# Electronic Supplementary Information

# Comprehensive understanding of Methyl 2-Naphthyl Ether Molecule by Ab Initio Calculation method

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**Table 1.** Geometrical parameters optimized by methyl 2 naphthalene ether in (FA), bond length (A°), bond angle (◦) and dihedral angle (º)

| **Parameters** | **HF** | **B3LYP** | **Parameters** | **HF** | **B3LYP** |
|---|---|---|---|---|---|
| C(1)-C(2) | 1.383 | 1.364 | C(1)-C(6)-H(12) | 120.572 | 120.716 |
| C(1)-C(6) | 1.42 | 1.416 | C(5)-C(6)-H(12) | 119.593 | 119.485 |
| C(1)-O(18) | 1.368 | 1.351 | C(3)-C(9)-C(14) | 120.825 | 120.714 |
| C(2)-C(3) | 1.414 | 1.412 | C(3)-C(9)-H(7) | 118.697 | 118.841 |
| C(2)-H(8) | 1.085 | 1.075 | H(7)-C(9)-C(14) | 120.478 | 120.445 |
| C(3)-C(4) | 1.435 | 1.41 | C(4)-C(10)-C(13) | 120.831 | 120.75 |
| C(3)-C(9) | 1.424 | 1.424 | C(4)-C(10)-H(15) | 118.654 | 118.815 |
| C(4)-C(5) | 1.417 | 1.413 | C(13)-C(10)-H(15) | 120.515 | 120.435 |
| C(4)-C(10) | 1.421 | 1.422 | C(10)-C(13)-C(14) | 120.061 | 119.969 |
| C(5)-C(6) | 1.378 | 1.361 | C(10)-C(13)-H(16) | 120.276 | 120.449 |
| C(5)-H(11) | 1.087 | 1.076 | C(14)-C(13)-H(16) | 119.663 | 119.582 |
| C(6)-H(12) | 1.083 | 1.073 | C(9)-C(14)-C(13) | 120.592 | 120.652 |
| C(9)-C(14) | 1.375 | 1.356 | C(9)-C(14)-H(17) | 119.943 | 120.015 |
| C(10)-C(13) | 1.375 | 1.356 | C(13)-C(14)-H(17) | 119.465 | 119.333 |
| C(10)-H(15) | 1.087 | 1.077 | C(1)-O(18)-C(19) | 118.72 | 120.372 |
| C(13)-C(14) | 1.419 | 1.419 | O(18)-C(19)-H(20) | 105.855 | 106.184 |
| C(13)-H(16) | 1.086 | 1.075 | O(18)-C(19)-H(21) | 111.868 | 111.696 |
| C(14)-H(17) | 1.086 | 1.076 | O(18)-C(19)-H(22) | 111.869 | 111.695 |
| O(18)-C(19) | 1.418 | 1.399 | H(20)-C(19)-H(21) | 109.025 | 108.943 |
| C(19)-H(20) | 1.091 | 1.08 | H(20)-C(19)-H(22) | 109.025 | 108.943 |
| C(19)-H(21) | 1.097 | 1.086 | H(21)-C(19)-H(22) | 109.092 | 109.274 |
| C(19)-H(22) | 1.097 | 1.086 | C(1)-C(6)-H(12) | 120.572 | 120.716 |
| H(7)-C(9) | 1.087 | 1.076 | C(5)-C(6)-H(12) | 119.593 | 119.485 |
| | | | C(3)-C(9)-C(14) | 120.825 | 120.714 |
| **Bond angle (o)** | | | C(3)-C(9)-H(7) | 118.697 | 118.841 |
| C(2)-C(1)-C(6) | 120.071 | 119.973 | H(7)-C(9)-C(14) | 120.478 | 120.445 |
| C(2)-C(1)-O(18) | 116.257 | 116.798 | C(4)-C(10)-C(13) | 120.831 | 120.75 |
| C(6)-C(1)-O(18) | 123.673 | 123.229 | C(4)-C(10)-H(15) | 118.654 | 118.815 |

| | | | | | |
|---|---|---|---|---|---|
| C(1)-C(2)-C(3) | 120.899 | 120.853 | C(13)-C(10)-H(15) | 120.515 | 120.435 |
| C(1)-C(2)-H(8) | 118.827 | 118.849 | C(10)-C(13)-C(14) | 120.061 | 119.969 |
| C(3)-C(2)-H(8) | 120.274 | 120.298 | C(10)-C(13)-H(16) | 120.276 | 120.449 |
| C(2)-C(3)-C(4) | 119.3 | 119.49 | C(14)-C(13)-H(16) | 119.663 | 119.582 |
| C(2)-C(3)-C(9) | 122.194 | 121.947 | C(9)-C(14)-C(13) | 120.592 | 120.652 |
| C(4)-C(3)-C(9) | 118.506 | 118.563 | C(9)-C(14)-H(17) | 119.943 | 120.015 |
| C(3)-C(4)-C(5) | 118.291 | 118.27 | C(13)-C(14)-H(17) | 119.465 | 119.333 |
| C(3)-C(4)-C(10) | 119.184 | 119.351 | C(1)-O(18)-C(19) | 118.72 | 120.372 |
| C(5)-C(4)-C(10) | 122.524 | 122.38 | O(18)-C(19)-H(20) | 105.855 | 106.184 |
| C(4)-C(5)-C(6) | 121.604 | 121.616 | O(18)-C(19)-H(21) | 111.868 | 111.696 |
| C(4)-C(5)-H(11) | 118.833 | 118.976 | O(18)-C(19)-H(22) | 111.869 | 111.695 |
| C(6)-C(5)-H(11) | 119.563 | 119.408 | H(20)-C(19)-H(21) | 109.025 | 108.943 |
| C(1)-C(6)-C(5) | 119.835 | 119.799 | H(20)-C(19)-H(22) | 109.025 | 108.943 |

