|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Molecule No. | Molecular structure | Atom | X | Y | Z |
| 1 |  | C | 0.00 | 0.19 | 0.00 |
| O | 0.00 | 1.40 | 0.00 |
| C | 1.29 | -0.61 | 0.00 |
| H | 1.34 | -1.26 | 0.88 |
| H | 1.34 | -1.26 | -0.88 |
| H | 2.15 | 0.06 | 0.00 |
| C | -1.29 | -0.61 | 0.00 |
| H | -1.34 | -1.26 | -0.88 |
| H | -1.34 | -1.27 | 0.88 |
| H | -2.15 | 0.06 | 0.00 |
| 2 |  | C | -0.14 | 0.11 | 0.00 |
| C | -1.19 | -0.79 | 0.00 |
| H | -2.21 | -0.44 | 0.00 |
| H | -1.02 | -1.86 | 0.00 |
| C | 1.29 | -0.48 | 0.00 |
| H | 1.32 | -1.58 | 0.00 |
| H | 1.84 | -0.12 | -0.88 |
| H | 1.84 | -0.11 | 0.88 |
| O | -0.20 | 1.38 | 0.00 |
| 3 |  | O | -0.55 | -0.71 | 0.00 |
| C | 0.46 | 0.18 | 0.00 |
| O | 0.30 | 1.37 | 0.00 |
| C | 1.80 | -0.52 | 0.00 |
| H | 1.89 | -1.16 | 0.88 |
| H | 1.89 | -1.16 | -0.88 |
| H | 2.60 | 0.21 | 0.00 |
| C | -1.88 | -0.16 | 0.00 |
| H | -2.55 | -1.02 | 0.00 |
| H | -2.04 | 0.45 | 0.89 |
| H | -2.04 | 0.45 | -0.89 |
| 4 |  | C | -0.60 | 0.13 | 0.00 |
| C | -1.79 | -0.57 | 0.00 |
| H | -2.72 | -0.02 | 0.00 |
| H | -1.80 | -1.65 | 0.00 |
| O | -0.36 | 1.36 | 0.00 |
| O | 0.55 | -0.76 | 0.00 |
| C | 1.80 | -0.11 | 0.00 |
| H | 2.56 | -0.90 | -0.01 |
| H | 1.94 | 0.53 | -0.88 |
| H | 1.94 | 0.52 | 0.89 |
| 5 |  | C | -0.46 | 0.24 | 0.00 |
| O | -0.79 | 1.39 | 0.00 |
| C | -1.41 | -0.94 | 0.00 |
| H | -1.24 | -1.56 | -0.88 |
| H | -1.24 | -1.56 | 0.88 |
| H | -2.43 | -0.57 | 0.00 |
| S | 1.29 | -0.26 | 0.00 |
| H | 1.76 | 1.00 | 0.00 |

**Table S1** Coordinates of 29 molecules optimized at the B3LYP/6-311+G(d) level (continue)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Molecule No. | Molecular structure | Atom | X | Y | Z |
| 6 |  | C | -0.66 | 0.12 | 0.00 |
| C | -1.31 | -1.08 | 0.02 |
| H | -2.39 | -1.10 | -0.01 |
| H | -0.77 | -2.02 | 0.09 |
| O | -1.00 | 1.30 | -0.02 |
| S | 1.34 | -0.16 | -0.02 |
| H | 1.59 | 1.11 | 0.36 |
| 7 |  | C | 0.76 | 0.28 | 0.00 |
| O | 0.64 | 1.48 | 0.00 |
| C | 2.09 | -0.44 | 0.00 |
| H | 2.18 | -1.08 | 0.88 |
| H | 2.18 | -1.08 | -0.88 |
| H | 2.90 | 0.30 | 0.00 |
| C | -2.01 | 0.40 | 0.00 |
| H | -2.94 | -0.17 | 0.00 |
| H | -1.95 | 1.02 | 0.89 |
| H | -1.95 | 1.02 | -0.89 |
| S | -0.66 | -0.83 | 0.00 |
