  | 174.742  | 176.459  | 175.894  |
| C5-C4-N1-H36              | -10.036 | -29.839  | -32.176  | -28.802  | -29.793  | -32.006  |
| C5-C4-C9-C8               | 58.858  | 60.243  | 60.394   | 58.831   | 60.225   | 60.596  |
| C5-C4-C9-C17              | -64.619 | -63.095  | -63.194  | -64.766  | -63.183  | -62.791  |
| C5-C6-C7-C8               | -56.075 | -52.708  | -52.360  | -52.378  | -52.857  | -51.757  |
| C5-C6-C7-C13              | -178.114 | -174.570  | -174.197  | -174.598  | -174.735  | -173.654  |
| C6-C5-C4-C9               | -58.610  | -60.003  | -59.988  | -57.997  | -60.041  | -59.874  |
| C6-C7-C8-C9               | 57.308  | 53.954  | 53.956   | 54.552   | 54.083   | 53.588  |
| C6-C7-C8-C10              | -175.300 | -177.294  | -176.623  | -175.037  | -177.100  | -177.106  |
| C6-C7-C13-C14             | -56.251 | -53.665  | -53.478  | -53.308  | -53.845  | -53.287  |
| C6-C7-C13-C12             | -177.636 | -177.549  | -177.958  | -178.739  | -177.738  | -177.708  |
| C7-C8-C9-C17              | 67.511  | 67.419  | 67.556   | 67.578   | 67.418   | 67.248  |
| C7-C8-C10-C11             | 50.352  | 53.136  | 52.827   | 50.756   | 53.099   | 52.800  |
| C7-C13-C12-C11            | -62.276 | -60.064  | -59.827  | -59.585  | -60.007  | -59.722  |
| C7-C13-C12-C16            | 175.796 | 179.111  | 179.597  | 179.922  | 179.189  | 179.713  |
| C7-C13-C12-C18            | 59.552  | 62.611  | 62.796   | 62.748   | 62.647   | 62.843  |
| Bond          | C7-C13-C14-C15 | C8-C10-C11-C12 | C8-C7-C13-C12 | C8-C7-C14-C14 | C9-C8-C10-C11 | C9-C8-C7-C13 | C10-C8-C7-C13 | C10-C11-C12-C13 | C10-C11-C12-C18 | C10-C11-C12-C16 | C11-C12-C13-C14 | C11-C12-C16-C15 | C11-C12-C16-C19 | C12-C13-C14-C15 | C12-C16-C15-C14 | C12-C16-C19-O2 | C12-C16-C19-N2 | C13-C12-C16-C15 | C13-C14-C15-C16 | C14-C13-C12-C16 | C14-C15-C16-C19 | C15-C16-C12-C18 | C15-C16-C19-O2 | C15-C16-C19-N2 | C16-C19-N2-H35 | C16-C19-N2-C20 | C18-C12-C16-C19 | C19-N2-C20-C21 | C19-N2-C20-C22 | C19-N2-C20-C23 | C20-N2-C19-O2 |