**Table 1.** (Contd.) Geometrical parameters optimized for methyl 2 naphthalene ether (bond length (A°), bond angle (◦) and dihedral angle (°))

| **Parameters** | **HF 6-31G(d,p)** | **B3LYP 6-31G(d,p)** | **Parameters** | **HF 6-31G(d,p)** | **B3LYP 6-31G(d,p)** |
|---|---|---|---|---|---|
| Dihedral angle (o) | | | | | |
| C(2)-C(1)-C(6)-C(5) | 0 | 0 | C(3)-C(4)-C(5)-C(6) | 0 | 0 |
| C(2)-C(1)-C(6)-H(12) | -179 | -179 | C(3)-C(4)-C(5)-H(11) | 180 | 180 |
| O(18)-C(1)-C(6)-C(5) | -179 | 180 | C(10)-C(4)-C(5)-C(6) | -179 | 180 |
| O(18)-C(1)-C(6)-H(12) | 0.001 | 0 | C(10)-C(4)-C(5)-H(11) | 0 | 0 |
| C(2)-C(1)-O(18)-C(19) | -179.996 | -179.997 | C(3)-C(4)-C(10)-C(13) | 0 | 0 |
| C(6)-C(1)-O(18)-C(19) | 0.003 | 0.003 | C(3)-C(4)-C(10)-H(15) | -179 | -179 |
| C(1)-C(2)-C(3)-C(4) | 0 | 0 | C(5)-C(4)-C(10)-C(13) | -179 | 180 |
| C(1)-C(2)-C(3)-C(9) | -179 | 180 | C(5)-C(4)-C(10)-H(15) | 0 | 0 |
| H(8)-C(2)-C(3)-C(4) | -179 | 180 | C(4)-C(5)-C(6)-C(1) | 0 | 0 |
| H(8)-C(2)-C(3)-C(9) | 0 | 0 | C(4)-C(5)-C(6)-H(12) | 180 | 180 |
| C(2)-C(3)-C(4)-C(5) | 0 | 0 | H(11)-C(5)-C(6)-C(1) | -179 | -179 |
| C(2)-C(3)-C(4)-C(10) | 180 | -179 | H(11)-C(5)-C(6)-H(12) | 0 | 0 |
| C(9)-C(3)-C(4)-C(5) | 180 | 180 | C(3)-C(9)-C(14)-C(13) | 0 | 0 |
| C(9)-C(3)-C(4)-C(10) | 0 | 0 | C(3)-C(9)-C(14)-H(17) | 180 | 180 |
| C(2)-C(3)-C(9)-C(14) | -179 | 180 | C(1)-O(18)-C(19)-H(20) | 179.997 | 179.998 |
| C(2)-C(3)-C(9)-H(7) | 0 | 0 | C(1)-O(18)-C(19)-H(21) | -61.374 | -61.365 |
| C(4)-C(3)-C(9)-C(14) | 0 | 0 | C(1)-O(18)-C(19)-H(22) | 61.368 | 61.362 |
| C(4)-C(3)-C(9)-H(7) | 180 | -179 | | | |

**Table 7–**NBO analysis ofmethyl 2 naphthalene ether calculated by B3LYP/6-31G (d,p) method

| Donor NBO (i) | Acceptor NBO (j) | E(2) kcal/mol | E(j)-E(i) a.u. | F(i,j) a.u. |
|---|---|---|---|---|
| C 1 - C 2 | C 2 | 0.85 | 3.21 | 0.047 |
| C 1 - C 2 | C 3 | 3.06 | 1.97 | 0.07 |
| C 1 - C 2 | C 6 | 0.79 | 1.56 | 0.032 |
| C 1 - C 2 | O 18 | 0.83 | 1.35 | 0.03 |
| C 1 - C 2 | C 1 - C 6 | 3.19 | 1.24 | 0.056 |
| C 1 - C 2 | C 2 - C 3 | 3.23 | 1.28 | 0.058 |
| C 1 - C 2 | C 2 - H 8 | 1.37 | 1.19 | 0.036 |
| C 1 - C 2 | C 3 - C 9 | 3.22 | 1.29 | 0.058 |
| C 1 - C 2 | C 6 - H12 | 1.79 | 1.19 | 0.041 |
| C 1 - C 2 | O18 - C19 | 2.77 | 0.99 | 0.047 |
| C 1 - C 2 | C 3 | 1.02 | 1.29 | 0.035 |
| C 1 - C 2 | C 6 | 1.27 | 0.64 | 0.028 |
| C 1 - C 2 | O18 | 0.95 | 0.97 | 0.029 |
| C 1 - C 2 | O18 | 0.54 | 1.76 | 0.03 |
| C 1 - C 2 | C 1 - C 2 | 0.61 | 0.3 | 0.012 |
| C 1 - C 2 | C 3 - C 4 | 11.22 | 0.48 | 0.069 |
| C 1 - C 2 | C 5 - C 6 | 16.25 | 0.29 | 0.061 |
| C 1 - C 6 | C 2 | 0.99 | 1.99 | 0.04 |
| C 1 - C 6 | C 2 | 0.68 | 1.49 | 0.029 |
| C 1 - C 6 | C 5 | 0.72 | 1.92 | 0.033 |
| C 1 - C 6 | C 5 | 1.67 | 1.42 | 0.044 |
| C 1 - C 6 | O18 | 0.52 | 1.34 | 0.024 |
| C 1 - C 6 | C 1 - C 2 | 3.45 | 1.3 | 0.06 |
| C 1 - C 6 | C 2 - H 8 | 2.08 | 1.18 | 0.044 |
| C 1 - C 6 | C 5 - C 6 | 2.44 | 1.3 | 0.05 |
| C 1 - C 6 | C 5 - H 11 | 2.22 | 1.17 | 0.046 |
| C 1 - C 6 | C 6 - H 12 | 0.9 | 1.18 | 0.029 |
| C 1 - C 6 | C 19 - H 20 | 0.6 | 3.48 | 0.041 |
| C 1 - O 18 | C 2 | 0.59 | 2.18 | 0.032 |
| C 1 - O 18 | C19 | 1.11 | 1.8 | 0.04 |
| C 1 - O 18 | C 2 - C 3 | 1.4 | 1.47 | 0.041 |
| C 1 - O 18 | C 5 - C6 | 0.97 | 1.49 | 0.034 |
| C 1 - O 18 | C19 - H 20 | 2.28 | 3.68 | 0.082 |
| C 1 - O 18 | C19 - H21 | 1.7 | 4.05 | 0.074 |
| C 1 - O 18 | C19 - H 22 | 1.23 | 4.68 | 0.068 |
| C 2 - C 3 | C 1 | 2.29 | 1.68 | 0.056 |
| C 2 - C 3 | C 4 | 0.8 | 1.93 | 0.035 |

