Supplementary information for

**Excited-State Polarizabilities: A Combined Density Functional Theory and Information-Theoretic Approach Study**

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**Table S1.** Excited-State ITA Quantities (in a.u.) Based on the Ground-State Geometry, with the Transition Density Matrix as Input.

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| **index** | **SS** | **IF** | **SGBP** | **rR2** | **rR3** | **IG** | **G1** | **G2** | **G3** |
| 1 | 96.62 | 4343.66 | 747.19 | 112.60 | 117.73 | 1.36 | **–**35.10 | 23.95 | 139.60 |
| 2 | 20.91 | 13967.03 | 974.35 | 146.55 | 151.56 | 1.33 | **–**34.68 | 23.61 | 141.54 |
| 3 | 143.16 | 5692.57 | 1017.29 | 154.00 | 161.88 | 2.08 | **–**50.74 | 34.87 | 195.88 |
| 4 | 98.03 | 4793.24 | 802.00 | 120.73 | 126.10 | 1.43 | **–**34.22 | 22.38 | 147.61 |
| 5 | 108.23 | 5045.39 | 855.88 | 129.04 | 135.06 | 1.58 | **–**38.87 | 25.61 | 159.66 |
| 6 | 93.25 | 4917.75 | 802.25 | 120.55 | 125.53 | 1.33 | **–**34.34 | 22.72 | 143.99 |
| 7 | 81.99 | 6523.98 | 855.67 | 128.54 | 133.50 | 1.32 | **–**34.65 | 22.09 | 141.99 |
| 8 | 20.86 | 13966.83 | 974.31 | 146.55 | 151.55 | 1.33 | **–**34.70 | 23.58 | 141.63 |
| 9 | 102.64 | 4928.22 | 829.73 | 124.72 | 130.02 | 1.42 | **–**36.45 | 23.07 | 150.98 |
| 10 | 106.75 | 4595.15 | 801.16 | 120.89 | 126.54 | 1.51 | **–**38.84 | 25.82 | 150.78 |
| 11 | 108.29 | 5045.38 | 855.91 | 128.99 | 134.82 | 1.56 | **–**38.84 | 23.73 | 159.47 |
| 12 | 81.97 | 6524.04 | 855.65 | 128.58 | 133.67 | 1.34 | **–**34.70 | 22.48 | 142.14 |
| 13 | 20.92 | 13967.07 | 974.34 | 146.59 | 151.71 | 1.35 | **–**34.76 | 22.69 | 141.71 |
| 14 | 102.61 | 4928.35 | 829.69 | 124.75 | 130.11 | 1.44 | **–**36.47 | 23.40 | 151.04 |
| 15 | 106.74 | 4595.21 | 801.16 | 120.89 | 126.62 | 1.51 | **–**38.89 | 24.50 | 150.86 |
| 16 | 96.60 | 6318.28 | 966.13 | 144.77 | 150.18 | 1.45 | **–**37.41 | 23.14 | 164.95 |
| 17 | 135.43 | 5825.99 | 1018.15 | 153.64 | 160.79 | 1.89 | **–**52.49 | 36.56 | 192.01 |
| 18 | 135.35 | 5825.83 | 1018.08 | 153.64 | 160.85 | 1.89 | **–**52.56 | 36.86 | 192.38 |
| 19 | 147.02 | 6527.75 | 1126.86 | 170.06 | 178.02 | 2.11 | **–**56.25 | 38.42 | 212.03 |
| 20 | 153.40 | 7224.94 | 1222.48 | 184.28 | 192.65 | 2.23 | **–**58.67 | 39.73 | 226.62 |
| 21 | 146.95 | 6527.57 | 1126.80 | 170.07 | 178.12 | 2.12 | **–**56.26 | 39.01 | 212.40 |
| 22 | 153.33 | 7224.81 | 1222.41 | 184.28 | 192.70 | 2.23 | **–**58.74 | 39.64 | 226.87 |
| 23 | 92.09 | 6775.55 | 909.62 | 136.86 | 142.49 | 1.49 | **–**38.38 | 26.23 | 153.09 |
| 24 | 106.73 | 6569.76 | 1020.10 | 153.06 | 159.01 | 1.60 | **–**41.10 | 26.28 | 176.00 |
| 25 | 174.15 | 7308.13 | 1289.03 | 194.68 | 203.90 | 2.43 | **–**69.91 | 50.12 | 244.61 |
| 26 | 191.13 | 7329.96 | 1328.91 | 201.27 | 211.66 | 2.74 | **–**74.36 | 52.65 | 255.14 |
| 27 | 83.02 | 6639.96 | 967.30 | 144.45 | 149.26 | 1.28 | **–**32.81 | 20.06 | 158.31 |

Cartesian coordinates optimized at the CAM-B3LYP/6-311+G(d) level

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| 26 |  |  |  |
| **1** |  |  |  |
| C | 1.85598 | 0.58956 | -0.00015 |
| C | 3.22436 | -1.39818 | 0.00039 |
| C | 4.34370 | -0.63354 | 0.00024 |
| C | 4.24113 | 0.78375 | -0.00011 |
| C | 3.01965 | 1.38770 | -0.00030 |
| C | -0.13442 | -0.25313 | -0.00001 |
| C | 0.72884 | -1.32570 | 0.00029 |
| H | 3.22658 | -2.47964 | 0.00065 |
| H | 5.31191 | -1.11632 | 0.00039 |
| H | 5.14365 | 1.38262 | -0.00023 |
| H | 2.90424 | 2.46360 | -0.00057 |
| H | 0.56850 | -2.38996 | 0.00059 |
| N | 1.99656 | -0.79204 | 0.00020 |
| N | 0.57604 | 0.91819 | -0.00027 |
| C | -1.59991 | -0.25338 | -0.00005 |
| C | -2.31178 | -1.45782 | -0.00011 |
| C | -2.32937 | 0.95069 | -0.00002 |
| C | -3.69174 | -1.49056 | -0.00010 |
| H | -1.76322 | -2.39371 | -0.00018 |
| C | -3.72485 | 0.91407 | -0.00001 |
| C | -4.39904 | -0.28972 | -0.00004 |
| H | -4.21526 | -2.43927 | -0.00014 |
| H | -4.25321 | 1.86009 | 0.00003 |
| H | -5.48357 | -0.29658 | -0.00003 |
| O | -1.75109 | 2.16494 | 0.00000 |
| H | -0.77442 | 2.06413 | -0.00013 |

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| 26 |  |  |  |
| **2** |  |  |  |
| C | -3.36093 | 0.56690 | 0.00001 |
| C | -4.67708 | -1.45576 | 0.00003 |
| C | -5.81550 | -0.72027 | 0.00003 |
| C | -5.74970 | 0.69929 | 0.00001 |
| C | -4.54468 | 1.33504 | -0.00000 |
| C | -1.35009 | -0.22431 | 0.00002 |
| C | -2.18433 | -1.31887 | 0.00003 |
| H | -4.65107 | -2.53687 | 0.00005 |
| H | -6.77094 | -1.22778 | 0.00003 |
| H | -6.66753 | 1.27437 | 0.00000 |
| H | -4.45737 | 2.41355 | -0.00002 |
| H | -1.99681 | -2.37875 | 0.00003 |
| N | -3.46532 | -0.81746 | 0.00003 |
| N | -2.08960 | 0.92849 | -0.00000 |
| C | 0.11423 | -0.18263 | 0.00002 |
| C | 0.86416 | -1.36135 | 0.00000 |
| C | 0.80757 | 1.04296 | 0.00002 |
| C | 2.24474 | -1.36019 | -0.00002 |
| H | 0.34941 | -2.31584 | 0.00000 |
| C | 2.20401 | 1.05467 | -0.00000 |
| C | 2.89941 | -0.13368 | -0.00002 |
| H | 2.80242 | -2.28698 | -0.00003 |
| O | 0.19635 | 2.23707 | 0.00005 |
| H | 2.70863 | 2.01170 | 0.00000 |
| Br | 4.80185 | -0.09673 | -0.00004 |
| H | -0.77851 | 2.10762 | 0.00009 |

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| 40 |  |  |  |
| **3** |  |  |  |
| C | -3.53893 | 0.55033 | 0.00009 |
| C | -4.81954 | -1.49493 | -0.00026 |
| C | -5.97122 | -0.77976 | -0.00014 |
| C | -5.93035 | 0.64056 | 0.00011 |
| C | -4.73622 | 1.29706 | 0.00022 |
| C | -1.51354 | -0.20490 | -0.00004 |
| C | -2.32939 | -1.31409 | -0.00023 |
| H | -4.77476 | -2.57547 | -0.00045 |
| H | -6.91751 | -1.30421 | -0.00022 |
| H | -6.85805 | 1.19966 | 0.00020 |
| H | -4.66772 | 2.37696 | 0.00040 |
| H | -2.12277 | -2.37037 | -0.00041 |
| N | -3.61934 | -0.83607 | -0.00015 |
| N | -2.27447 | 0.93444 | 0.00015 |
| C | -0.05031 | -0.14008 | -0.00003 |
| C | 0.71876 | -1.30901 | -0.00027 |
| C | 0.62797 | 1.09220 | 0.00022 |
| C | 2.09730 | -1.27936 | -0.00026 |
| H | 0.21600 | -2.27047 | -0.00048 |
| C | 2.02400 | 1.11661 | 0.00023 |
| C | 2.76325 | -0.04856 | -0.00001 |
| H | 2.65787 | -2.20687 | -0.00046 |
| H | 2.52735 | 2.07516 | 0.00043 |
| O | -0.00060 | 2.28098 | 0.00047 |
| N | 4.19888 | 0.03852 | 0.00002 |
| C | 4.81062 | -0.50513 | -1.21243 |
| H | 5.89217 | -0.39699 | -1.09561 |
| H | 4.61690 | -1.58684 | -1.31601 |
| C | 4.36863 | 0.21748 | -2.47337 |
| H | 4.58206 | 1.28561 | -2.40031 |
| H | 4.89939 | -0.18083 | -3.34132 |
| H | 3.29911 | 0.10053 | -2.65466 |
| C | 4.81062 | -0.50572 | 1.21219 |
| H | 4.61691 | -1.58749 | 1.31525 |
| H | 5.89217 | -0.39752 | 1.09543 |
| C | 4.36863 | 0.21627 | 2.47349 |
| H | 4.58207 | 1.28443 | 2.40096 |
| H | 3.29910 | 0.09924 | 2.65471 |
| H | 4.89936 | -0.18248 | 3.34125 |
| H | -0.97187 | 2.13815 | 0.00043 |