|--------------|----------------|----------------|---------------|---------------|---------------|---------------|---------------|----------------|----------------|----------------|----------------|----------------|----------------|---------------|----------------|----------------|---------------|----------------|----------------|---------------|----------------|---------------|---------------|----------------|---------------|---------------|----------------|---------------|
|              | -160.911       | -163.787       | -164.328      | -165.133      | -163.765      | -164.351      | -53.579        | 58.932         | -179.683       | 176.279         | -178.080       | -155.424       | 82.758         | -34.955         | 19.021         | 90.225         | -39.672         | 9.554          | 141.383        | 79.293         | -26.938        | 156.234        | -5.601         | 173.015        | -42.525        | 61.357         | -59.317        | -3.783         | -0.949         | 0.097          | -2.301         | -0.547         | 0.483          |
**Table 3S.** All of the observed and calculated vibrational frequencies of finasteride using by GGA method with different functionals

| Vib. no. | Assignments | Exp | Calculated with GGA/ |  |
|----------|-------------|-----|----------------------|---|
|          |             |     | PW91     | PBE | RPBE | BLYP | HCTH |
| 1        | νN₂H₃₅      | 3429 | 3523.52  | 3517.12 | 3533.87 | 3503.01 | 3667.07 |
| 2        | νN₁H₆       | 3240 | 3517.57  | 3514.26 | 3505.29 | 3473.15 | 3634.81 |
| 3        | νC₂H₂       | 3201.78 | 3218.12 | 3217.38 | 3150.47 | 3126.47 |
| 4        | νC₁H₁      | 3116 | 3138.43  | 3146.81 | 3143.32 | 3110.35 | 3271.74 |
| 5        | νₙC₂₋₁,₂₂H  |     | 3119.13  | 3123.82 | 3139.69 | 3086.35 | 3247.78 |
| 6        | νₙC₂₋₁,₂₂H  |     | 3117.50  | 3122.25 | 3129.45 |            | 3247.78 |
| 7        | νₙC₁₈H₂₃-2₅ |     | 3115.47  | 3122.16 | 3125.50 | 3082.91 | 3190.46 |
| 8        | νₙC₂₃H₂₂-₂₄  |   | 3100.07  | 3107.15 | 3114.27 | 3066.25 | 3203.17 |
| 9        | νₙC₁₇H₂₁-₂₂   | | 3096.47  | 3100.72 | 3111.17 | 3069.79 | 3184.78 |
| 10       | νₙC₁₇H₂₀-₂₂   | | 3092.62  | 3096.56 | 3105.83 | 3066.20 | 3184.78 |
| 11       | νₙC₁₈H₂₃-2₅  | | 3084.99  | 3086.91 | 3095.89 | 3057.87 | 3170.07 |
| 12       | νₙC₂₁,₂₂H₂₆-₂₇,₂₉-₃₁ | | 3083.77  | 3085.05 | 3094.68 | 3053.07 | 3189.94 |
| 13       | νₙC₂₁,₂₂H₂₆-₂₇,₂₉-₃₁ | | 3082.64  | 3082.34 | 3084.79 | 3053.07 | 3167.05 |