| | | | | |
|---|---|---|---|---|
| C 2 - C 3 | C 9 | 0.86 | 1.94 | 0.037 |
| C 2 - C 3 | C1 - C 2 | 3.05 | 1.28 | 0.056 |
| C 2 - C 3 | C 1 - O 18 | 3.83 | 1.03 | 0.056 |
| C 2 - C 3 | C 2 - H 8 | 1.31 | 1.16 | 0.035 |
| C 2 - C 3 | C 3 - C 4 | 1.83 | 1.25 | 0.043 |
| C 2 - C 3 | C 3 - C 9 | 2.15 | 1.26 | 0.047 |
| C 2 - C 3 | C 4 - C 10 | 2.47 | 1.22 | 0.049 |
| C 2 - C 3 | C 9 - C 14 | 1.47 | 1.28 | 0.039 |
| C 2 - C 3 | C 19 - H 20 | 3.24 | 3.46 | 0.095 |
| C 2 - C 3 | C 19 - H 21 | 1.87 | 3.83 | 0.076 |
| C 2 - C 3 | C 19 - H 22 | 1.03 | 4.46 | 0.061 |
| C 2 - H 8 | C 1 | 0.76 | 2.47 | 0.039 |
| C 2 - H 8 | C 3 | 0.7 | 1.78 | 0.032 |
| C 2 - H 8 | C 3 | 0.72 | 1.74 | 0.032 |
| C 2 - H 8 | C 1 - C 2 | 1.38 | 1.12 | 0.035 |
| C 2 - H 8 | C 1 - C 6 | 4.81 | 1.04 | 0.063 |
| C 2 - H 8 | C 1 - O 18 | 0.9 | 0.86 | 0.025 |
| C 2 - H 8 | C 2 - C 3 | 1.35 | 1.09 | 0.034 |
| C 2 - H 8 | C 3 - C 4 | 4.24 | 1.09 | 0.061 |
| C 3 - C 4 | C 2 | 0.95 | 1.46 | 0.033 |
| C 3 - C 4 | C 5 | 0.52 | 1.88 | 0.028 |
| C 3 - C 4 | C 5 | 0.67 | 1.39 | 0.027 |
| C 3 - C 4 | C 9 | 0.66 | 1.93 | 0.032 |
| C 3 - C 4 | C 10 | 0.63 | 1.92 | 0.031 |
| C 3 - C 4 | C 10 | 0.52 | 1.44 | 0.025 |
| C 3 - C 4 | C 2 - C 3 | 2.51 | 1.24 | 0.05 |
| C 3 - C 4 | C 2 - H 8 | 1.9 | 1.15 | 0.042 |
| C 3 - C 4 | C 3 - C 9 | 2.26 | 1.25 | 0.048 |
| C 3 - C 4 | C 4 - C 5 | 2.24 | 1.3 | 0.048 |
| C 3 - C 4 | C 4 - C 10 | 2.48 | 1.21 | 0.049 |
| C 3 - C 4 | C 5 - H 11 | 1.86 | 1.13 | 0.041 |
| C 3 - C 4 | H 7 - C 9 | 1.73 | 1.14 | 0.04 |
| C 3 - C 4 | C 10 - H 15 | 1.72 | 1.14 | 0.04 |
| C 3 - C 4 | C 2 | 1.03 | 0.69 | 0.027 |
| C 3 - C 4 | C 4 | 0.58 | 1.45 | 0.03 |
| C 3 - C 4 | C 5 | 0.82 | 0.7 | 0.025 |
| C 3 - C 4 | C 5 | 0.51 | 2.14 | 0.034 |
| C 3 - C 4 | C 9 | 1.47 | 0.66 | 0.032 |
| C 3 - C 4 | C 10 | 1.56 | 0.66 | 0.033 |
| C 3 - C 4 | C 1 - C 2 | 15.79 | 0.27 | 0.061 |
| C 3 - C 4 | C 5 - C 6 | 19.17 | 0.26 | 0.067 |
| C 3 - C 4 | C 9 - C 14 | 15.51 | 0.27 | 0.062 |
| C 3 - C 4 | C 10 - C 13 | 16.73 | 0.28 | 0.064 |