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| 27 |  |  |  |
| **4** |  |  |  |
| C | 2.25803 | 0.58123 | -0.00003 |
| C | 3.60812 | -1.41782 | 0.00003 |
| C | 4.73498 | -0.66335 | -0.00001 |
| C | 4.64499 | 0.75411 | -0.00005 |
| C | 3.42827 | 1.36875 | -0.00006 |
| C | 0.25890 | -0.24415 | 0.00001 |
| C | 1.11325 | -1.32425 | 0.00004 |
| H | 3.60077 | -2.49927 | 0.00006 |
| H | 5.69867 | -1.15510 | 0.00000 |
| H | 5.55256 | 1.34533 | -0.00008 |
| H | 3.32258 | 2.44566 | -0.00010 |
| H | 0.94379 | -2.38715 | 0.00009 |
| N | 2.38624 | -0.80131 | 0.00001 |
| N | 0.98044 | 0.92101 | -0.00003 |
| C | -1.20359 | -0.22673 | 0.00001 |
| C | -1.94010 | -1.41633 | 0.00004 |
| C | -1.92055 | 0.98490 | -0.00002 |
| C | -3.31726 | -1.43738 | 0.00005 |
| H | -1.41008 | -2.36267 | 0.00006 |
| C | -3.31482 | 0.97229 | -0.00001 |
| C | -4.00496 | -0.22471 | 0.00003 |
| H | -3.87383 | -2.36576 | 0.00008 |
| O | -1.32915 | 2.19045 | -0.00006 |
| H | -3.83086 | 1.92712 | -0.00003 |
| O | -5.36493 | -0.27905 | 0.00004 |
| H | -5.73691 | 0.60892 | 0.00003 |
| H | -0.35243 | 2.07460 | -0.00006 |

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| 30 |  |  |  |
| **5** |  |  |  |
| C | -2.63606 | 0.61229 | -0.00014 |
| C | -4.05484 | -1.33874 | 0.00009 |
| C | -5.15496 | -0.54568 | -0.00001 |
| C | -5.01582 | 0.86778 | -0.00018 |
| C | -3.77844 | 1.43979 | -0.00024 |
| C | -0.66664 | -0.28191 | -0.00003 |
| C | -1.55820 | -1.33178 | 0.00010 |
| H | -4.08505 | -2.41981 | 0.00022 |
| H | -6.13512 | -1.00373 | 0.00005 |
| H | -5.90232 | 1.49017 | -0.00026 |
| H | -3.63542 | 2.51239 | -0.00038 |
| H | -1.42557 | -2.39989 | 0.00026 |
| N | -2.81234 | -0.76513 | 0.00003 |
| N | -1.34761 | 0.90764 | -0.00017 |
| C | 0.79500 | -0.31623 | -0.00002 |
| C | 1.49014 | -1.53324 | -0.00004 |
| C | 1.55596 | 0.86438 | 0.00003 |
| C | 2.86247 | -1.59941 | 0.00000 |
| H | 0.92802 | -2.46095 | -0.00010 |
| C | 2.95252 | 0.80952 | 0.00008 |
| C | 3.60206 | -0.41106 | 0.00006 |
| H | 3.38747 | -2.54618 | -0.00002 |
| H | 3.48109 | 1.75251 | 0.00011 |
| O | 1.00956 | 2.09221 | 0.00004 |
| O | 4.95085 | -0.55433 | 0.00010 |
| C | 5.75124 | 0.60889 | 0.00018 |
| H | 5.57213 | 1.21519 | 0.89258 |
| H | 6.78258 | 0.26393 | 0.00022 |
| H | 5.57221 | 1.21525 | -0.89219 |
| H | 0.02969 | 2.01283 | -0.00005 |

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| 26 |  |  |  |
| **6** |  |  |  |
| C | -2.21599 | 0.54922 | 0.00013 |
| C | -3.37670 | -1.56717 | -0.00015 |
| C | -4.56699 | -0.91928 | -0.00003 |
| C | -4.60811 | 0.50146 | 0.00018 |
| C | -3.45449 | 1.22604 | 0.00026 |
| C | -0.15247 | -0.08828 | -0.00000 |
| C | -0.90152 | -1.24273 | -0.00015 |
| H | -3.26940 | -2.64326 | -0.00031 |
| H | -5.48163 | -1.49710 | -0.00010 |
| H | -5.56666 | 1.00575 | 0.00027 |
| H | -3.44849 | 2.30806 | 0.00042 |
| H | -0.63412 | -2.28539 | -0.00031 |
| N | -2.21627 | -0.83938 | -0.00007 |
| N | -0.97589 | 1.00581 | 0.00018 |
| C | 1.30530 | 0.06024 | -0.00002 |
| C | 2.12803 | -1.07227 | -0.00020 |
| C | 1.90972 | 1.33060 | 0.00015 |
| C | 3.49213 | -0.93530 | -0.00022 |
| H | 1.70534 | -2.06965 | -0.00033 |
| C | 3.30198 | 1.43267 | 0.00012 |
| C | 4.10117 | 0.30720 | -0.00006 |
| H | 3.73541 | 2.42529 | 0.00025 |
| H | 5.18188 | 0.38013 | -0.00008 |
| O | 1.21407 | 2.48309 | 0.00034 |
| F | 4.26506 | -2.04825 | -0.00040 |
| H | 0.25235 | 2.28633 | 0.00035 |

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| 26 |  |  |  |
| **7** |  |  |  |
| C | 2.57735 | 0.47242 | 0.00009 |
| C | 3.52470 | -1.74744 | -0.00006 |
| C | 4.77279 | -1.21941 | 0.00002 |
| C | 4.95306 | 0.19038 | 0.00013 |
| C | 3.87609 | 1.02466 | 0.00017 |
| C | 0.46104 | 0.03998 | 0.00000 |
| C | 1.09329 | -1.18217 | -0.00007 |
| H | 3.31230 | -2.80779 | -0.00014 |
| H | 5.62634 | -1.88415 | -0.00001 |
| H | 5.95644 | 0.59823 | 0.00019 |
| H | 3.97632 | 2.10204 | 0.00026 |
| H | 0.72549 | -2.19378 | -0.00016 |
| N | 2.44129 | -0.90930 | -0.00002 |
| N | 1.38770 | 1.04818 | 0.00011 |
| C | -0.97501 | 0.33342 | -0.00001 |
| C | -1.90668 | -0.70913 | -0.00006 |
| C | -1.44857 | 1.65850 | 0.00003 |
| C | -3.25893 | -0.45103 | -0.00007 |
| H | -1.56813 | -1.73778 | -0.00010 |
| C | -2.82375 | 1.89731 | 0.00003 |
| C | -3.72884 | 0.85664 | -0.00003 |
| H | -3.15845 | 2.92754 | 0.00006 |
| H | -4.79390 | 1.05230 | -0.00003 |
| O | -0.64193 | 2.73262 | 0.00007 |
| Cl | -4.39642 | -1.78320 | -0.00014 |
| H | 0.29606 | 2.43994 | 0.00007 |

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| 26 |  |  |  |
| **8** |  |  |  |
| C | 2.88003 | -0.71195 | 0.00021 |
| C | 4.69066 | 0.88305 | 0.00062 |
| C | 5.58958 | -0.13114 | 0.00059 |
| C | 5.14507 | -1.48101 | 0.00037 |
| C | 3.81372 | -1.76997 | 0.00018 |
| C | 1.15501 | 0.59012 | 0.00019 |
| C | 2.25271 | 1.42030 | 0.00041 |
| H | 4.95587 | 1.93143 | 0.00078 |
| H | 6.64622 | 0.10111 | 0.00073 |
| H | 5.87484 | -2.28133 | 0.00034 |
| H | 3.43980 | -2.78533 | 0.00001 |
| H | 2.35708 | 2.49147 | 0.00056 |
| N | 3.35189 | 0.59345 | 0.00043 |
| N | 1.55840 | -0.71830 | 0.00007 |
| C | -0.26736 | 0.94907 | 0.00008 |
| C | -0.65748 | 2.28943 | 0.00020 |
| C | -1.26101 | -0.05217 | -0.00014 |
| C | -1.98812 | 2.65707 | 0.00010 |
| H | 0.10367 | 3.06150 | 0.00037 |
| C | -2.60509 | 0.34065 | -0.00024 |
| C | -2.96894 | 1.67195 | -0.00012 |
| H | -2.26947 | 3.70311 | 0.00019 |
| H | -4.01879 | 1.93697 | -0.00020 |
| O | -0.98352 | -1.35916 | -0.00026 |
| Br | -3.95024 | -0.99588 | -0.00054 |
| H | -0.00741 | -1.48821 | -0.00016 |

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| 27 |  |  |  |
| **9** |  |  |  |
| C | 2.44898 | 0.46707 | 0.00004 |
| C | 3.42787 | -1.73884 | -0.00010 |
| C | 4.66779 | -1.19260 | -0.00006 |
| C | 4.82768 | 0.21971 | 0.00004 |
| C | 3.73925 | 1.03868 | 0.00009 |
| C | 0.33946 | 0.00290 | 0.00001 |
| C | 0.98865 | -1.20938 | -0.00008 |
| H | 3.23049 | -2.80204 | -0.00017 |
| H | 5.53093 | -1.84475 | -0.00010 |
| H | 5.82512 | 0.64179 | 0.00007 |
| H | 3.82422 | 2.11734 | 0.00016 |
| H | 0.63612 | -2.22649 | -0.00015 |
| N | 2.33248 | -0.91575 | -0.00005 |
| N | 1.25027 | 1.02507 | 0.00008 |
| C | -1.10062 | 0.27901 | 0.00002 |
| C | -2.02263 | -0.76328 | -0.00006 |
| C | -1.58791 | 1.60339 | 0.00011 |
| C | -3.39117 | -0.52822 | -0.00006 |
| H | -1.67234 | -1.78853 | -0.00012 |
| C | -2.96664 | 1.83622 | 0.00010 |
| C | -3.85998 | 0.79119 | 0.00002 |
| H | -3.30446 | 2.86517 | 0.00017 |
| H | -4.92600 | 0.98355 | 0.00002 |
| O | -0.79075 | 2.67537 | 0.00020 |
| C | -4.30617 | -1.62605 | -0.00014 |
| N | -5.03956 | -2.51168 | -0.00021 |
| H | 0.15229 | 2.38876 | 0.00021 |