| 8 |  | C | -0.96 | 0.25 | 0.00 |
| C | -2.06 | -0.55 | 0.00 |
| H | -3.05 | -0.09 | 0.00 |
| H | -1.98 | -1.63 | 0.00 |
| O | -0.77 | 1.48 | 0.00 |
| C | 1.93 | 0.49 | 0.00 |
| H | 2.56 | 0.46 | -0.89 |
| H | 1.35 | 1.42 | 0.00 |
| H | 2.56 | 0.46 | 0.89 |
| S | 0.70 | -0.85 | 0.00 |
| 9 |  | O | 0.00 | 0.00 | 0.11 |
| H | 0.00 | 0.77 | -0.46 |
| H | 0.00 | -0.77 | -0.46 |
| 10 |  | O | 0.00 | 0.00 | 0.11 |
| H | 0.00 | 0.00 | -0.86 |
| 11 |  | O | 0.79 | -1.04 | 0.00 |
| C | 0.09 | 0.13 | 0.00 |
| O | 0.63 | 1.21 | 0.00 |
| C | -1.39 | -0.12 | 0.00 |
| H | -1.67 | -0.70 | -0.88 |
| H | -1.67 | -0.70 | 0.88 |
| H | -1.93 | 0.83 | 0.00 |
| H | 1.73 | -0.82 | 0.00 |
| 12 |  | O | -0.70 | 1.16 | 0.00 |
| C | -0.21 | 0.00 | 0.00 |
| O | -0.81 | -1.10 | 0.00 |
| C | 1.35 | -0.05 | 0.00 |
| H | 1.74 | 0.47 | -0.88 |
| H | 1.74 | 0.47 | 0.88 |
| H | 1.73 | -1.08 | 0.00 |

**Table S1** Coordinates of 29 molecules optimized at the B3LYP/6-311+G(d) level (continue)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Molecule No. | Molecular structure | Atom | X | Y | Z |
| 13 |  | C | 1.35 | 0.39 | 0.00 |
| H | 2.08 | -0.41 | 0.00 |
| H | 1.70 | 1.42 | 0.00 |
| C | 0.00 | 0.13 | 0.00 |
| O | -0.33 | -1.27 | 0.00 |
| H | -1.29 | -1.25 | 0.00 |
| O | -1.00 | 0.90 | 0.00 |
| 14 |  | C | -0.16 | 0.39 | 0.00 |
| H | -0.14 | 1.49 | 0.00 |
| O | -1.20 | -0.25 | 0.00 |
| N | 1.08 | -0.16 | 0.00 |
| H | 1.19 | -1.16 | 0.00 |
| H | 1.91 | 0.42 | 0.00 |
| 15 |  | C | -1.48 | 0.41 | 0.00 |
| H | -2.05 | 1.36 | 0.00 |
| O | -2.05 | -0.65 | 0.00 |
| C | 0.01 | 0.60 | 0.00 |
| H | 0.36 | 1.64 | 0.00 |
| N | 0.81 | -0.39 | 0.00 |
| C | 2.23 | -0.13 | 0.00 |
| H | 2.67 | -0.62 | -0.88 |
| H | 2.50 | 0.93 | 0.00 |
| H | 2.67 | -0.62 | 0.88 |
| 16 |  | C | -1.36 | 0.40 | 0.00 |
| H | -1.91 | 1.38 | 0.00 |
| O | -2.04 | -0.65 | 0.00 |
| C | 0.04 | 0.60 | 0.00 |
| H | 0.38 | 1.65 | 0.00 |
| N | 0.96 | -0.39 | 0.00 |
| C | 2.23 | -0.16 | 0.00 |
| H | 2.93 | -1.00 | 0.00 |
| H | 2.66 | 0.86 | 0.00 |
| 17 |  | C | 0.00 | 0.00 | 0.00 |
| N | -1.09 | -0.77 | 0.00 |
| H | -2.00 | -0.40 | -0.22 |
| H | -1.04 | -1.75 | 0.22 |
| N | 1.21 | -0.56 | 0.00 |
| H | 2.04 | -0.02 | 0.22 |
| H | 1.35 | -1.53 | -0.22 |