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|---|---|---|---|---|
| C 3 - C 9 | C 2 | 0.85 | 1.96 | 0.037 |
| C 3 - C 9 | C 4 | 1.28 | 1.93 | 0.045 |
| C 3 - C 9 | C 14 | 0.68 | 1.94 | 0.033 |
| C 3 - C 9 | C 14 | 1.65 | 1.39 | 0.043 |
| C 3 - C 9 | C 1 - C 2 | 1.59 | 1.28 | 0.04 |
| C 3 - C 9 | C 2 - C 3 | 2.84 | 1.25 | 0.053 |
| C 3 - C 9 | C 3 - C 4 | 2.57 | 1.25 | 0.051 |
| C 3 - C 9 | C 4 - C 5 | 2.41 | 1.31 | 0.05 |
| C 3 - C 9 | H 7 - C 9 | 0.69 | 1.16 | 0.025 |
| C 3 - C 9 | C 9 - C 14 | 2.29 | 1.28 | 0.048 |
| C 3 - C 9 | C 14 - H 17 | 2.17 | 1.16 | 0.045 |
| C 4 - C 5 | C 3 | 1.1 | 1.94 | 0.041 |
| C 4 - C 5 | C 6 | 1.29 | 1.93 | 0.045 |
| C 4 - C 5 | C 6 | 0.81 | 1.53 | 0.032 |
| C 4 - C 5 | C 10 | 1.24 | 1.94 | 0.044 |
| C 4 - C 5 | C 3 - C 4 | 2.59 | 1.26 | 0.051 |
| C 4 - C 5 | C 3 - C 9 | 2.46 | 1.26 | 0.05 |
| C 4 - C 5 | C 4 - C 10 | 2.73 | 1.23 | 0.052 |
| C 4 - C 5 | C 5 - C 6 | 2.39 | 1.29 | 0.05 |
| C 4 - C 5 | C 5 - H 11 | 0.78 | 1.15 | 0.027 |
| C 4 - C 5 | C 6 - H 12 | 2.23 | 1.16 | 0.045 |
| C 4 - C 5 | C 10 - C 13 | 1.6 | 1.3 | 0.041 |
| C 4 - C 10 | C 3 | 1.05 | 1.94 | 0.04 |
| C 4 - C 10 | C 5 | 1.03 | 1.89 | 0.04 |
| C 4 - C 10 | C 13 | 0.71 | 1.94 | 0.033 |
| C 4 - C 10 | C 13 | 1.63 | 1.39 | 0.043 |
| C 4 - C 10 | C 2 - C 3 | 2.44 | 1.25 | 0.049 |
| C 4 - C 10 | C 3 - C 4 | 2.84 | 1.25 | 0.053 |
| C 4 - C 10 | C 4 - C 5 | 1.94 | 1.31 | 0.045 |
| C 4 - C 10 | C 5 - C 6 | 1.79 | 1.28 | 0.043 |
| C 4 - C 10 | C 10 - C 13 | 2.54 | 1.29 | 0.051 |
| C 4 - C 10 | C 10 - H 15 | 0.76 | 1.15 | 0.027 |
| C 4 - C 10 | C 13 - H 16 | 2.2 | 1.16 | 0.045 |
| C 4 - C 10 | C 19 - H 22 | 2.17 | 4.47 | 0.088 |
| C 5 - C 6 | C 1 | 1.75 | 1.93 | 0.052 |
| C 5 - C 6 | C 4 | 2.38 | 1.93 | 0.061 |
| C 5 - C 6 | C 1 - C 6 | 2.46 | 1.24 | 0.049 |
| C 5 - C 6 | C 1 - O 18 | 4.09 | 1.06 | 0.059 |
| C 5 - C 6 | C 4 - C 5 | 2.47 | 1.35 | 0.052 |
| C 5 - C 6 | C 4 - C 10 | 3.21 | 1.26 | 0.057 |
| C 5 - C 6 | C 5 - H 11 | 1.16 | 1.18 | 0.033 |
| C 5 - C 6 | C 6 - H 12 | 1.43 | 1.19 | 0.037 |
| C 5 - C 6 | C 1 | 0.76 | 1.89 | 0.036 |