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| 29 |  |  |  |
| **10** |  |  |  |
| C | -2.24173 | 0.53292 | 0.00003 |
| C | -3.36354 | -1.60377 | -0.00003 |
| C | -4.56617 | -0.97810 | 0.00000 |
| C | -4.63325 | 0.44129 | 0.00005 |
| C | -3.49238 | 1.18649 | 0.00006 |
| C | -0.16491 | -0.06640 | -0.00003 |
| C | -0.89440 | -1.23429 | -0.00003 |
| H | -3.23690 | -2.67781 | -0.00006 |
| H | -5.46991 | -1.57289 | -0.00000 |
| H | -5.60071 | 0.92837 | 0.00007 |
| H | -3.50602 | 2.26848 | 0.00009 |
| H | -0.60836 | -2.27183 | -0.00005 |
| N | -2.21677 | -0.85574 | -0.00002 |
| N | -1.01030 | 1.01191 | 0.00002 |
| C | 1.28970 | 0.10911 | -0.00003 |
| C | 2.13993 | -1.00486 | -0.00001 |
| C | 1.86805 | 1.38853 | -0.00003 |
| C | 3.51740 | -0.89766 | 0.00002 |
| H | 1.69757 | -1.99637 | -0.00000 |
| C | 3.25903 | 1.50830 | -0.00001 |
| C | 4.06416 | 0.39021 | 0.00002 |
| H | 3.67984 | 2.50695 | -0.00002 |
| H | 5.14318 | 0.51362 | 0.00003 |
| O | 1.15397 | 2.53014 | -0.00010 |
| C | 4.40639 | -2.11249 | 0.00008 |
| H | 3.82233 | -3.03447 | -0.00020 |
| H | 5.05558 | -2.13503 | -0.87929 |
| H | 5.05512 | -2.13528 | 0.87978 |
| H | 0.19628 | 2.31628 | -0.00019 |

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| 30 |  |  |  |
| **11** |  |  |  |
| C | -2.63839 | 0.46038 | -0.00003 |
| C | -3.60464 | -1.75171 | -0.00003 |
| C | -4.84858 | -1.21347 | -0.00005 |
| C | -5.01711 | 0.19779 | -0.00006 |
| C | -3.93287 | 1.02280 | -0.00005 |
| C | -0.52563 | 0.01087 | 0.00001 |
| C | -1.16860 | -1.20614 | -0.00001 |
| H | -3.40130 | -2.81388 | -0.00003 |
| H | -5.70757 | -1.87124 | -0.00007 |
| H | -6.01704 | 0.61416 | -0.00007 |
| H | -4.02394 | 2.10104 | -0.00005 |
| H | -0.80758 | -2.22012 | -0.00001 |
| N | -2.51418 | -0.92322 | -0.00002 |
| N | -1.44466 | 1.02636 | -0.00001 |
| C | 0.91436 | 0.28720 | 0.00002 |
| C | 1.82862 | -0.76563 | 0.00002 |
| C | 1.40446 | 1.60745 | 0.00002 |
| C | 3.19501 | -0.54728 | 0.00001 |
| H | 1.48581 | -1.79370 | 0.00003 |
| C | 2.77802 | 1.81707 | 0.00001 |
| C | 3.67362 | 0.76026 | 0.00000 |
| H | 3.13301 | 2.84080 | 0.00001 |
| H | 4.73493 | 0.97101 | -0.00001 |
| O | 0.61004 | 2.69934 | 0.00006 |
| O | 3.98416 | -1.66472 | 0.00000 |
| C | 5.38157 | -1.48864 | 0.00006 |
| H | 5.81286 | -2.48735 | 0.00009 |
| H | 5.71960 | -0.95235 | -0.89241 |
| H | 5.71953 | -0.95233 | 0.89255 |
| H | -0.32912 | 2.41922 | 0.00011 |

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| 26 |  |  |  |
| **12** |  |  |  |
| C | -1.02496 | 0.86945 | 0.00024 |
| C | -2.57142 | -0.98680 | -0.00036 |
| C | -3.60611 | -0.11157 | -0.00017 |
| C | -3.38411 | 1.28978 | 0.00023 |
| C | -2.10987 | 1.77034 | 0.00044 |
| C | 0.87694 | -0.15487 | 0.00008 |
| C | -0.08416 | -1.14288 | -0.00028 |
| H | -2.68910 | -2.06076 | -0.00067 |
| H | -4.23390 | 1.95962 | 0.00037 |
| H | -1.89904 | 2.83147 | 0.00075 |
| H | -0.02446 | -2.21741 | -0.00064 |
| N | -1.29478 | -0.49293 | -0.00015 |
| N | 0.27945 | 1.07673 | 0.00037 |
| C | 2.33519 | -0.29485 | 0.00013 |
| C | 2.92801 | -1.56249 | 0.00019 |
| C | 3.17662 | 0.83367 | 0.00007 |
| C | 4.29813 | -1.72719 | 0.00014 |
| H | 2.29267 | -2.44174 | 0.00028 |
| C | 4.56211 | 0.66335 | 0.00002 |
| C | 5.11734 | -0.59950 | 0.00005 |
| H | 4.72836 | -2.72160 | 0.00019 |
| H | 5.17881 | 1.55425 | -0.00003 |
| H | 6.19613 | -0.71049 | 0.00001 |
| O | 2.71854 | 2.09824 | 0.00008 |
| Cl | -5.23590 | -0.71992 | -0.00044 |
| H | 1.73778 | 2.09416 | 0.00031 |

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| 26 |  |  |  |
| **13** |  |  |  |
| C | 0.29386 | 0.98681 | 0.00007 |
| C | 1.91774 | -0.80229 | -0.00004 |
| C | 2.91561 | 0.11487 | 0.00001 |
| C | 2.63367 | 1.50625 | 0.00010 |
| C | 1.34002 | 1.93251 | 0.00013 |
| C | -1.56304 | -0.11733 | 0.00001 |
| C | -0.56132 | -1.06360 | -0.00004 |
| H | 2.07505 | -1.87114 | -0.00010 |
| H | 3.45107 | 2.21501 | 0.00014 |
| H | 1.08471 | 2.98390 | 0.00019 |
| H | -0.57543 | -2.13970 | -0.00011 |
| N | 0.62111 | -0.36286 | -0.00001 |
| N | -1.01780 | 1.13884 | 0.00008 |
| C | -3.01414 | -0.31814 | 0.00000 |
| C | -3.55338 | -1.60955 | 0.00007 |
| C | -3.90209 | 0.77414 | -0.00006 |
| C | -4.91534 | -1.83157 | 0.00008 |
| H | -2.88166 | -2.46131 | 0.00013 |
| C | -5.27927 | 0.54578 | -0.00005 |
| C | -5.78108 | -0.73918 | 0.00001 |
| H | -5.30360 | -2.84311 | 0.00013 |
| H | -5.93276 | 1.41004 | -0.00010 |
| H | -6.85428 | -0.89536 | 0.00002 |
| O | -3.49758 | 2.05684 | -0.00015 |
| Br | 4.71498 | -0.47575 | -0.00003 |
| H | -2.51746 | 2.09430 | -0.00017 |

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| 27 |  |  |  |
| **14** |  |  |  |
| C | 1.16629 | 0.85916 | -0.00002 |
| C | 2.70292 | -1.00083 | -0.00009 |
| C | 3.75457 | -0.13165 | -0.00010 |
| C | 3.52358 | 1.27745 | -0.00007 |
| C | 2.25286 | 1.76026 | -0.00003 |
| C | -0.73639 | -0.16727 | 0.00001 |
| C | 0.22005 | -1.15646 | -0.00004 |
| H | 2.81630 | -2.07595 | -0.00011 |
| H | 4.37253 | 1.94853 | -0.00008 |
| H | 2.04126 | 2.82112 | -0.00001 |
| H | 0.15778 | -2.23080 | -0.00006 |
| N | 1.43521 | -0.50938 | -0.00006 |
| N | -0.13304 | 1.06613 | 0.00001 |
| C | -2.19399 | -0.30106 | 0.00004 |
| C | -2.78942 | -1.56831 | -0.00004 |
| C | -3.03284 | 0.82943 | 0.00015 |
| C | -4.15913 | -1.72999 | -0.00002 |
| H | -2.15626 | -2.44904 | -0.00013 |
| C | -4.41881 | 0.66144 | 0.00017 |
| C | -4.97596 | -0.60003 | 0.00009 |
| H | -4.59162 | -2.72329 | -0.00009 |
| H | -5.03379 | 1.55343 | 0.00026 |
| H | -6.05489 | -0.70893 | 0.00010 |
| O | -2.57511 | 2.09385 | 0.00026 |
| C | 5.08662 | -0.64821 | -0.00014 |
| N | 6.16113 | -1.05421 | -0.00017 |
| H | -1.59558 | 2.09287 | 0.00026 |

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| 29 |  |  |  |
| **15** |  |  |  |
| C | 1.41013 | 0.77135 | 0.00003 |
| C | 2.89940 | -1.12847 | 0.00004 |
| C | 3.98555 | -0.31482 | 0.00007 |
| C | 3.77894 | 1.09787 | 0.00009 |
| C | 2.52770 | 1.63286 | 0.00007 |
| C | -0.52513 | -0.18827 | -0.00003 |
| C | 0.40355 | -1.20573 | 0.00000 |
| H | 2.95856 | -2.20895 | 0.00003 |
| H | 4.64445 | 1.75143 | 0.00011 |
| H | 2.35517 | 2.70118 | 0.00008 |
| H | 0.30917 | -2.27790 | 0.00000 |
| N | 1.63511 | -0.59469 | 0.00002 |
| N | 0.11189 | 1.02376 | 0.00001 |
| C | -1.98807 | -0.27906 | -0.00005 |
| C | -2.62493 | -1.52459 | 0.00002 |
| C | -2.79006 | 0.87793 | -0.00010 |
| C | -4.00053 | -1.64178 | 0.00006 |
| H | -2.02007 | -2.42515 | 0.00006 |
| C | -4.18060 | 0.75617 | -0.00006 |
| C | -4.78009 | -0.48670 | 0.00002 |
| H | -4.46487 | -2.62085 | 0.00012 |
| H | -4.76585 | 1.66813 | -0.00011 |
| H | -5.86219 | -0.55990 | 0.00004 |
| O | -2.28643 | 2.12520 | -0.00025 |
| C | 5.37860 | -0.87623 | 0.00010 |
| H | 5.93631 | -0.54621 | -0.87969 |
| H | 5.93626 | -0.54627 | 0.87993 |
| H | 5.37387 | -1.96693 | 0.00006 |
| H | -1.30521 | 2.08326 | -0.00037 |