| N | -0.12 | 1.33 | 0.00 |
| H | -1.00 | 1.78 | 0.23 |
| H | 0.65 | 1.93 | -0.22 |

**Table S1** Coordinates of 29 molecules optimized at the B3LYP/6-311+G(d) level (continue)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Molecule No. | Molecular structure | Atom | X | Y | Z |
| 18 |  | C | -0.01 | 0.12 | 0.00 |
| N | -0.12 | 1.40 | 0.03 |
| H | -1.09 | 1.70 | -0.08 |
| N | -1.05 | -0.80 | -0.06 |
| H | -0.85 | -1.78 | -0.07 |
| H | -1.93 | -0.54 | 0.35 |
| N | 1.25 | -0.47 | -0.07 |
| H | 1.98 | 0.23 | -0.01 |
| H | 1.41 | -1.25 | 0.54 |
| 19 |  | C | 0.56 | 0.01 | 0.00 |
| C | -0.54 | 1.09 | 0.00 |
| C | -1.93 | 0.61 | 0.00 |
| C | -2.22 | -0.71 | 0.00 |
| C | -1.18 | -1.72 | 0.00 |
| C | 0.13 | -1.39 | 0.00 |
| H | -2.70 | 1.37 | 0.00 |
| H | -3.25 | -1.04 | 0.00 |
| H | -1.47 | -2.76 | 0.00 |
| H | 0.88 | -2.17 | 0.00 |
| O | -0.28 | 2.28 | 0.00 |
| N | 1.77 | 0.45 | 0.00 |
| C | 2.92 | -0.41 | 0.00 |
| H | 3.53 | -0.15 | -0.87 |
| H | 3.53 | -0.15 | 0.87 |
| H | 2.75 | -1.49 | 0.00 |
| 20 |  | C | 0.55 | -0.06 | -0.11 |
| C | -0.35 | 1.10 | -0.01 |
| C | -1.75 | 0.76 | 0.08 |
| C | -2.22 | -0.54 | 0.08 |
| C | -1.33 | -1.63 | -0.02 |
| C | 0.03 | -1.36 | -0.11 |
| H | -2.44 | 1.59 | 0.14 |
| H | -3.29 | -0.73 | 0.13 |
| H | -1.70 | -2.65 | -0.07 |
| H | 0.73 | -2.19 | -0.24 |
| O | 0.06 | 2.29 | 0.02 |
| N | 1.92 | 0.19 | -0.27 |
| C | 2.80 | -0.57 | 0.24 |
| H | 2.57 | -1.42 | 0.91 |
| H | 3.85 | -0.38 | 0.03 |
| 21 |  | C | 0.54 | 0.00 | 0.00 |
| H | 1.03 | -0.38 | 0.96 |
| H | 1.03 | -0.64 | -0.80 |
| H | 1.03 | 1.02 | -0.15 |
| O | -0.79 | 0.00 | 0.00 |

**Table S1** Coordinates of 29 molecules optimized at the B3LYP/6-311+G(d) level (continue)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Molecule No. | Molecular structure | Atom | X | Y | Z |
| 22 |  | N | 1.71 | -0.67 | 0.00 |
| H | 1.39 | -1.63 | 0.00 |
| H | 1.94 | -0.43 | -0.97 |
| C | 0.57 | 0.20 | 0.34 |
| H | 0.40 | 0.12 | 1.45 |
| O | -0.69 | -0.72 | -0.15 |
| O | 0.57 | 1.37 | -0.17 |
| C | -1.89 | -0.04 | -0.01 |
| H | -1.85 | 0.96 | -0.48 |
| H | -2.70 | -0.62 | -0.49 |
| H | -2.18 | 0.11 | 1.05 |
| 23 |  | C | -0.03 | 0.43 | 0.18 |
| O | -1.35 | 0.23 | -0.47 |
| O | 0.03 | 0.18 | 1.42 |