| | | | | |
|---|---|---|---|---|
| C 5 - C 6 | C 1 - C 2 | 18.21 | 0.3 | 0.068 |
| C 5 - C 6 | C 3 - C 4 | 8.22 | 0.49 | 0.06 |
| C 5 - H 11 | C 4 | 0.51 | 1.74 | 0.027 |
| C 5 - H 11 | C 4 | 0.96 | 1.78 | 0.037 |
| C 5 - H 11 | C 6 | 1.07 | 1.77 | 0.039 |
| C 5 - H 11 | C 1 - C 6 | 4.1 | 1.05 | 0.059 |
| C 5 - H 11 | C 3 - C 4 | 4.44 | 1.1 | 0.063 |
| C 5 - H 11 | C 4 - C 5 | 0.77 | 1.16 | 0.027 |
| C 5 - H 11 | C 5 - C 6 | 1 | 1.13 | 0.03 |
| C 6 - H 12 | C 1 | 0.86 | 1.54 | 0.033 |
| C 6 - H 12 | C 5 | 1.25 | 1.75 | 0.042 |
| C 6 - H 12 | C 1 - C 2 | 3.68 | 1.13 | 0.058 |
| C 6 - H 12 | C 1 - C 6 | 0.58 | 1.06 | 0.022 |
| C 6 - H 12 | C 4 - C 5 | 3.97 | 1.17 | 0.061 |
| C 6 - H 12 | C 5 - C 6 | 1.23 | 1.14 | 0.033 |
| H 7 - C 9 | C 3 | 1.43 | 1.77 | 0.045 |
| H 7 - C 9 | C 14 | 1.19 | 1.78 | 0.041 |
| H 7 - C 9 | C 3 - C 4 | 4.2 | 1.09 | 0.061 |
| H 7 - C 9 | C 3 - C 9 | 0.61 | 1.1 | 0.023 |
| H 7 - C 9 | C 9 - C 14 | 1.07 | 1.13 | 0.031 |
| H 7 - C 9 | C 13 - C 14 | 4.14 | 1.07 | 0.059 |
| C 9 - C 14 | C 3 | 0.61 | 1.97 | 0.031 |
| C 9 - C 14 | C 3 | 1.87 | 1.96 | 0.054 |
| C 9 - C 14 | C 13 | 0.62 | 1.97 | 0.031 |
| C 9 - C 14 | C 13 | 1.26 | 1.42 | 0.038 |
| C 9 - C 14 | C 2 - C 3 | 3.14 | 1.28 | 0.057 |
| C 9 - C 14 | C 3 - C 9 | 2.46 | 1.29 | 0.05 |
| C 9 - C 14 | H 7 - C 9 | 1.27 | 1.19 | 0.035 |
| C 9 - C 14 | C 13 - C 14 | 2.17 | 1.26 | 0.047 |
| C 9 - C 14 | C 13 - H 16 | 1.78 | 1.19 | 0.041 |
| C 9 - C 14 | C 14 - H 17 | 1.15 | 1.19 | 0.033 |
| C 9 - C 14 | C 13 | 1.69 | 0.75 | 0.034 |
| C 9 - C 14 | C 3 - C 4 | 9.56 | 0.48 | 0.064 |
| C 9 - C 14 | C 10 - C 13 | 16.2 | 0.3 | 0.062 |
| C 10 - C 13 | C 4 | 2.49 | 1.92 | 0.062 |
| C 10 - C 13 | C 14 | 0.66 | 1.97 | 0.032 |
| C 10 - C 13 | C 14 | 1.22 | 1.42 | 0.037 |
| C 10 - C 13 | C 4 - C 5 | 2.81 | 1.34 | 0.055 |
| C 10 - C 13 | C 4 - C 10 | 2.54 | 1.25 | 0.05 |
| C 10 - C 13 | C 10 - H 15 | 1.23 | 1.18 | 0.034 |
| C 10 - C 13 | C 13 - C 14 | 2.2 | 1.26 | 0.047 |
| C 10 - C 13 | C 13 - H 16 | 1.18 | 1.19 | 0.033 |
| C 10 - C 13 | C 14 - H 17 | 1.8 | 1.19 | 0.041 |

| | | | | |
|---|---|---|---|---|
| C 10 - C 13 | C 4 | 0.51 | 1.48 | 0.026 |
| C 10 - C 13 | C 14 | 1.63 | 0.91 | 0.037 |
| C 10 - C 13 | C 3 - C 4 | 8.98 | 0.48 | 0.062 |
| C 10 - C 13 | C 9 - C 14 | 17.51 | 0.29 | 0.064 |
| C 10 - H 15 | C 4 | 0.62 | 1.73 | 0.029 |
| C 10 - H 15 | C 4 | 0.84 | 1.77 | 0.035 |
| C 10 - H 15 | C 13 | 1.19 | 1.78 | 0.041 |
| C 10 - H 15 | C 3 - C 4 | 4.3 | 1.1 | 0.061 |
| C 10 - H 15 | C 4 - C 10 | 0.64 | 1.07 | 0.023 |
| C 10 - H 15 | C 10 - C 13 | 1.04 | 1.13 | 0.031 |
| C 10 - H 15 | C 13 - C 14 | 4.04 | 1.07 | 0.059 |
| C 13 - C 14 | C 9 | 1.75 | 1.47 | 0.045 |
| C 13 - C 14 | C 10 | 1.68 | 1.45 | 0.044 |
| C 13 - C 14 | H 7 - C 9 | 2.46 | 1.16 | 0.048 |
| C 13 - C 14 | C 9 - C 14 | 2.29 | 1.29 | 0.049 |
| C 13 - C 14 | C 10 - C 13 | 2.29 | 1.29 | 0.049 |
| C 13 - C 14 | C 10 - H 15 | 2.53 | 1.15 | 0.048 |
| C 13 - C 14 | C 13 - H 16 | 0.81 | 1.16 | 0.027 |
| C 13 - C 14 | C 14 - H 17 | 0.79 | 1.16 | 0.027 |
| C 13 - H 16 | C 10 | 1.09 | 1.77 | 0.039 |
| C 13 - H 16 | C 14 | 1.09 | 1.78 | 0.039 |
| C 13 - H 16 | C 4 - C 10 | 4.2 | 1.06 | 0.06 |
| C 13 - H 16 | C 9 - C 14 | 3.41 | 1.13 | 0.055 |
| C 13 - H 16 | C 10 - C 13 | 0.95 | 1.13 | 0.029 |
| C 13 - H 16 | C 13 - C 14 | 0.6 | 1.07 | 0.023 |
| C 13 - H 16 | C 19 - H 21 | 1.19 | 3.67 | 0.059 |
| C 14 - H 17 | C 9 | 1.07 | 1.78 | 0.039 |
| C 14 - H 17 | C 13 | 1.07 | 1.78 | 0.039 |
| C 14 - H 17 | C 3 - C 9 | 4.18 | 1.1 | 0.061 |
| C 14 - H 17 | C 9 - C 14 | 0.97 | 1.13 | 0.03 |
| C 14 - H 17 | C 10 - C 13 | 3.4 | 1.13 | 0.055 |
| O 18 - C 19 | C 1 | 0.93 | 1.84 | 0.037 |
| O 18 - C 19 | C 1 | 1.57 | 2.04 | 0.051 |
| O 18 - C 19 | H 22 | 13.23 | 1.19 | 0.112 |
| O 18 - C 19 | C 1 - C 2 | 2.66 | 1.43 | 0.055 |
| O 18 - C 19 | C 19 - H 20 | 1.05 | 3.61 | 0.055 |
| O 18 - C 19 | C 19 - H 21 | 2.25 | 3.98 | 0.085 |
| O 18 - C 19 | C 19 - H 22 | 0.77 | 4.62 | 0.053 |
| C 19 - H 20 | O 18 | 0.66 | 1.54 | 0.028 |
| C 19 - H 20 | C 19 | 0.78 | 2.3 | 0.038 |
| C 19 - H 20 | C 19 | 0.84 | 2.9 | 0.044 |
| C 19 - H 20 | H 22 | 4.02 | 0.68 | 0.047 |
| C 19 - H 20 | H 22 | 7.2 | 0.67 | 0.062 |