| 14       | νₙC₁₅H₁₇-₁₈   | | 3079.38  | 3081.74 | 3080.78 |            | 3209.23 |
| 15       | νₙC₂₃H₃₃-₃₄  | | 3064.71  | 3066.56 | 3076.26 | 3030.93 | 3145.59 |
| 16       | νₙC₁₄H₁₅-₁₆  | | 3059.17  | 3061.99 | 3069.63 | 3038.08 | 3159.86 |
| 17       | νₙC₁₀H₁₀-₁₁   | | 3053.51  | 3060.65 | 3066.55 | 3024.62 | 3194.69 |
| 18       | νₙC₆H₆-₇      | | 3045.63  | 3052.07 | 3060.83 | 3022.24 | 3130.18 |
| 19       | νₙC₁₁H₁₂-₁₃   | | 3035.79  | 3036.59 | 3038.54 |            | 3101.20 |
| 20       | νₙC₅H₄-₅      | | 3033.09  | 3032.53 | 3038.05 | 3012.15 | 3086.08 |
| 21       | νₙC₁₀H₁₀-₁₁   | | 3029.51  | 3029.35 | 3034.48 |            | 3095.65 |
| 22       | νₙC₁₈H₂₃-2₅   | | 3025.57  | 3027.64 | 3033.28 | 3008.52 | 3086.74 |
| 23       | νₙC₁₇H₂₀-₂₂   | | 3020.58  | 3022.93 | 3030.96 | 3005.47 | 3116.47 |
| 24       | νₙC₁₄H₁₅-₁₆   | | 3014.43  | 3017.73 | 3027.58 | 2996.55 | 3033.56 |
| 25       | νₙC₁₀H₁₀-₁₁   | | 3013.27  | 3017.05 | 3024.41 | 2999.87 |            |
| 26       | νₙC₂₂H₂₉-₃₁   | | 3012.34  | 3014.82 | 3023.52 | 2995.81 | 3090.44 |
| 27       | νₙC₂₁H₂₆-₂₇; νₙC₁₅H₁₇-₁₈ | | 3009.45  | 3007.99 | 3023.11 | 2989.99 | 2987.80 |
| 28       | νC₁₁H₆     | | 2997.08  | 3000.67 | 3011.55 | 2981.95 | 3023.44 |
| 29       | ν₂C₂₃H₃₃-₃₄ | | 2986    | 2994.88 | 2992.67 | 2994.43 | 2973.46 | 3053.52 |
| 30       | ν₁C₂₃H₃₃-₃₄ | | 2969    | 2972.46 | 2977.34 | 2971.53 | 2950.33 | 3074.22 |
| 31       | ν₁C₆H₆-₇    | | 2967.02  | 2973.26 | 2968.76 | 2946.50 | 3033.93 |
| 32       | ν₂C₁₁H₁₂-₁₃ | | 2962.53  | 2963.08 | 2965.52 | 2955.85 |            |
| 33       | ν₁C₁₈H₁₉    | | 2936    | 2924.59 | 2924.11 | 2955.08 | 2907.17 | 2932.14 |
| 34       | ν₁C₁₃H₁₄    | | 2904    | 2917.88 | 2917.30 | 2928.69 | 2923.26 | 3075.97 |
| C4H3 | 2866 | 2888.82 | 2885.14 | 2887.32 | 2897.14 | 2945.62 |
| C3O2; B11H36; B2H2 | 1688 | 1698.01 | 1695.16 | 1686.55 | 1667.94 | 1775.34 |
| C19O2; B2H3 | 1668 | 1686.02 | 1693.63 | 1682.14 | 1653.36 | 1740.00 |
| C1 | 1600 | 1634.60 | 1635.8 | 1620.95 | 1607.62 | 1661.61 |
| δaC21,22,23H26-28-29-31-32-34; | 1505 | 1500.91 | 1501.91 | 1514.41 | 1506.00 | 1556.08 |
| B2H3; δaC21,22,23H26-28-29-31-32-34; | 1495.46 | 1499.02 | 1502.48 | 1488.60 | 1539.70 |