| C | -1.99 | -0.95 | -0.06 |
| H | -2.04 | -1.02 | 1.03 |
| H | -3.01 | -0.92 | -0.47 |
| H | -1.48 | -1.84 | -0.45 |
| C | 0.38 | 1.84 | -0.29 |
| H | 1.43 | 2.02 | -0.01 |
| H | 0.28 | 1.96 | -1.37 |
| H | -0.24 | 2.58 | 0.22 |
| O | 0.84 | -0.54 | -0.70 |
| C | 1.97 | -1.03 | -0.05 |
| H | 2.30 | -1.95 | -0.57 |
| H | 2.82 | -0.32 | -0.06 |
| H | 1.75 | -1.27 | 1.00 |
| 24 |  | C | 1.42 | -1.08 | 1.19 |
| H | 1.06 | -2.04 | 0.80 |
| H | 2.26 | -1.28 | 1.86 |
| H | 0.61 | -0.62 | 1.77 |
| C | 2.31 | 1.21 | 0.57 |
| H | 3.13 | 1.10 | 1.28 |
| H | 2.67 | 1.83 | -0.26 |
| H | 1.48 | 1.74 | 1.06 |
| O | 2.87 | -0.76 | -0.69 |
| C | 1.93 | -0.19 | 0.02 |
| C | 0.59 | 0.06 | -1.03 |
| H | 0.47 | -0.90 | -1.51 |
| H | 0.99 | 0.80 | -1.73 |
| C | -0.67 | 0.55 | -0.46 |
| O | -0.93 | 1.67 | -0.06 |
| S | -1.96 | -0.80 | -0.31 |
| C | -3.27 | 0.10 | 0.60 |
| H | -4.21 | 0.03 | 0.07 |
| H | -3.38 | -0.31 | 1.61 |
| H | -2.95 | 1.14 | 0.66 |

**Table S1** Coordinates of 29 molecules optimized at the B3LYP/6-311+G(d) level (continue)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Molecule No. | Molecular structure | Atom | X | Y | Z |
| 25 |  | C | 1.14 | -1.22 | 1.02 |
| H | 0.75 | -2.13 | 0.56 |
| H | 2.04 | -1.50 | 1.59 |
| H | 0.39 | -0.84 | 1.72 |
| C | 1.98 | 1.14 | 0.59 |
| H | 2.86 | 0.96 | 1.22 |
| H | 2.27 | 1.85 | -0.19 |
| H | 1.20 | 1.59 | 1.21 |
| O | 2.42 | -0.67 | -0.93 |
| C | 1.57 | -0.21 | -0.07 |
| C | 0.10 | 0.17 | -0.97 |
| H | -0.07 | -0.75 | -1.53 |
| H | 0.47 | 0.96 | -1.63 |
| C | -1.08 | 0.63 | -0.26 |
| O | -1.31 | 1.73 | 0.22 |
| S | -2.37 | -0.73 | 0.00 |
| H | -3.17 | 0.04 | 0.77 |
| 26 |  | C | 1.14 | -1.35 | 0.85 |
| H | 0.85 | -2.19 | 0.21 |
| H | 1.99 | -1.66 | 1.46 |
| H | 0.30 | -1.12 | 1.52 |
| C | 1.87 | 1.08 | 0.87 |
| H | 2.69 | 0.82 | 1.55 |
| H | 2.20 | 1.91 | 0.25 |
| H | 1.00 | 1.40 | 1.46 |
| O | 2.61 | -0.46 | -0.83 |
| C | 1.60 | -0.15 | -0.05 |
| C | 0.29 | 0.26 | -1.02 |
| H | 0.24 | -0.57 | -1.73 |
| H | 0.62 | 1.17 | -1.52 |
| C | -1.02 | 0.49 | -0.37 |
| O | -1.41 | 1.50 | 0.19 |
| O | -1.82 | -0.64 | -0.40 |
| C | -3.04 | -0.55 | 0.32 |
| H | -3.53 | -1.51 | 0.21 |
| H | -2.85 | -0.35 | 1.38 |
| H | -3.67 | 0.25 | -0.07 |