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| 29 |  |  |  |
| **16** |  |  |  |
| C | 0.36293 | 0.97468 | 0.00014 |
| C | 1.96916 | -0.82652 | -0.00028 |
| C | 2.97950 | 0.07834 | -0.00017 |
| C | 2.70329 | 1.47503 | 0.00010 |
| C | 1.41685 | 1.91466 | 0.00025 |
| C | -1.50145 | -0.11914 | 0.00004 |
| C | -0.50909 | -1.07230 | -0.00019 |
| H | 2.11916 | -1.89647 | -0.00049 |
| H | 3.52552 | 2.17962 | 0.00017 |
| H | 1.16768 | 2.96733 | 0.00046 |
| H | -0.53155 | -2.14826 | -0.00039 |
| N | 0.68082 | -0.38059 | -0.00013 |
| N | -0.94413 | 1.13510 | 0.00024 |
| C | -2.95382 | -0.30651 | 0.00008 |
| C | -3.50305 | -1.59407 | -0.00014 |
| C | -3.83305 | 0.79277 | 0.00035 |
| C | -4.86634 | -1.80534 | -0.00011 |
| H | -2.83825 | -2.45120 | -0.00035 |
| C | -5.21200 | 0.57496 | 0.00038 |
| C | -5.72351 | -0.70593 | 0.00016 |
| H | -5.26248 | -2.81375 | -0.00028 |
| H | -5.85879 | 1.44420 | 0.00059 |
| H | -6.79785 | -0.85367 | 0.00019 |
| O | -3.42031 | 2.07279 | 0.00057 |
| C | 4.40043 | -0.38569 | -0.00027 |
| F | 5.06870 | 0.06481 | -1.07802 |
| F | 4.50104 | -1.72478 | -0.00096 |
| F | 5.06848 | 0.06366 | 1.07812 |
| H | -2.44085 | 2.10552 | 0.00052 |

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| 36 |  |  |  |
| **17** |  |  |  |
| C | -0.23230 | 1.08470 | -0.13534 |
| C | 1.48195 | -0.60242 | 0.06319 |
| C | 2.45970 | 0.33746 | -0.05411 |
| C | 2.07682 | 1.70449 | -0.21338 |
| C | 0.76717 | 2.07254 | -0.25474 |
| C | -2.03017 | -0.10397 | 0.01558 |
| C | -0.98111 | -0.99019 | 0.11794 |
| H | 1.67960 | -1.65472 | 0.21532 |
| H | 2.85161 | 2.45317 | -0.32535 |
| H | 0.46119 | 3.10217 | -0.38576 |
| H | -0.93903 | -2.05782 | 0.24723 |
| N | 0.16429 | -0.23477 | 0.01931 |
| N | -1.55115 | 1.17010 | -0.13994 |
| C | -3.46965 | -0.37561 | 0.05425 |
| C | -3.94393 | -1.68274 | 0.20922 |
| C | -4.41136 | 0.66433 | -0.06199 |
| C | -5.29344 | -1.97000 | 0.25036 |
| H | -3.23013 | -2.49458 | 0.29967 |
| C | -5.77539 | 0.37045 | -0.01987 |
| C | -6.21274 | -0.92905 | 0.13424 |
| H | -5.63044 | -2.99270 | 0.37144 |
| H | -6.47125 | 1.19589 | -0.11225 |
| H | -7.27685 | -1.13648 | 0.16448 |
| O | -4.07006 | 1.95631 | -0.21479 |
| C | 3.88820 | -0.05495 | -0.01132 |
| C | 4.34870 | -1.16839 | -0.71455 |
| C | 4.80318 | 0.68496 | 0.73879 |
| C | 5.68465 | -1.53911 | -0.66031 |
| H | 3.65946 | -1.73474 | -1.33149 |
| C | 6.13929 | 0.31681 | 0.79056 |
| H | 4.46182 | 1.54443 | 1.30541 |
| C | 6.58466 | -0.79787 | 0.09261 |
| H | 6.02529 | -2.40388 | -1.21880 |
| H | 6.83425 | 0.89948 | 1.38493 |
| H | 7.62929 | -1.08505 | 0.13251 |
| H | -3.09171 | 2.03846 | -0.23141 |

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| 36 |  |  |  |
| **18** |  |  |  |
| C | 0.65407 | 1.05443 | 0.04337 |
| C | 0.81497 | 3.46777 | 0.06609 |
| C | 2.16610 | 3.37619 | 0.07249 |
| C | 2.79573 | 2.10621 | 0.06882 |
| C | 2.07311 | 0.94210 | 0.05375 |
| C | -1.49273 | 0.77767 | 0.00217 |
| C | -1.28873 | 2.13749 | 0.02438 |
| H | 0.26257 | 4.39716 | 0.07342 |
| H | 2.75864 | 4.28129 | 0.09068 |
| H | 3.87728 | 2.05636 | 0.10155 |
| H | -1.96273 | 2.97661 | 0.01413 |
| N | 0.07479 | 2.31656 | 0.05122 |
| N | -0.28797 | 0.12684 | 0.01342 |
| C | -2.75541 | 0.03478 | -0.03274 |
| C | -3.98002 | 0.70855 | 0.02668 |
| C | -2.77237 | -1.36947 | -0.13011 |
| C | -5.18562 | 0.03713 | -0.01079 |
| H | -3.98191 | 1.79032 | 0.10828 |
| C | -3.99318 | -2.04538 | -0.16779 |
| C | -5.18529 | -1.35293 | -0.10956 |
| H | -6.11830 | 0.58655 | 0.03802 |
| H | -3.96818 | -3.12597 | -0.24423 |
| H | -6.12313 | -1.89684 | -0.13977 |
| O | -1.65752 | -2.11999 | -0.19070 |
| C | 2.72880 | -0.38530 | 0.04214 |
| C | 3.84342 | -0.60544 | -0.76799 |
| C | 2.27115 | -1.42759 | 0.84952 |
| C | 4.49099 | -1.83202 | -0.76555 |
| H | 4.19240 | 0.18430 | -1.42418 |
| C | 2.92170 | -2.65196 | 0.85427 |
| H | 1.40375 | -1.27673 | 1.47911 |
| C | 4.03301 | -2.85902 | 0.04788 |
| H | 5.34988 | -1.98806 | -1.40887 |
| H | 2.55498 | -3.44990 | 1.49012 |
| H | 4.53564 | -3.81976 | 0.04840 |
| H | -0.86670 | -1.53852 | -0.15569 |

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| **19** |  |  |  |
| C | -1.08927 | 1.13335 | -0.15434 |
| C | 0.67801 | -0.50306 | 0.00075 |
| C | 1.62649 | 0.46515 | -0.12839 |
| C | 1.19872 | 1.82107 | -0.27166 |
| C | -0.12161 | 2.15104 | -0.28418 |
| C | -2.84829 | -0.10905 | 0.01757 |
| C | -1.77152 | -0.96440 | 0.09328 |
| H | 0.90812 | -1.55016 | 0.14287 |
| H | 1.94850 | 2.59310 | -0.39524 |
| H | -0.46002 | 3.17212 | -0.40194 |
| H | -1.69532 | -2.03132 | 0.21264 |
| N | -0.65121 | -0.17426 | -0.01876 |
| N | -2.41046 | 1.17983 | -0.13487 |
| C | -4.27825 | -0.42382 | 0.07998 |
| C | -4.71103 | -1.74605 | 0.22731 |
| C | -5.25213 | 0.58917 | -0.00527 |
| C | -6.05061 | -2.07349 | 0.29085 |
| H | -3.97207 | -2.53749 | 0.29333 |
| C | -6.60588 | 0.25480 | 0.05946 |
| C | -7.00206 | -1.05882 | 0.20565 |
| H | -6.35507 | -3.10712 | 0.40523 |
| H | -7.32724 | 1.06045 | -0.00924 |
| H | -8.05888 | -1.29785 | 0.25371 |
| O | -4.95136 | 1.89233 | -0.14844 |
| C | 3.06551 | 0.11601 | -0.11737 |
| C | 3.55100 | -0.98824 | -0.82582 |
| C | 3.98006 | 0.87582 | 0.60318 |
| C | 4.88982 | -1.32180 | -0.80357 |
| H | 2.86975 | -1.58162 | -1.42601 |
| C | 5.33231 | 0.55490 | 0.63356 |
| H | 3.63524 | 1.72918 | 1.17707 |
| C | 5.79287 | -0.55167 | -0.07160 |
| H | 5.26591 | -2.17186 | -1.36023 |
| H | 6.00677 | 1.16933 | 1.21477 |
| O | 7.08748 | -0.95464 | -0.11175 |
| C | 8.05029 | -0.20620 | 0.60054 |
| H | 7.83874 | -0.20264 | 1.67369 |
| H | 9.00348 | -0.69885 | 0.42517 |
| H | 8.10418 | 0.82362 | 0.23585 |
| H | -3.97606 | 2.00246 | -0.18431 |

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| 42 |  |  |  |
| **20** |  |  |  |
| C | 1.81114 | 1.17026 | 0.19164 |
| C | -0.00338 | -0.40948 | 0.00316 |
| C | -0.92037 | 0.58467 | 0.16175 |
| C | -0.45464 | 1.92356 | 0.33833 |
| C | 0.87511 | 2.21232 | 0.35599 |
| C | 3.53117 | -0.11856 | -0.02875 |
| C | 2.42964 | -0.93958 | -0.12261 |
| H | -0.26659 | -1.44498 | -0.16425 |
| H | -1.18019 | 2.71438 | 0.48452 |
| H | 1.24470 | 3.21895 | 0.50067 |
| H | 2.32172 | -1.99993 | -0.27195 |
| N | 1.33335 | -0.12090 | 0.02025 |
| N | 3.13163 | 1.17795 | 0.16466 |
| C | 4.95049 | -0.47292 | -0.10955 |
| C | 5.34223 | -1.80211 | -0.30393 |
| C | 5.95479 | 0.50690 | 0.00475 |
| C | 6.67072 | -2.16731 | -0.38509 |
| H | 4.57956 | -2.56830 | -0.39349 |
| C | 7.29753 | 0.13406 | -0.07780 |
| C | 7.65282 | -1.18508 | -0.27019 |
| H | 6.94338 | -3.20505 | -0.53609 |
| H | 8.04329 | 0.91470 | 0.01441 |
| H | 8.70165 | -1.45417 | -0.33152 |
| O | 5.69527 | 1.81313 | 0.19314 |
| C | -2.36875 | 0.27691 | 0.14241 |
| C | -2.87579 | -0.83907 | 0.81110 |
| C | -3.25798 | 1.10009 | -0.55064 |
| C | -4.22811 | -1.13020 | 0.77747 |
| H | -2.20757 | -1.47029 | 1.38600 |
| C | -4.61230 | 0.81420 | -0.58334 |
| H | -2.88264 | 1.96198 | -1.09064 |
| C | -5.10559 | -0.30586 | 0.08014 |
| H | -4.62403 | -1.99211 | 1.30037 |
| H | -5.29117 | 1.45480 | -1.13082 |
| C | -6.54941 | -0.66147 | 0.07837 |
| O | -7.01305 | -1.62196 | 0.63812 |
| O | -7.29455 | 0.20736 | -0.62024 |
| C | -8.69567 | -0.07153 | -0.66767 |
| H | -9.13252 | 0.72307 | -1.26612 |
| H | -8.87486 | -1.04176 | -1.12930 |
| H | -9.11762 | -0.07128 | 0.33656 |
| H | 4.72475 | 1.95360 | 0.23586 |