| δC14H15-16 | 1488.82 | 1490.38 | 1491.79 | 1493.64 | 1601.99 |
| δC10H10-11; δaC18H23-25 | 1482.71 | 1480.27 | 1490.61 | 1495.85 | 1576.07 |
| δaC21,22,23H26-28-29-31-32-34; | 1480.01 | 1479.87 | 1488.31 | 1487.40 | 1529.81 |
| δC11H12-13, δC18H23-25 | 1473.83 | 1475.15 | 1481.71 | 1479.41 | 1549.98 |
| δaC17H20-22 | 1471.75 | 1470.6 | 1478.67 | 1480.22 | 1532.42 |
| δaC21,23H26-28-32-34 | 1468.06 | 1466.4 | 1476.78 | 1470.34 | 1510.52 |
| δaC21,22,23H26-28-29-31-32-34; δaC18H23-25 | 1465.01 | 1461.61 | 1476.07 | 1473.7 | 1495.66 |
| δaC17H20-22; δC3,6H4-5,6-7 | 1463.39 | 1460.6 | 1474.29 | 1476.47 |
| δC18H23-25; δC6,10H6-7,10-11 | 1461.70 | 1460.07 | 1472.68 | 1473.63 | 1526.51 |
| δC13H17-18 | 1461.44 | 1459.02 | 1469.73 | 1470.21 |
| δaC17H20-22; δC6H6-7 | 1458.86 | 1457.6 | 1465.98 | 1476.47 |
| δaC21,22,23H26-28-29-31; B2H3 | 1456.99 | 1455.36 | 1465.13 | 1455.55 | 1489.29 |
| δaC18H23-25; δC10,15H10-11,17-18 | 1450 | 1450.76 | 1448.03 | 1451.86 | 1462.99 |
| δC3H4-5; δaC17H20-22 | 1449.48 | 1440.15 | 1448.64 | 1463.92 | 1490.47 |
| δaC21,22,23H26-28-29-31-32-34; | 1439.70 | 1436.38 | 1442.11 | 1455.97 |
| βC1H1; B2H3; γC6H3 | 1401.43 | 1395.65 | 1405.07 | 1399.90 | 1454.72 |
| δC21,22,23H26-28-29-31-32-34 | 1392 | 1395.47 | 1391.59 | 1402.34 | 1419.03 |
| C3H4-5; γC6H3 | 1385.66 | 1383.81 | 1392.84 | 1484.35 | 1409.49 |
| δC18H23-25; γC4,13H5,14 | 1383 | 1383.03 | 1382.59 | 1382.64 | 1388.30 | 1445.43 |
| δC17H20-22; βC1,2,7,13H1,2,8,14; γC10H10-11 | 1376.69 | 1370.93 | 1379.24 | 1373.12 |
| βC1,7,13H1,8,14; δC18H23-25; | 1373.07 | 1368.81 | 1376.53 | 1370.15 | 1449.96 |
| δC22,23H29-31-32-34 | 1368.82 | 1364.04 | 1374.31 | 1368.42 | 1430.32 |
| δC21,22,23H26-28-29-31-32-34 | 1364 | 1363.23 | 1361.62 | 1369.55 | 1368.42 | 1428.95 |
| γC6H3 | 1358.85 | 1353.6 | 1367.68 | 1357.35 | 1421.09 |
| δC17H20-22 | 1353.85 | 1347.88 | 1360.54 | 1353.28 | 1409.49 |
| γC4,7,8,11,13H3,8,9,13,14; γC10H10-11; C10H10 | 1344.65 | 1341.62 | 1355.77 | 1344.04 | 1381.35 |
| γC7,13H8,14 | 1336.85 | 1333.89 | 1347.59 | 1343.46 |
| γC4,7,13,16H3,8,9,14,19; γC5,11H4,5,12-13; | 1334.97 | 1330.51 | 1338.04 | 1340.40 | 1378.70 |
| γC4,6,15H3,6,17,19; γC3H4-5 | 1330 | 1331.26 | 1326.9 | 1329.08 | 1336.54 | 1364.80 |