**Table S1** Coordinates of 29 molecules optimized at the B3LYP/6-311+G(d) level (continue)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Molecule No. | Molecular structure | Atom | X | Y | Z |
| 27 |  | C | 1.03 | -1.16 | 1.00 |
| H | 0.85 | -2.13 | 0.51 |
| H | 1.97 | -1.25 | 1.56 |
| H | 0.22 | -0.97 | 1.71 |
| C | 1.36 | 1.32 | 0.63 |
| H | 2.27 | 1.30 | 1.24 |
| H | 1.48 | 2.10 | -0.13 |
| H | 0.51 | 1.59 | 1.26 |
| O | 2.19 | -0.31 | -0.93 |
| C | 1.22 | -0.06 | -0.08 |
| C | -0.22 | 0.01 | -0.96 |
| H | -0.21 | -0.91 | -1.54 |
| H | -0.08 | 0.87 | -1.62 |
| C | -1.49 | 0.16 | -0.23 |
| O | -2.00 | 1.18 | 0.20 |
| H | -2.88 | -0.82 | 0.58 |
| O | -2.12 | -1.05 | 0.02 |
| 28 |  | C | -0.99 | 0.84 | 0.72 |
| C | 0.19 | 1.33 | -0.13 |
| C | 1.45 | 0.50 | 0.14 |
| C | 1.13 | -0.95 | -0.22 |
| C | -0.06 | -1.42 | 0.63 |
| H | -0.04 | 1.22 | -1.20 |
| H | -1.04 | 1.47 | 1.61 |
| H | 0.87 | -0.98 | -1.28 |
| H | 0.20 | -2.24 | 1.29 |
| H | 1.73 | 0.58 | 1.20 |
| O | -0.78 | -0.51 | 1.28 |
| C | -2.34 | 0.87 | 0.03 |
| H | -3.14 | 0.62 | 0.72 |
| H | -2.50 | 1.88 | -0.37 |
| O | -2.32 | -0.08 | -1.07 |
| H | -3.05 | 0.07 | -1.68 |
| O | 2.17 | -1.86 | 0.07 |
| H | 2.92 | -1.67 | -0.51 |
| O | 2.50 | 0.93 | -0.70 |
| H | 3.21 | 1.33 | -0.19 |
| O | 0.34 | 2.70 | 0.19 |
| H | 0.91 | 3.12 | -0.46 |
| H | -1.68 | -1.48 | -0.80 |
| O | -1.05 | -2.19 | -0.43 |
| H | -1.55 | -2.90 | 0.00 |

**Table S1** Coordinates of 29 molecules optimized at the B3LYP/6-311+G(d) level (continue)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Molecule No. | Molecular structure | Atom | X | Y | Z |
| 29 |  | C | 1.35 | 0.25 | -0.60 |
| C | 0.29 | 1.15 | 0.05 |
| C | -1.15 | 0.65 | -0.12 |
| C | -1.20 | -0.87 | 0.19 |
| H | 0.48 | 1.19 | 1.13 |
| H | 1.77 | 0.74 | -1.48 |
| H | -0.78 | -1.02 | 1.20 |
| H | -1.47 | 0.81 | -1.16 |
| O | 0.77 | -1.02 | -1.20 |
| C | 2.44 | -0.24 | 0.33 |
| H | 3.17 | -0.85 | -0.21 |
| H | 2.95 | 0.64 | 0.73 |
| O | 1.79 | -0.99 | 1.35 |
| H | 2.42 | -1.34 | 1.99 |
| O | -2.49 | -1.39 | 0.03 |
| H | -2.84 | -1.74 | 0.86 |
| O | -1.94 | 1.38 | 0.78 |
| H | -2.86 | 1.39 | 0.49 |
| O | 0.49 | 2.42 | -0.54 |
| H | 0.01 | 3.09 | -0.03 |
| C | -0.29 | -1.53 | -0.78 |
| H | -0.57 | -2.47 | -1.27 |