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|---|---|---|---|---|
| C 19 - H 20 | H 22 | 16.9 | 0.88 | 0.109 |
| C 19 - H 20 | C 1 - O 18 | 3.57 | 0.87 | 0.05 |
| C 19 - H 20 | C 3 - C 4 | 3.38 | 0.75 | 0.051 |
| C 19 - H 20 | C 4 - C 5 | 0.93 | 1.16 | 0.029 |
| C 19 - H 20 | C 19 - H 20 | 0.82 | 3.31 | 0.046 |
| C 19 - H 20 | C 19 - H 21 | 3.58 | 3.68 | 0.103 |
| C 19 - H 20 | C 19 - H 22 | 10 | 4.31 | 0.186 |
| C 19 - H 21 | O 18 | 0.9 | 1.25 | 0.03 |
| C 19 - H 21 | H 22 | 7.64 | 0.64 | 0.063 |
| C 19 - H 21 | H 22 | 2.06 | 0.68 | 0.034 |
| C 19 - H 21 | H 22 | 14.83 | 0.89 | 0.103 |
| C 19 - H 21 | C 3 - C 4 | 1.17 | 0.76 | 0.03 |
| C 19 - H 21 | C 19 - H 22 | 5.18 | 4.32 | 0.134 |
| C 19 - H 22 | O 18 | 0.92 | 1.25 | 0.03 |
| C 19 - H 22 | C 19 | 0.68 | 2.31 | 0.036 |
| C 19 - H 22 | C 19 | 1.54 | 2.91 | 0.06 |
| C 19 - H 22 | C 19 | 0.69 | 2.94 | 0.04 |
| C 19 - H 22 | H 22 | 1.49 | 0.69 | 0.029 |
| C 19 - H 22 | H 22 | 1.37 | 0.64 | 0.026 |
| C 19 - H 22 | H 22 | 5.41 | 0.68 | 0.054 |
| C 19 - H 22 | H 22 | 72.66 | 0.89 | 0.227 |
| C 19 - H 22 | C 3 - C 4 | 5.17 | 0.75 | 0.064 |
| C 19 - H 22 | C 3 - C 9 | 0.62 | 1.11 | 0.024 |
| C 19 - H 22 | C 4 - C 5 | 1.6 | 1.17 | 0.039 |
| C 19 - H 22 | C 19 - H 21 | 7.75 | 3.69 | 0.151 |
| C 19 - H 22 | C 19 - H 22 | 15.64 | 4.32 | 0.233 |
| C 1 | C 2 | 1.46 | 10.91 | 0.113 |
| C 1 | C 6 | 0.63 | 11.37 | 0.075 |
| C 1 | C 6 | 0.7 | 10.96 | 0.078 |
| C 1 | C 1 - C 2 | 1.18 | 10.72 | 0.101 |
| C 1 | C 1 - O 18 | 1.34 | 10.47 | 0.107 |
| C 1 | C 2 - C 3 | 0.62 | 10.69 | 0.073 |
| C 1 | C 2 - H 8 | 0.51 | 10.6 | 0.066 |
| C 1 | C 5 - C 6 | 0.52 | 10.72 | 0.067 |
| C 1 | C 6 - H 12 | 0.51 | 10.59 | 0.066 |
| C 1 | O 18 - C 19 | 0.91 | 10.4 | 0.087 |
| C 2 | C 1 | 2.19 | 11.25 | 0.14 |
| C 2 | C 1 | 0.65 | 12.03 | 0.079 |
| C 2 | C 3 | 1.8 | 11.3 | 0.127 |
| C 2 | C 3 | 0.73 | 11.09 | 0.08 |
| C 2 | C 1 - C 6 | 1.11 | 10.56 | 0.097 |
| C 2 | C 1 - O 18 | 0.64 | 10.39 | 0.073 |
| C 2 | C 3 - C 4 | 0.78 | 10.61 | 0.082 |