| γC4,7,8,13H3,8,9,14; γC11H12-13 | 1328.93 | 1324.52 | 1321.96 | 1340.40 | 1381.81 |
| γC4,7,15,16H3,8,17,19; γC5,11H4,5,12-13; | 1322.14 | 1318.87 | 1317.68 | 1326.74 | 1333.10 |
| βN1H6; γC4,10,11H13,11,12; γC3H4-5 | 1317.07 | 1310.21 | 1315.38 | 1323.09 | 1344.17 |
| βN1H6, C2H2; γC8H9; τC11H12-13 | 1306.20 | 1301.54 | 1305.83 | 1311.85 |
75 βC₂H₅; γC₄,7,16H₃,8,19; δC₁₄H₁₅-16   1299.34 1295.94 1302.58 1300.24 1354.83
76 γC₄,6,7,8,11H₃,6,8,9,14   1291 1292.38 1288.78 1290.29 1296.93 1320.47
77 γC₈,13,16H₉,13,19; δC₁₄H₁₅-16,17,18   1290.22 1285.45 1284.93 1289.73 1305.38
78 γC₈,14,15,16H₉,15,18,19   1277 1274.40 1268.44 1274.32 1282.12 1324.15
79 δC₁₄H₁₅-16,17-18   1264.24 1262.69 1263.45 1259.41 1286.65
80 γC₇,11H₈,13; τC₁₀H₁₀-11   1257 1250.16 1247.23 1247.02 1250.71 1279.97
81 γC₈,14,15,16H₆,6C₁₅H₁₅-16; δasC₂₁,2₂H₂₆-2₈,2₉,3₁,3₂,3₄   1245.53 1238.99 1301.04
82 γC₄,5H₃,5; τC₆H₆-7   1243.47 1239.61 1235.32 1237.10 1269.61
83 γC₈,13,16H₉,13,19; δC₁₄H₁₅-16   1230.85 1230.86 1225.76 1235.53 1257.36
84 γC₁₄H₁₆; τC₁₅H₁₇-18; δasC₂₁,2₂,2₃H₂₆-2₈,2₉,3₁,3₂,3₃,3₄   1227.94 1227.42 1223.17 1228.25 1270.72
85 τC₁₄,1₅H₁₅-16,17-1₈   1225 1225.56 1225.35 1217.17 1224.96
86 τC₁₄,1₅H₁₅-16,17-1₈; γC₁₆H₁₉;   1203 1220.53 1217.41 1213.03 1210.22 1237.60
87 βC₁₁H₇; τC₅H₅   1213.14 1207.87 1205.79 1208.79
88 τC₁₀,1₄H₁₀-1₁,1₅-1₆; δC₁₆H₁₉; δasC₁₈H₂₃-2₅;   1209.11 1206.75 1202.35 1206.65 1234.82
89 γC₇,1₃H₈,1₄; τC₁₀H₁₀-1₁; βN₂H₃₅   1191.03 1189.47 1186.67 1201.21 1224.77
90 βC₁₁H₇; βN₂H₃₅; γC₄,6,1₆H₃,7,1₉; τC₅H₄₅   1186.76 1183.79 1180.24 1185.10 1199.03
91 βN₂H₃₅; γC₁₆H₁₉   1168 1170.58 1167.75 1164.15 1182.65
92 βC₁₂H₁₂; τC₅,8,₁₂H₄,₉,₁₂; νC₆C₉   1157.20 1153.71 1148.79 1154.19 1189.71
93 βC₁₂H₁₂; γC₄,₁₀H₃,₁₁; τC₁₁H₁₂-₁₃; νC₆C₉   1150.21 1145.9 1141.19 1147.03 1254.11
94 γC₇Hₘ; νC₇C₁₃   1143.50 1141.43 1127.24
95 βC₁₂H₁₂;   1125 1123.38 1120.32 1117.23 1124.49 1180.98
96 βC₁₂H₁₂; βN₁H₃₆; νC₄N₁   1113.72 1110.81 1109.13 1112.38 1173.47
97 γC₇,₁₆H₈,₁₉; δasC₁₈H₂₃-2₅; C₇; C₁₂; νC₁₃C₁₄   1103.49 1101.86 1096.05 1105.50 1148.38
98 βC₁₂H₁₂; νC₆H₆-₇; γC₁₃H₁₄; βN₁H₃₆; C₉;   1097.89 1095.59 1085.77 1092.13 1152.23
99 γC₁₁,₁₃,₁₆H₁₂,₁₄,₁₉; τC₁₄,₁₅H₁₅-1₆,1₇-₁₈   1091.94 1088.9 1079.36 1081.57 1144.63
100 γC₄,₅,₇H₃₅,₈   1077.42 1075.76 1066.54 1074.45 1115.73