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| **21** |  |  |  |
| C | -0.29160 | 1.44992 | 0.04634 |
| C | -0.84352 | 3.80482 | 0.00760 |
| C | 0.47519 | 4.11156 | 0.03283 |
| C | 1.44815 | 3.08155 | 0.07330 |
| C | 1.09895 | 1.75594 | 0.07848 |
| C | -2.26288 | 0.55637 | -0.01502 |
| C | -2.46518 | 1.91653 | -0.02460 |
| H | -1.64346 | 4.53171 | -0.01683 |
| H | 0.77746 | 5.15051 | 0.03420 |
| H | 2.49584 | 3.35170 | 0.12514 |
| H | -3.35444 | 2.52156 | -0.06576 |
| N | -1.21420 | 2.48687 | 0.01523 |
| N | -0.92114 | 0.28658 | 0.02787 |
| C | -3.25317 | -0.52343 | -0.04854 |
| C | -4.62179 | -0.23631 | -0.01124 |
| C | -2.85798 | -1.87243 | -0.12338 |
| C | -5.57818 | -1.23118 | -0.04974 |
| H | -4.94051 | 0.79862 | 0.05393 |
| C | -3.82746 | -2.87605 | -0.16214 |
| C | -5.17058 | -2.56156 | -0.12649 |
| H | -6.63125 | -0.97774 | -0.01819 |
| H | -3.48680 | -3.90302 | -0.22079 |
| H | -5.90816 | -3.35614 | -0.15685 |
| O | -1.57177 | -2.26470 | -0.16149 |
| C | 2.11029 | 0.67818 | 0.10614 |
| C | 3.26320 | 0.77523 | -0.66464 |
| C | 1.95863 | -0.45210 | 0.91851 |
| C | 4.24775 | -0.20579 | -0.63326 |
| H | 3.39426 | 1.62342 | -1.32767 |
| C | 2.92948 | -1.42974 | 0.96432 |
| H | 1.06892 | -0.56090 | 1.52509 |
| C | 4.08287 | -1.31515 | 0.18802 |
| H | 5.12306 | -0.09524 | -1.25922 |
| H | 2.81475 | -2.30232 | 1.59609 |
| O | 4.97625 | -2.33032 | 0.29707 |
| C | 6.15533 | -2.27788 | -0.47700 |
| H | 6.71309 | -3.17977 | -0.23668 |
| H | 5.92967 | -2.26839 | -1.54731 |
| H | 6.76027 | -1.40202 | -0.22443 |
| H | -0.98611 | -1.47698 | -0.12408 |

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| 42 |  |  |  |
| **22** |  |  |  |
| C | -1.06596 | 1.55370 | 0.04851 |
| C | -2.00557 | 3.78242 | 0.04880 |
| C | -0.75763 | 4.30844 | 0.07310 |
| C | 0.37503 | 3.45687 | 0.08884 |
| C | 0.25105 | 2.09219 | 0.07797 |
| C | -2.85875 | 0.34252 | -0.01885 |
| C | -3.28726 | 1.64929 | -0.00782 |
| H | -2.91637 | 4.36502 | 0.04043 |
| H | -0.63532 | 5.38323 | 0.09021 |
| H | 1.36305 | 3.89832 | 0.13553 |
| H | -4.26605 | 2.09598 | -0.03724 |
| N | -2.15024 | 2.42195 | 0.03552 |
| N | -1.48990 | 0.30219 | 0.01526 |
| C | -3.65410 | -0.88710 | -0.06482 |
| C | -5.05119 | -0.83322 | -0.01036 |
| C | -3.04009 | -2.14936 | -0.16973 |
| C | -5.82815 | -1.97290 | -0.06125 |
| H | -5.53767 | 0.13230 | 0.07899 |
| C | -3.82877 | -3.30002 | -0.22112 |
| C | -5.20483 | -3.21485 | -0.16839 |
| H | -6.90827 | -1.89986 | -0.01566 |
| H | -3.32212 | -4.25430 | -0.30287 |
| H | -5.79970 | -4.12078 | -0.20871 |
| O | -1.70711 | -2.32128 | -0.22591 |
| C | 1.43389 | 1.20261 | 0.09434 |
| C | 2.54519 | 1.50685 | -0.69369 |
| C | 1.47844 | 0.06876 | 0.90802 |
| C | 3.67696 | 0.70991 | -0.66436 |
| H | 2.51417 | 2.36518 | -1.35514 |
| C | 2.61059 | -0.72533 | 0.94376 |
| H | 0.62337 | -0.18786 | 1.51936 |
| C | 3.71677 | -0.41088 | 0.15961 |
| H | 4.52950 | 0.95015 | -1.28591 |
| H | 2.65148 | -1.60105 | 1.57955 |
| C | 4.90651 | -1.29919 | 0.23518 |
| O | 4.99138 | -2.26554 | 0.94873 |
| O | 5.89582 | -0.90944 | -0.58439 |
| C | 7.07185 | -1.72029 | -0.56687 |
| H | 6.83441 | -2.74177 | -0.86163 |
| H | 7.75269 | -1.26516 | -1.28099 |
| H | 7.51251 | -1.73099 | 0.42938 |
| H | -1.25930 | -1.44968 | -0.17358 |

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| 29 |  |  |  |
| **23** |  |  |  |
| C | 1.41461 | 0.94381 | 0.00001 |
| C | 2.78360 | -1.04704 | 0.00011 |
| C | 3.89459 | -0.27086 | 0.00011 |
| C | 3.80268 | 1.14490 | 0.00006 |
| C | 2.57804 | 1.74074 | 0.00001 |
| C | -0.57372 | 0.09911 | -0.00002 |
| C | 0.29253 | -0.97327 | 0.00004 |
| H | 2.80192 | -2.12728 | 0.00014 |
| H | 4.71054 | 1.73364 | 0.00007 |
| H | 2.46587 | 2.81679 | -0.00003 |
| H | 0.13408 | -2.03769 | 0.00007 |
| N | 1.55796 | -0.43780 | 0.00006 |
| N | 0.13502 | 1.27050 | -0.00003 |
| C | -2.03831 | 0.09504 | -0.00006 |
| C | -2.74475 | -1.11564 | -0.00006 |
| C | -2.76955 | 1.29349 | -0.00011 |
| C | -4.12461 | -1.17870 | -0.00010 |
| H | -2.18409 | -2.04533 | -0.00003 |
| C | -4.16468 | 1.24108 | -0.00016 |
| C | -4.82561 | 0.03243 | -0.00016 |
| H | -4.70526 | 2.18025 | -0.00022 |
| H | -5.91155 | 0.02198 | -0.00022 |
| O | -2.20253 | 2.51485 | -0.00012 |
| Cl | 5.46146 | -1.02686 | 0.00018 |
| C | -4.85771 | -2.49336 | -0.00000 |
| H | -4.16515 | -3.33682 | -0.00086 |
| H | -5.49822 | -2.59549 | 0.88000 |
| H | -5.49963 | -2.59484 | -0.87905 |
| H | -1.22664 | 2.42345 | -0.00009 |

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| 32 |  |  |  |
| **24** |  |  |  |
| C | -0.74480 | -1.10391 | 0.00004 |
| C | -2.20381 | 0.81854 | -0.00009 |
| C | -3.28266 | -0.00360 | -0.00007 |
| C | -3.11764 | -1.41771 | 0.00001 |
| C | -1.86985 | -1.95752 | 0.00006 |
| C | 1.20034 | -0.16081 | 0.00003 |
| C | 0.28610 | 0.86779 | -0.00006 |
| H | -2.26891 | 1.89699 | -0.00015 |
| H | -3.99293 | -2.05519 | 0.00001 |
| H | -1.70464 | -3.02660 | 0.00012 |
| H | 0.39348 | 1.93857 | -0.00013 |
| N | -0.95484 | 0.27242 | -0.00004 |
| N | 0.54530 | -1.36722 | 0.00008 |
| C | 2.66261 | -0.08978 | 0.00004 |
| C | 3.31114 | 1.15337 | 0.00003 |
| C | 3.44941 | -1.25250 | 0.00005 |
| C | 4.68608 | 1.28151 | 0.00003 |
| H | 2.70738 | 2.05563 | 0.00004 |
| C | 4.84064 | -1.13396 | 0.00005 |
| C | 5.44341 | 0.10440 | 0.00005 |
| H | 5.42500 | -2.04648 | 0.00008 |
| H | 6.52760 | 0.16613 | 0.00006 |
| O | 2.94259 | -2.49998 | 0.00009 |
| C | -4.66228 | 0.57137 | -0.00006 |
| F | -5.36442 | 0.17550 | -1.07785 |
| F | -4.65679 | 1.91434 | -0.00054 |
| F | -5.36408 | 0.17629 | 1.07825 |
| C | 5.35670 | 2.62901 | -0.00005 |
| H | 4.62554 | 3.43917 | 0.00067 |
| H | 5.99305 | 2.76020 | 0.87906 |
| H | 5.99184 | 2.76069 | -0.87997 |
| H | 1.96402 | -2.45802 | 0.00014 |

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| 46 |  |  |  |
| **25** |  |  |  |
| C | 0.24166 | 0.04452 | 0.02300 |
| C | -1.46386 | -1.67029 | -0.01402 |
| C | -2.44335 | -0.72732 | 0.01234 |
| C | -2.06629 | 0.64658 | 0.04450 |
| C | -0.75968 | 1.05464 | 0.05204 |
| C | 2.04189 | -1.15471 | -0.04201 |
| C | 0.99384 | -2.04557 | -0.05002 |
| H | -1.65147 | -2.73393 | -0.06408 |
| H | -2.84873 | 1.39268 | 0.11150 |
| H | 0.94986 | -3.12023 | -0.09077 |
| N | -0.15134 | -1.28483 | -0.00547 |
| N | 1.56156 | 0.12689 | 0.00217 |
| C | 3.48180 | -1.42419 | -0.07689 |
| C | 3.96142 | -2.73816 | -0.05200 |
| C | 4.41830 | -0.37498 | -0.13936 |
| C | 5.31152 | -3.02372 | -0.09050 |
| H | 3.25129 | -3.55648 | 0.00238 |
| C | 5.78273 | -0.66711 | -0.17832 |
| C | 6.22560 | -1.97380 | -0.15457 |
| H | 5.65294 | -4.05189 | -0.06906 |
| H | 6.47463 | 0.16534 | -0.22763 |
| H | 7.29002 | -2.17966 | -0.18500 |
| O | 4.07157 | 0.92470 | -0.16521 |
| C | -0.39054 | 2.48805 | 0.09217 |
| C | -1.08810 | 3.41081 | -0.68824 |
| C | 0.63424 | 2.94979 | 0.91936 |
| C | -0.77783 | 4.76166 | -0.63725 |
| H | -1.86617 | 3.06417 | -1.35944 |
| C | 0.94090 | 4.30089 | 0.97280 |
| H | 1.19099 | 2.24737 | 1.52606 |
| C | 0.23705 | 5.21135 | 0.19582 |
| H | -1.32451 | 5.46303 | -1.25782 |
| H | 1.73766 | 4.64299 | 1.62366 |
| H | 0.48361 | 6.26652 | 0.23441 |
| C | -3.87120 | -1.12509 | 0.01284 |
| C | -4.32515 | -2.17071 | 0.81714 |
| C | -4.79191 | -0.45993 | -0.79769 |
| C | -5.66006 | -2.54879 | 0.80311 |
| H | -3.63140 | -2.67620 | 1.48013 |
| C | -6.12701 | -0.83503 | -0.80962 |
| H | -4.45567 | 0.34548 | -1.44149 |
| C | -6.56576 | -1.88232 | -0.01044 |
| H | -5.99545 | -3.35970 | 1.44010 |
| H | -6.82654 | -0.31108 | -1.45143 |
| H | -7.60964 | -2.17487 | -0.01904 |
| H | 3.09317 | 1.00513 | -0.13292 |