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|---|---|---|---|---|
| C 2 | C 3 - C 9 | 0.85 | 10.62 | 0.085 |
| C 3 | C 2 | 0.98 | 10.84 | 0.092 |
| C 3 | C 4 | 1.74 | 11.26 | 0.125 |
| C 3 | C 9 | 1.5 | 10.84 | 0.114 |
| C 3 | C 1 - C 2 | 0.53 | 10.65 | 0.067 |
| C 3 | C 4 - C 5 | 0.63 | 10.68 | 0.074 |
| C 3 | C 4 - C 10 | 0.68 | 10.59 | 0.076 |
| C 3 | C 9 - C 14 | 0.58 | 10.65 | 0.07 |
| C 4 | C 3 | 0.86 | 11.31 | 0.088 |
| C 4 | C 3 | 0.94 | 11.3 | 0.092 |
| C 4 | C 5 | 1.33 | 10.76 | 0.107 |
| C 4 | C 10 | 1.5 | 10.82 | 0.114 |
| C 4 | C 2 - C 3 | 0.63 | 10.62 | 0.073 |
| C 4 | C 5 - C 6 | 0.63 | 10.64 | 0.073 |
| C 4 | C 10 - C 13 | 0.58 | 10.65 | 0.071 |
| C 5 | C 4 | 1.22 | 11.3 | 0.105 |
| C 5 | C 4 | 0.58 | 11.21 | 0.072 |
| C 5 | C 6 | 1.9 | 10.89 | 0.128 |
| C 5 | C 1 - C 6 | 0.72 | 10.57 | 0.079 |
| C 5 | C 3 - C 4 | 0.74 | 10.63 | 0.08 |
| C 5 | C 4 - C 10 | 0.9 | 10.6 | 0.087 |
| C 5 | C 6 - H 12 | 0.6 | 10.53 | 0.071 |
| C 6 | C 1 | 2.01 | 11.06 | 0.133 |
| C 6 | C 5 | 1.6 | 10.77 | 0.117 |
| C 6 | C 5 | 0.58 | 11.07 | 0.071 |
| C 6 | C 1 - C 2 | 0.77 | 10.65 | 0.081 |
| C 6 | C 1 - O 18 | 0.79 | 10.4 | 0.081 |
| C 6 | C 4 - C 5 | 0.76 | 10.69 | 0.081 |
| C 6 | C 5 - C 6 | 0.55 | 10.65 | 0.068 |
| C 6 | C 5 - H 11 | 0.55 | 10.52 | 0.068 |
| C 9 | C 3 | 1.58 | 11.31 | 0.12 |
| C 9 | C 14 | 1.98 | 10.75 | 0.13 |
| C 9 | C 2 - C 3 | 0.84 | 10.62 | 0.085 |
| C 9 | C 3 - C 4 | 0.7 | 10.62 | 0.078 |
| C 9 | C 13 - C 14 | 0.74 | 10.59 | 0.079 |
| C 9 | C 14 - H 17 | 0.54 | 10.52 | 0.068 |
| C 10 | C 4 | 1.29 | 11.3 | 0.108 |
| C 10 | C 4 | 0.51 | 11.2 | 0.068 |
| C 10 | C 13 | 1.97 | 10.76 | 0.13 |
| C 10 | C 3 - C 4 | 0.73 | 10.62 | 0.079 |
| C 10 | C 4 - C 5 | 0.85 | 10.68 | 0.086 |
| C 10 | C 13 - C 14 | 0.72 | 10.59 | 0.078 |