101 γC₈H₉; τC₁₁H₁₂-₁₃   1065 1056.01 1055.08 1058.67 1060.70 1107.54
102 δasC₂₁,₂₂,₂₃H₂₆-₂₈,₂₉,₃₁-₃₄   1053.57 1053.43 1045.31 1047.06 1102.30
103 γC₈H₉; δC₁₀H₁₀-₁₁; δasC₂₃H₃₂-₃₄; ring relaxation vibration   1051.32 1050.28 1041.49 1039.20
104 δasC₂₁,₂₂,₂₃H₂₆-₂₈,₂₉,₃₁-₃₄   1040.91 1039.57 1037.85 1036.09 1084.19
105 γC₁₆H₁₉; νC₁₅₁₆   1027 1028.16 1028.04 1013.01 1032.29 1074.95
106 γC₆,₈,₁₁H₆,₉,₁₄; τC₁₄H₁₅-₁₆; νC₅C₆   1024.14 1023.45 1011.75 1008.89 1070.43
107 γC₈,₁₁,₁₆H₉,₁₂,₁₉; βC₁₄H₁₅-₁₆; γC₁₅H₁₇-₁₈   1021.76 1020.63 1008.26 1002.55 1050.14
108 δasC₅H₅₆; νC₅H₆   995.65 995.97 985.95 996.92 1042.38
109 γC₄,₁₁H₃,₁₃; τC₃H₄-₅; δasC₁₈H₂₃-₂₅   991 992.30 988.64 985.22 980.25 1036.42
110 γC₁₁H₁₃; δasC₁₇H₂₀-₂₂   985.02 983.28 981.42 978.00
111 γC₁₂H₁₂   976.07 978.29 971.37 971.16 1014.62
112 γC₁₁,₁₄,₁₆H₁₃,₁₆,₁₉; δasC₁₈H₂₃,₂₄,₂₅   968 965.32 965.38 966.38 962.83
113 $\delta_{as}C_{21,22,23}H_{26-28,29-31,32-34}$ 960 960.90 957.44 951.82 957.43 1019.13
114 $\nu C_{14}C_{15}$ 952.56 951.75 942.66 945.45 987.96
115 $\gamma C_{5,7,10,14,15}H_{4-5,8,10-11,15,17}$; $\delta_{as}C_{17}H_{20-22}$ 940.40 938.4 935.43 933.02 1002.46
116 $\delta_{as}C_{17}H_{20-22}$ 937 933.86 929.97 926.18 925.07 965.39
117 $\gamma C_{6}H_{6-7}$; $\delta_{as}C_{17}H_{20-22}$ 929.04 925.62 914.51 924.00 974.00
118 $\delta_{as}C_{20,21,22,23}H_{26-28,29-31,32-33}$ 925.04 924.11 914.04 912.61
119 $\delta_{as}C_{21,22,23}H_{26-28,29-31,32-34}$ 914 914.18 914.04 907.11 909.10 952.86
120 $\rho C_{5,11}H_{4-5,12-13}$ 910.90 910.68 904.78 896.65 955.99
121 $\rho C_{6}H_{6-7}$; $\gamma C_{10,11}H_{10,12-13}$; $\delta_{as}C_{18,23}H_{23-25,32-34}$ 907.26 906.36 898.94 894.27 945.40
122 $\delta_{as}C_{23}H_{32-34}$ 898.64 899.42 886.65 892.84 927.02
123 $\beta N_{1}H_{36}$; $\gamma C_{6}H_{6-7}$; $\rho C_{10}H_{10-11}$; $\delta_{as}C_{17}H_{20-22}$ 890 881.87 881.36 873.24 873.09 915.85
124 $\gamma C_{5,14}H_{4-5,15-16}$; $\delta_{as}C_{17}H_{20-22}$ 848.71 846.64 837.69 866.70 872.74
125 $\rho C_{14}H_{15-16}$; $\gamma C_{15}H_{17-18}$ 836.93 838.37 831.66 828.59 878.75
126 $\gamma C_{11}H_{12-13}$ 833.08 838.35 819.96 813.86 831.59
127 $\gamma C_{12}H_{1,2}$ 810.02 808.83 815.5 803.72 849.33
128 $\gamma C_{1,6,16}H_{1,6-7,10-11}$ 803.48 803.96 798.23 786.95