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| 52 |  |  |  |
| **26** |  |  |  |
| C | 0.48884 | 3.11874 | -0.15642 |
| C | 2.84132 | 2.85572 | 0.29590 |
| C | 3.00736 | 4.20018 | 0.23953 |
| C | 1.89861 | 5.04832 | -0.02503 |
| C | 0.65888 | 4.51825 | -0.21940 |
| C | -0.19261 | 1.06853 | -0.13778 |
| C | 1.16402 | 1.00321 | 0.12658 |
| H | 3.64452 | 2.16001 | 0.49062 |
| H | 3.99410 | 4.61555 | 0.39608 |
| H | 2.04645 | 6.12036 | -0.07133 |
| H | -0.20982 | 5.13100 | -0.42178 |
| N | 1.59542 | 2.31945 | 0.09778 |
| N | -0.58827 | 2.37257 | -0.29777 |
| C | -1.18534 | -0.01248 | -0.22199 |
| C | -0.81491 | -1.32771 | -0.52217 |
| C | -2.54923 | 0.25487 | -0.00009 |
| C | -1.74451 | -2.34677 | -0.54900 |
| H | 0.21614 | -1.54687 | -0.76613 |
| C | -3.50345 | -0.77580 | -0.00624 |
| C | -3.08064 | -2.06623 | -0.27699 |
| H | -1.43844 | -3.35835 | -0.78969 |
| H | -3.80199 | -2.87438 | -0.29599 |
| O | -3.01716 | 1.49661 | 0.23951 |
| C | 2.10079 | -0.10812 | 0.45717 |
| H | 2.76800 | 0.20500 | 1.26803 |
| H | 1.53043 | -0.94288 | 0.86569 |
| C | 2.95452 | -0.59738 | -0.73076 |
| H | 2.29141 | -0.95894 | -1.52095 |
| H | 3.50075 | 0.24558 | -1.16321 |
| C | 3.92417 | -1.67923 | -0.33005 |
| C | 5.25082 | -1.37886 | -0.03241 |
| C | 3.50360 | -3.00277 | -0.21256 |
| C | 6.13509 | -2.36994 | 0.37340 |
| H | 5.60245 | -0.35569 | -0.12935 |
| C | 4.38219 | -3.99737 | 0.19236 |
| H | 2.47519 | -3.26090 | -0.44755 |
| C | 5.70233 | -3.68333 | 0.48830 |
| H | 7.16574 | -2.11552 | 0.59549 |
| H | 4.03611 | -5.02198 | 0.27327 |
| H | 6.39092 | -4.45979 | 0.80217 |
| C | -4.93924 | -0.40172 | 0.26759 |
| H | -4.98260 | 0.13110 | 1.22333 |
| H | -5.25556 | 0.34044 | -0.47184 |
| C | -5.93773 | -1.55866 | 0.28359 |
| H | -5.95071 | -2.06883 | -0.68419 |
| H | -5.62335 | -2.30078 | 1.02721 |
| C | -7.32252 | -1.09437 | 0.61993 |
| H | -7.43393 | -0.59145 | 1.57980 |
| C | -8.38924 | -1.24161 | -0.15267 |
| H | -9.36596 | -0.87942 | 0.14839 |
| H | -8.32882 | -1.73148 | -1.12030 |
| H | -2.30254 | 2.14830 | 0.07133 |

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| 26 |  |  |  |
| **27** |  |  |  |
| C | 2.78803 | 0.66884 | -0.00005 |
| C | 4.10110 | -1.35611 | 0.00003 |
| C | 5.23949 | -0.62221 | 0.00004 |
| C | 5.17549 | 0.79861 | -0.00000 |
| C | 3.97280 | 1.43711 | -0.00005 |
| C | 0.77922 | -0.12393 | -0.00001 |
| C | 1.61071 | -1.21982 | -0.00005 |
| H | 4.07174 | -2.43706 | 0.00006 |
| H | 6.19447 | -1.13045 | 0.00007 |
| H | 6.09444 | 1.37189 | -0.00001 |
| H | 3.88782 | 2.51577 | -0.00009 |
| H | 1.41729 | -2.27673 | -0.00005 |
| N | 2.88990 | -0.71428 | -0.00001 |
| N | 1.51775 | 1.03123 | -0.00010 |
| C | -0.68360 | -0.05024 | 0.00002 |
| C | -1.47232 | -1.19847 | 0.00001 |
| C | -1.34268 | 1.19771 | 0.00003 |
| C | -2.84802 | -1.16163 | 0.00001 |
| C | -2.73741 | 1.22883 | 0.00001 |
| C | -3.48310 | 0.06987 | 0.00000 |
| O | -0.71402 | 2.37342 | 0.00006 |
| F | -0.88674 | -2.40757 | 0.00001 |
| F | -3.56326 | -2.28888 | -0.00000 |
| F | -4.81119 | 0.12847 | -0.00000 |
| F | -3.36843 | 2.40368 | 0.00002 |
| H | 0.26139 | 2.21783 | 0.00012 |

Cartesian coordinates optimized at the TD-CAM-B3LYP/6-311+G(d) level

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| 26 |  |  |  |
| **1** |  |  |  |
| C | 1.95124 | 0.27266 | -0.63568 |
| C | 3.20149 | -0.77538 | 1.15188 |
| C | 4.35162 | -0.32444 | 0.55158 |
| C | 4.34005 | 0.41760 | -0.62521 |
| C | 3.08705 | 0.71910 | -1.24493 |
| C | -0.16034 | -0.20808 | 0.03017 |
| C | 0.68287 | -0.73678 | 0.93224 |
| H | 3.14824 | -1.34407 | 2.06527 |
| H | 5.29431 | -0.56398 | 1.02929 |
| H | 5.26274 | 0.76115 | -1.06951 |
| H | 3.02435 | 1.27803 | -2.16803 |
| H | 0.47539 | -1.30183 | 1.82449 |
| N | 1.97732 | -0.45539 | 0.53683 |
| N | 0.61858 | 0.38339 | -0.97126 |
| C | -1.63592 | -0.23355 | -0.04584 |
| C | -2.30628 | -1.29473 | -0.59352 |
| C | -2.38818 | 0.91259 | 0.44954 |
| C | -3.70888 | -1.32041 | -0.65015 |
| H | -1.74430 | -2.13744 | -0.97712 |
| C | -3.83156 | 0.83995 | 0.38272 |
| C | -4.46190 | -0.24840 | -0.15478 |
| H | -4.20983 | -2.18165 | -1.07378 |
| H | -4.37934 | 1.68797 | 0.77452 |
| H | -5.54408 | -0.28699 | -0.20111 |
| O | -1.81308 | 1.92128 | 0.89183 |
| H | 0.27833 | 1.10165 | -1.58585 |

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| 26 |  |  |  |
| **2** |  |  |  |
| C | -3.45332 | 0.26419 | 0.64280 |
| C | -4.70337 | -0.85955 | -1.09873 |
| C | -5.85514 | -0.42926 | -0.48784 |
| C | -5.84478 | 0.33903 | 0.67252 |
| C | -4.59068 | 0.68959 | 1.26169 |
| C | -1.34113 | -0.16678 | -0.05343 |
| C | -2.18478 | -0.74142 | -0.92736 |
| H | -4.65016 | -1.44674 | -2.00041 |
| H | -6.79845 | -0.70667 | -0.94318 |
| H | -6.76888 | 0.66576 | 1.12619 |
| H | -4.52850 | 1.27003 | 2.17155 |
| H | -1.97620 | -1.32129 | -1.80997 |
| N | -3.47838 | -0.49148 | -0.51398 |
| N | -2.11739 | 0.42193 | 0.95342 |
| C | 0.13426 | -0.15001 | -0.00743 |
| C | 0.85000 | -1.19159 | 0.52218 |
| C | 0.84433 | 1.01673 | -0.51523 |
| C | 2.25115 | -1.18400 | 0.54744 |
| H | 0.32545 | -2.05193 | 0.91870 |
| C | 2.29246 | 0.99035 | -0.48497 |
| C | 2.95190 | -0.08379 | 0.03466 |
| H | 2.79239 | -2.02706 | 0.95429 |
| O | 0.23539 | 2.01069 | -0.94034 |
| H | 2.81014 | 1.85161 | -0.88535 |
| Br | 4.85051 | -0.11358 | 0.07863 |
| H | -1.79158 | 1.18179 | 1.52490 |