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|---|---|---|---|---|
| C 10 | C 13 - H 16 | 0.56 | 10.52 | 0.068 |
| C 13 | C 10 | 0.57 | 11.3 | 0.072 |
| C 13 | C 10 | 1.14 | 10.82 | 0.099 |
| C 13 | C 10 | 0.69 | 11.05 | 0.078 |
| C 13 | C 14 | 1.32 | 10.76 | 0.107 |
| C 13 | C 4 - C 10 | 0.74 | 10.59 | 0.079 |
| C 13 | C 9 - C 14 | 0.62 | 10.65 | 0.073 |
| C 13 | C 10 - C 13 | 0.5 | 10.66 | 0.066 |
| C 13 | C 10 - H 15 | 0.62 | 10.52 | 0.072 |
| C 14 | C 9 | 0.57 | 11.31 | 0.072 |
| C 14 | C 9 | 1.11 | 10.84 | 0.098 |
| C 14 | C 9 | 0.73 | 11.04 | 0.08 |
| C 14 | C 13 | 1.3 | 10.76 | 0.106 |
| C 14 | C 3 - C 9 | 0.74 | 10.63 | 0.08 |
| C 14 | H 7 - C 9 | 0.61 | 10.53 | 0.072 |
| C 14 | C 9 - C 14 | 0.5 | 10.65 | 0.065 |
| C 14 | C 10 - C 13 | 0.61 | 10.66 | 0.072 |
| O 18 | C 1 | 1.98 | 19.99 | 0.178 |
| O 18 | C 19 | 1.01 | 20.19 | 0.127 |
| O 18 | C 1 - C 6 | 0.56 | 19.51 | 0.094 |
| C 19 | C 19 | 1.07 | 11.89 | 0.101 |
| C 19 | C 19 | 2.16 | 12.49 | 0.147 |
| C 19 | C 19 | 1.19 | 12.52 | 0.109 |
| C 19 | H 22 | 0.73 | 10.85 | 0.079 |
| C 19 | H 22 | 1.49 | 10.27 | 0.111 |
| C 19 | H 22 | 0.96 | 10.22 | 0.088 |
| C 19 | H 22 | 3.19 | 10.26 | 0.162 |
| C 19 | H 22 | 56.91 | 10.47 | 0.689 |
| C 19 | C 1 - O 18 | 0.9 | 10.46 | 0.087 |
| C 19 | C 3 - C 4 | 2.83 | 10.34 | 0.175 |
| C 19 | C 4 - C 5 | 1.27 | 10.75 | 0.105 |
| C 19 | O 18 - C 19 | 1.31 | 10.39 | 0.104 |
| C 19 | C 19 - H 21 | 14.76 | 13.27 | 0.397 |
| C 19 | C 19 - H 22 | 32.5 | 13.9 | 0.603 |
| O 18 | C 1 | 2.96 | 1.55 | 0.061 |
| O 18 | C 1 | 0.69 | 1.76 | 0.031 |
| O 18 | C 1 | 0.88 | 2.56 | 0.043 |
| O 18 | C 19 | 3.1 | 1.75 | 0.066 |
| O 18 | C 1 - C 2 | 0.63 | 1.15 | 0.024 |
| O 18 | C 1 - C 6 | 7.77 | 1.07 | 0.082 |
| O 18 | C 19 - H 20 | 0.75 | 3.33 | 0.045 |
| O 18 | C 1 | 2.31 | 2.14 | 0.065 |
| O 18 | C 19 | 1.48 | 2.09 | 0.052 |

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|---|---|---|---|---|
| O 18 | C 19 | 0.56 | 1 | 0.022 |
| O 18 | H 22 | 1.9 | 0.67 | 0.033 |
| O 18 | C 1 - C 2 | 27.39 | 0.35 | 0.092 |
| O 18 | C 19 - H 21 | 0.77 | 3.47 | 0.048 |
| O 18 | C 19 - H 22 | 0.52 | 4.1 | 0.043 |
| C 1 - C 2 | C 1 | 1.06 | 0.91 | 0.068 |
| C 1 - C 2 | C 2 | 3.22 | 0.42 | 0.081 |
| C 1 - C 2 | C 3 - C 4 | 30.15 | 0.19 | 0.105 |
| C 1 - C 2 | C 19 - H 22 | 0.87 | 3.75 | 0.122 |
| C 3 - C 4 | C 2 | 0.65 | 0.23 | 0.022 |
| C 3 - C 4 | C 3 | 0.9 | 1.12 | 0.058 |
| C 3 - C 4 | C 3 | 1.15 | 0.36 | 0.037 |
| C 3 - C 4 | C 4 | 1.36 | 1.12 | 0.071 |
| C 3 - C 4 | C 4 | 0.87 | 0.29 | 0.029 |
| C 3 - C 4 | C 9 | 1.6 | 0.21 | 0.033 |
| C 3 - C 4 | C 10 | 1.73 | 0.2 | 0.034 |
| C 3 - C 4 | C 19 | 1.69 | 0.98 | 0.074 |
| C 3 - C 4 | C 19 | 3.63 | 1.55 | 0.136 |
| C 3 - C 4 | C 19 | 0.83 | 0.91 | 0.05 |
| C 3 - C 4 | C 19 | 1.04 | 0.91 | 0.056 |
| C 3 - C 4 | C 19 | 1.76 | 3.7 | 0.147 |
| C 3 - C 4 | C 19 | 5.53 | 2.16 | 0.199 |
| C 3 - C 4 | C 19 | 2.44 | 2.18 | 0.133 |
| C 3 - C 4 | H 22 | 3.36 | 0.51 | 0.075 |
| C 3 - C 4 | H 22 | 19.55 | 0.13 | 0.093 |
| C 3 - C 4 | C 3 - C 9 | 4.47 | 0.36 | 0.071 |
| C 3 - C 4 | C 4 - C 5 | 8.82 | 0.41 | 0.107 |
| C 3 - C 4 | C 10 - C 13 | 0.51 | 0.39 | 0.025 |
| C 3 - C 4 | C 19 - H 21 | 18.09 | 2.93 | 0.411 |
| C 3 - C 4 | C 19 - H 22 | 48.3 | 3.56 | 0.741 |
| C 5 - C 6 | C 5 | 2.82 | 0.44 | 0.083 |
| C 5 - C 6 | C 5 | 0.55 | 0.46 | 0.038 |
| C 5 - C 6 | C 6 | 2.45 | 0.35 | 0.069 |
| C 5 - C 6 | C 3 - C 4 | 12.99 | 0.19 | 0.072 |
| C 9 - C 14 | C 9 | 1.84 | 0.39 | 0.068 |
| C 9 - C 14 | C 14 | 0.64 | 1.66 | 0.082 |
| C 9 - C 14 | C 3 - C 4 | 11.97 | 0.18 | 0.069 |
| C 10 - C 13 | C 10 | 1.86 | 0.38 | 0.067 |
| C 10 - C 13 | C 10 | 0.56 | 0.48 | 0.041 |
| C 10 - C 13 | C 13 | 1.03 | 0.46 | 0.054 |
| C 10 - C 13 | C 3 - C 4 | 16.49 | 0.18 | 0.081 |