129 $\gamma C_{13,14,16}H_{14,16-19}$; $\nu C_{20}C_{21-22}$; $\nu C_{16}C_{19}$ 786.72 786.15 776.94 776.53 820.32
130 $\rho C_{15}H_{17-18}$; $\gamma C_{16}C_{19}$ 766 765.47 766.83 764.38 752.60 759.38
131 $\gamma C_{8,15}H_{4-7}$; $\delta C_{19}O_{2}$ 761.65 763.46 754.11 753.38
132 $\nu C_{20}C_{21-23}$; 741 733.68 732.96 719.8 716.41
133 $\nu C_{20}C_{18-17}$; $\rho C_{5}H_{4-5}$ 731.66 729.54 715.3 712.00 757.08
134 $\gamma C_{1,2}H_{1,2}$ 688 694.58 695.34 698.79 685.92 716.10
135 $\rho C_{10,14,15}H_{10-11,15-16,17-18}$; $\gamma C_{18}H_{25}$; $\nu$ ring prckering vibration 676.85 678.05 665.6 666.42 668.36
136 $\gamma C_{7}H_{8}$; ring prckering vibration 649.17 647.31 638.02 642.48
137 $\gamma N_{1}H_{36}$; ring prckering vibration 613 616.65 615.8 615.23 616.40 635.34
138 $\gamma N_{1}H_{36}$; $\rho C_{15}H_{17-18}$ 600 602.30 598.19 599.96 601.32 635.34
139 $\gamma N_{1}H_{36}$; $\rho C_{5}H_{4-5}$ 572 574.28 570.03 570.06 571.82 629.93
140 $\gamma N_{1}H_{36}$; $\rho C_{5,14}H_{4-5,15-16}$ 548.78 542.55 543.11 550.72 580.23
141 $\gamma N_{1}H_{36}$; $\delta C_{18}H_{23-25}$ 536 534.64 532.88 524.35 529.12 598.24
142 $\gamma N_{1,2}H_{36,35}$ 522.00 519.78 513.74 515.76 554.08
143 $\gamma N_{1}H_{36}$; $\nu C_{2}H_{2}$ 502 498.83 496.65 495.23 498.62 544.97
144 $\gamma N_{2}H_{35}; \nu C_{6,10}H_{6-7,10-11}$ 484 488.10 488.53 486.01 484.23 522.52
145 $\delta_{as}C_{21,22,23}H_{26-28,29-31,32-34}$; $\nu C_{19}$ 470.88 470.9 473.41 467.87 518.31
146 $\gamma N_{2}H_{35}$; $\gamma C_{19}O_{2}$ 463 458.40 460.74 460.29 453.19 489.16
147 $\gamma N_{1}H_{36}$; $\nu C_{4,5}H_{4}$ 448.63 445.88 449.29 447.19 444.70
148 $\gamma N_{1,2}H_{36,35}$; ring prckering vibration 432 429.69 428.79 427.73 427.43 459.89
149 $\delta_{as}C_{21,22,23}H_{26-28,29-31,32-34}$; $\gamma C_{1}H_{1}$; $\gamma N_{1}H_{36}$; $\nu C_{19}O_{2}$ 422.12 419.96 420.75 423.98 454.36
150 $\delta_{as}C_{21,22,23}H_{26-28,29-31,32-34}$; $\gamma N_{2}H_{35}$; $\nu C_{19}O_{2}$ 416.92 416.81 418.08 417.94
151 $\gamma N_{2}H_{35}; \gamma N_{1}H_{36}; \nu C_{10,11}H$ 411.62 413.59 412.34 413.78

1,10,11,15,16,17,18
| 152 γN₂H₃₅ | 402.23 | 408.27 | 409.22 | 406.07 | 403.76 |
| Mean Absolute Deviation | 14.405 | 14.846 | 16.696 | 15.632 | 61.174 |