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| 40 |  |  |  |
| **3** |  |  |  |
| C | -3.62106 | 0.68448 | -0.11120 |
| C | -4.87089 | -1.38534 | -0.21445 |
| C | -6.02342 | -0.63991 | -0.16802 |
| C | -6.01348 | 0.74943 | -0.09320 |
| C | -4.75897 | 1.43512 | -0.07265 |
| C | -1.50821 | -0.13455 | -0.10416 |
| C | -2.35163 | -1.17859 | -0.16634 |
| H | -4.81712 | -2.46022 | -0.26274 |
| H | -6.96686 | -1.17258 | -0.18903 |
| H | -6.93817 | 1.30629 | -0.05334 |
| H | -4.69654 | 2.51354 | -0.03197 |
| H | -2.14316 | -2.23344 | -0.21470 |
| N | -3.64604 | -0.69467 | -0.17645 |
| N | -2.28590 | 1.03000 | -0.11501 |
| C | -0.03243 | -0.08304 | -0.09229 |
| C | 0.69947 | -0.12958 | -1.25019 |
| C | 0.66263 | 0.04884 | 1.18068 |
| C | 2.10033 | -0.09713 | -1.22975 |
| H | 0.18607 | -0.20905 | -2.20081 |
| C | 2.10851 | 0.06839 | 1.15406 |
| C | 2.81150 | -0.00147 | -0.01742 |
| H | 2.64315 | -0.15493 | -2.16516 |
| H | 2.62650 | 0.14447 | 2.10135 |
| O | 0.03637 | 0.16283 | 2.24869 |
| N | 4.24546 | 0.02380 | 0.00890 |
| C | 4.81901 | 1.20100 | -0.64572 |
| H | 5.90432 | 1.09900 | -0.57643 |
| H | 4.58079 | 1.22596 | -1.72309 |
| C | 4.39764 | 2.50687 | 0.00574 |
| H | 4.65257 | 2.50794 | 1.06698 |
| H | 4.90885 | 3.34592 | -0.47069 |
| H | 3.32418 | 2.68254 | -0.08242 |
| C | 4.85624 | -1.22283 | -0.45686 |
| H | 4.61924 | -1.42179 | -1.51628 |
| H | 5.93778 | -1.07762 | -0.40870 |
| C | 4.47534 | -2.42433 | 0.39079 |
| H | 4.73025 | -2.25356 | 1.43820 |
| H | 3.40794 | -2.64456 | 0.33606 |
| H | 5.01251 | -3.31081 | 0.04738 |
| H | -1.96133 | 1.91229 | 0.23974 |

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| 27 |  |  |  |
| **4** |  |  |  |
| C | 2.35061 | 0.23349 | -0.65444 |
| C | 3.60201 | -0.73614 | 1.17600 |
| C | 4.75281 | -0.33143 | 0.54484 |
| C | 4.74111 | 0.34873 | -0.66873 |
| C | 3.48694 | 0.63360 | -1.29353 |
| C | 0.23829 | -0.18325 | 0.05236 |
| C | 1.08311 | -0.67571 | 0.97393 |
| H | 3.54933 | -1.25638 | 2.11789 |
| H | 5.69618 | -0.55804 | 1.02753 |
| H | 5.66428 | 0.65688 | -1.13729 |
| H | 3.42376 | 1.14476 | -2.24394 |
| H | 0.87576 | -1.19116 | 1.89580 |
| N | 2.37692 | -0.43343 | 0.55448 |
| N | 1.01660 | 0.34320 | -0.98625 |
| C | -1.23609 | -0.19750 | -0.01180 |
| C | -1.92528 | -1.27581 | -0.50882 |
| C | -1.98080 | 0.97475 | 0.43920 |
| C | -3.32024 | -1.29502 | -0.55534 |
| H | -1.37727 | -2.14076 | -0.86083 |
| C | -3.42302 | 0.91688 | 0.38381 |
| C | -4.06278 | -0.18777 | -0.09987 |
| H | -3.85632 | -2.15575 | -0.93258 |
| O | -1.39338 | 1.99239 | 0.83772 |
| H | -3.96057 | 1.78940 | 0.73861 |
| O | -5.41190 | -0.30825 | -0.18358 |
| H | -5.84870 | 0.48309 | 0.14887 |
| H | 0.68111 | 1.03755 | -1.63032 |

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| **5** |  |  |  |
| C | -2.75449 | 0.21582 | 0.66180 |
| C | -4.01572 | -0.59977 | -1.23567 |
| C | -5.16056 | -0.20350 | -0.58845 |
| C | -5.14102 | 0.39764 | 0.66603 |
| C | -3.88507 | 0.60637 | 1.31682 |
| C | -0.64815 | -0.21569 | -0.05429 |
| C | -1.49806 | -0.62395 | -1.01173 |
| H | -3.96900 | -1.05998 | -2.20862 |
| H | -6.10541 | -0.37216 | -1.09156 |
| H | -6.05947 | 0.70154 | 1.14653 |
| H | -3.81627 | 1.05387 | 2.29845 |
| H | -1.29677 | -1.08532 | -1.96312 |
| N | -2.78836 | -0.37180 | -0.58742 |
| N | -1.42109 | 0.26585 | 1.00992 |
| C | 0.82428 | -0.27547 | 0.02050 |
| C | 1.47898 | -1.40102 | 0.46101 |
| C | 1.60676 | 0.89759 | -0.35418 |
| C | 2.86932 | -1.45906 | 0.51712 |
| H | 0.90428 | -2.26936 | 0.75807 |
| C | 3.04901 | 0.80121 | -0.29280 |
| C | 3.65482 | -0.34769 | 0.13157 |
| H | 3.37918 | -2.35401 | 0.84866 |
| H | 3.59631 | 1.68294 | -0.59428 |
| O | 1.05070 | 1.95273 | -0.69638 |
| O | 4.98872 | -0.54151 | 0.22937 |
| C | 5.84502 | 0.52277 | -0.14086 |
| H | 5.67608 | 1.40073 | 0.48801 |
| H | 6.85780 | 0.15862 | 0.00864 |
| H | 5.70522 | 0.79317 | -1.19066 |
| H | -1.07195 | 0.91018 | 1.69730 |

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| **6** |  |  |  |
| C | -2.24682 | 0.02159 | -0.69362 |
| C | -3.47963 | -0.47451 | 1.32916 |
| C | -4.63701 | -0.35271 | 0.60021 |
| C | -4.63779 | -0.04839 | -0.75750 |
| C | -3.38902 | 0.13697 | -1.42867 |
| C | -0.13292 | -0.01922 | 0.11833 |
| C | -0.96625 | -0.28841 | 1.13674 |
| H | -3.41801 | -0.69871 | 2.38106 |
| H | -5.57580 | -0.50065 | 1.12075 |
| H | -5.56628 | 0.04457 | -1.30145 |
| H | -3.33452 | 0.35756 | -2.48551 |
| H | -0.74994 | -0.50303 | 2.16909 |
| N | -2.26129 | -0.27234 | 0.65590 |
| N | -0.91376 | 0.12998 | -1.03459 |
| C | 1.34156 | 0.06191 | 0.07224 |
| C | 2.10618 | -1.05998 | -0.10066 |
| C | 1.98226 | 1.36791 | 0.18203 |
| C | 3.49754 | -0.95093 | -0.12981 |
| H | 1.65519 | -2.03866 | -0.20146 |
| C | 3.42973 | 1.40101 | 0.15583 |
| C | 4.16967 | 0.26342 | 0.00133 |
| H | 3.89657 | 2.37193 | 0.26119 |
| H | 5.25232 | 0.27549 | -0.02299 |
| O | 1.31460 | 2.41042 | 0.27313 |
| F | 4.21509 | -2.06612 | -0.28082 |
| H | -0.61194 | 0.64779 | -1.84126 |

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| 26 |  |  |  |
| **7** |  |  |  |
| C | -2.54775 | -0.03827 | -0.69347 |
| C | -3.74182 | -0.62204 | 1.32936 |
| C | -4.90112 | -0.61601 | 0.59357 |
| C | -4.92177 | -0.32911 | -0.76792 |
| C | -3.69151 | -0.03775 | -1.43523 |
| C | -0.44370 | 0.12518 | 0.12922 |
| C | -1.25507 | -0.20820 | 1.14670 |
| H | -3.66608 | -0.82717 | 2.38423 |
| H | -5.82538 | -0.84352 | 1.11135 |
| H | -5.85167 | -0.32809 | -1.31734 |
| H | -3.65129 | 0.17434 | -2.49443 |
| H | -1.02577 | -0.39119 | 2.18236 |
| N | -2.54326 | -0.31660 | 0.65965 |
| N | -1.22843 | 0.18872 | -1.02915 |
| C | 1.01742 | 0.33824 | 0.09061 |
| C | 1.88112 | -0.71491 | -0.03143 |
| C | 1.53519 | 1.70066 | 0.15390 |
| C | 3.26851 | -0.50063 | -0.05090 |
| H | 1.50220 | -1.72627 | -0.09886 |
| C | 2.97414 | 1.85985 | 0.14276 |
| C | 3.81232 | 0.78782 | 0.04171 |
| H | 3.35407 | 2.87115 | 0.21509 |
| H | 4.88767 | 0.91418 | 0.03058 |
| O | 0.77625 | 2.68033 | 0.19312 |
| Cl | 4.32489 | -1.85789 | -0.17795 |
| H | -0.97066 | 0.72420 | -1.83958 |

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| 26 |  |  |  |
| **8** |  |  |  |
| C | 3.14120 | -0.19242 | 0.67771 |
| C | 4.42276 | 0.00661 | -1.36599 |
| C | 5.50103 | -0.50514 | -0.68717 |
| C | 5.43696 | -0.86722 | 0.65497 |
| C | 4.20787 | -0.69324 | 1.36385 |
| C | 1.12807 | 0.54829 | -0.05031 |
| C | 1.98120 | 0.59893 | -1.08698 |
| H | 4.41017 | 0.29378 | -2.40424 |
| H | 6.42776 | -0.62668 | -1.23538 |
| H | 6.30242 | -1.27187 | 1.15882 |
| H | 4.11094 | -0.94240 | 2.41121 |
| H | 1.81973 | 0.92571 | -2.09978 |
| N | 3.21672 | 0.15388 | -0.65728 |
| N | 1.84891 | 0.09881 | 1.06287 |
| C | -0.29646 | 0.92707 | 0.04489 |
| C | -0.68162 | 2.22356 | 0.22733 |
| C | -1.29715 | -0.13562 | -0.03155 |
| C | -2.04265 | 2.57582 | 0.29494 |
| H | 0.07189 | 2.99729 | 0.30483 |
| C | -2.69266 | 0.28842 | 0.02923 |
| C | -3.03819 | 1.60792 | 0.19088 |
| H | -2.32188 | 3.61416 | 0.42053 |
| H | -4.08151 | 1.89308 | 0.23763 |
| O | -0.96782 | -1.32187 | -0.11852 |
| Br | -4.01419 | -1.02960 | -0.11754 |
| H | 1.41816 | -0.33880 | 1.85837 |

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| 27 |  |  |  |
| **9** |  |  |  |
| C | 2.44854 | 0.09747 | -0.66227 |
| C | 3.59527 | -0.90413 | 1.22007 |
| C | 4.77215 | -0.73729 | 0.53542 |
| C | 4.82511 | -0.16378 | -0.73290 |
| C | 3.61128 | 0.25844 | -1.35467 |
| C | 0.32402 | 0.07207 | 0.11780 |
| C | 1.11044 | -0.47187 | 1.06174 |
| H | 3.49438 | -1.33222 | 2.20364 |
| H | 5.68470 | -1.06779 | 1.01699 |
| H | 5.76891 | -0.04082 | -1.24333 |
| H | 3.59679 | 0.69160 | -2.34501 |
| H | 0.85432 | -0.88025 | 2.02437 |
| N | 2.41188 | -0.46692 | 0.59950 |
| N | 1.13579 | 0.38940 | -0.97884 |
| C | -1.13839 | 0.27294 | 0.08832 |
| C | -1.99859 | -0.76341 | -0.12057 |
| C | -1.66491 | 1.62565 | 0.26592 |
| C | -3.39978 | -0.56223 | -0.10403 |
| H | -1.61455 | -1.76251 | -0.28235 |
| C | -3.10536 | 1.78587 | 0.28804 |
| C | -3.93881 | 0.72318 | 0.10766 |
| H | -3.48322 | 2.78704 | 0.45215 |
| H | -5.01439 | 0.84956 | 0.12261 |
| O | -0.90607 | 2.59745 | 0.36578 |
| C | -4.26822 | -1.67008 | -0.29071 |
| N | -4.97280 | -2.56724 | -0.44307 |
| H | 0.90112 | 1.11208 | -1.63739 |

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| 29 |  |  |  |
| **10** |  |  |  |
| C | -2.25821 | 0.00796 | 0.69268 |
| C | -3.48731 | -0.50211 | -1.32867 |
| C | -4.64519 | -0.40404 | -0.59617 |
| C | -4.64793 | -0.10545 | 0.76258 |
| C | -3.40091 | 0.09988 | 1.43224 |
| C | -0.14442 | 0.00487 | -0.12347 |
| C | -0.97566 | -0.27393 | -1.14089 |
| H | -3.42388 | -0.71993 | -2.38177 |
| H | -5.58267 | -0.56622 | -1.11493 |
| H | -5.57687 | -0.03086 | 1.30875 |
| H | -3.34749 | 0.31837 | 2.48951 |
| H | -0.75849 | -0.47892 | -2.17491 |
| N | -2.27116 | -0.28072 | -0.65681 |
| N | -0.92777 | 0.13904 | 1.02870 |
| C | 1.32915 | 0.11203 | -0.07772 |
| C | 2.11718 | -0.99228 | 0.08225 |
| C | 1.94312 | 1.43012 | -0.17269 |
| C | 3.52697 | -0.91590 | 0.11799 |
| H | 1.64720 | -1.96579 | 0.17024 |
| C | 3.38678 | 1.47919 | -0.14515 |
| C | 4.13576 | 0.34391 | -0.00265 |
| H | 3.84291 | 2.45707 | -0.23823 |
| H | 5.21843 | 0.40952 | 0.01927 |
| O | 1.25762 | 2.46335 | -0.25030 |
| C | 4.33816 | -2.16341 | 0.26299 |
| H | 4.20688 | -2.81835 | -0.60360 |
| H | 5.40179 | -1.94734 | 0.35944 |
| H | 4.02686 | -2.73780 | 1.13935 |
| H | -0.62784 | 0.64029 | 1.84611 |

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| **11** |  |  |  |
| C | -2.60598 | -0.11608 | -0.69787 |
| C | -3.82986 | -0.52112 | 1.35014 |
| C | -4.97977 | -0.57395 | 0.59994 |
| C | -4.98076 | -0.40450 | -0.78053 |
| C | -3.74001 | -0.17493 | -1.45488 |
| C | -0.51028 | 0.10168 | 0.13534 |
| C | -1.33692 | -0.13664 | 1.16636 |
| H | -3.76857 | -0.63428 | 2.41962 |
| H | -5.91218 | -0.75291 | 1.12232 |
| H | -5.90361 | -0.44714 | -1.34034 |
| H | -3.68429 | -0.05340 | -2.52744 |
| H | -1.12324 | -0.22910 | 2.21707 |
| N | -2.62131 | -0.27725 | 0.67209 |
| N | -1.28321 | 0.07629 | -1.03062 |
| C | 0.95389 | 0.30465 | 0.09172 |
| C | 1.80495 | -0.75456 | 0.00587 |
| C | 1.47784 | 1.66568 | 0.10459 |
| C | 3.20569 | -0.57233 | -0.03306 |
| H | 1.42997 | -1.76998 | -0.01964 |
| C | 2.91542 | 1.80223 | 0.07828 |
| C | 3.75155 | 0.72108 | 0.00973 |
| H | 3.30699 | 2.81130 | 0.11207 |
| H | 4.82299 | 0.86989 | -0.01165 |
| O | 0.72874 | 2.65623 | 0.11606 |
| O | 3.92667 | -1.69952 | -0.10024 |
| C | 5.34303 | -1.62098 | -0.12522 |
| H | 5.69524 | -2.64706 | -0.17595 |
| H | 5.68897 | -1.07256 | -1.00379 |
| H | 5.72447 | -1.14845 | 0.78227 |
| H | -1.00118 | 0.50538 | -1.89395 |

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| 26 |  |  |  |
| **12** |  |  |  |
| C | -1.11364 | 0.79411 | -0.59252 |
| C | -2.54715 | -0.87404 | 0.41994 |
| C | -3.61482 | -0.09827 | 0.03873 |
| C | -3.49020 | 1.10247 | -0.64127 |
| C | -2.17747 | 1.55893 | -0.97618 |
| C | 0.91076 | -0.10947 | -0.13454 |
| C | -0.02526 | -0.93093 | 0.36975 |
| H | -2.60952 | -1.80441 | 0.95651 |
| H | -4.36441 | 1.67344 | -0.91270 |
| H | -2.02229 | 2.47940 | -1.51998 |
| H | 0.08197 | -1.86117 | 0.89993 |
| N | -1.26864 | -0.39137 | 0.09343 |
| N | 0.24204 | 0.94355 | -0.76395 |
| C | 2.38529 | -0.20897 | -0.13948 |
| C | 3.05154 | -0.92097 | -1.10066 |
| C | 3.14089 | 0.49273 | 0.89036 |
| C | 4.45206 | -1.02119 | -1.09212 |
| H | 2.48816 | -1.42899 | -1.87379 |
| C | 4.58062 | 0.35347 | 0.86864 |
| C | 5.20626 | -0.38262 | -0.09973 |
| H | 4.94943 | -1.60495 | -1.85621 |
| H | 5.12993 | 0.86163 | 1.65134 |
| H | 6.28608 | -0.47527 | -0.10490 |
| O | 2.57284 | 1.19866 | 1.74028 |
| Cl | -5.20932 | -0.68514 | 0.45091 |
| H | 0.66919 | 1.82148 | -0.99979 |

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| 26 |  |  |  |
| **13** |  |  |  |
| C | 0.37806 | 1.02102 | -0.47536 |
| C | 1.89884 | -0.75261 | 0.16271 |
| C | 2.92612 | 0.12780 | -0.07473 |
| C | 2.73987 | 1.43314 | -0.50085 |
| C | 1.40234 | 1.89062 | -0.71776 |
| C | -1.59896 | -0.03898 | -0.17169 |
| C | -0.62045 | -0.90369 | 0.14503 |
| H | 2.00466 | -1.76822 | 0.50125 |
| H | 3.58138 | 2.08685 | -0.66874 |
| H | 1.19901 | 2.89286 | -1.06622 |
| H | -0.67949 | -1.92362 | 0.48304 |
| N | 0.59438 | -0.26876 | -0.03981 |
| N | -0.98563 | 1.14438 | -0.59103 |
| C | -3.06828 | -0.19659 | -0.17133 |
| C | -3.73120 | -0.73402 | -1.24212 |
| C | -3.82362 | 0.25860 | 0.98892 |
| C | -5.12631 | -0.89184 | -1.22937 |
| H | -3.16870 | -1.05749 | -2.10939 |
| C | -5.25725 | 0.06683 | 0.96491 |
| C | -5.87886 | -0.49119 | -0.11821 |
| H | -5.62047 | -1.33520 | -2.08448 |
| H | -5.80549 | 0.38907 | 1.84137 |
| H | -6.95425 | -0.62570 | -0.12301 |
| O | -3.26114 | 0.80785 | 1.95084 |
| Br | 4.69374 | -0.51479 | 0.20915 |
| H | -1.45157 | 2.03249 | -0.64597 |

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| 27 |  |  |  |
| **14** |  |  |  |
| C | 1.25455 | 0.81847 | -0.51154 |
| C | 2.67872 | -0.92730 | 0.36774 |
| C | 3.76572 | -0.12575 | 0.04359 |
| C | 3.62479 | 1.12480 | -0.54439 |
| C | 2.32130 | 1.61632 | -0.84008 |
| C | -0.77288 | -0.11333 | -0.14297 |
| C | 0.15953 | -0.97415 | 0.30029 |
| H | 2.73157 | -1.89373 | 0.83676 |
| H | 4.49920 | 1.71372 | -0.77766 |
| H | 2.16509 | 2.57748 | -1.30643 |
| H | 0.04973 | -1.94050 | 0.76044 |
| N | 1.40407 | -0.41323 | 0.07896 |
| N | -0.09096 | 0.98726 | -0.66573 |
| C | -2.24815 | -0.20045 | -0.15805 |
| C | -2.91872 | -0.80545 | -1.18658 |
| C | -2.99731 | 0.39472 | 0.94109 |
| C | -4.32071 | -0.89317 | -1.18842 |
| H | -2.35988 | -1.23777 | -2.00764 |
| C | -4.43832 | 0.27254 | 0.90412 |
| C | -5.06965 | -0.35339 | -0.13575 |
| H | -4.82236 | -1.39050 | -2.00869 |
| H | -4.98386 | 0.70139 | 1.73537 |
| H | -6.15020 | -0.43495 | -0.15052 |
| O | -2.42304 | 0.99766 | 1.86264 |
| C | 5.07669 | -0.62513 | 0.33362 |
| N | 6.12675 | -1.02914 | 0.56570 |
| H | -0.51724 | 1.85699 | -0.93124 |

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| 29 |  |  |  |
| **15** |  |  |  |
| C | 1.50308 | 0.57591 | 0.67107 |
| C | 2.87299 | -0.87748 | -0.69489 |
| C | 3.99207 | -0.24421 | -0.21585 |
| C | 3.88396 | 0.80303 | 0.70768 |
| C | 2.59837 | 1.21491 | 1.16892 |
| C | -0.55556 | -0.15930 | 0.07943 |
| C | 0.34775 | -0.88433 | -0.60034 |
| H | 2.87660 | -1.68334 | -1.41154 |
| H | 4.77338 | 1.29734 | 1.07374 |
| H | 2.48144 | 2.00768 | 1.89486 |
| H | 0.20206 | -1.68694 | -1.30272 |
| N | 1.61176 | -0.45071 | -0.24575 |
| N | 0.14923 | 0.72038 | 0.91110 |
| C | -2.03149 | -0.22633 | 0.09670 |
| C | -2.69951 | -1.13355 | 0.87558 |
| C | -2.78875 | 0.71875 | -0.71436 |
| C | -4.10150 | -1.20227 | 0.87415 |
| H | -2.13482 | -1.82144 | 1.49284 |
| C | -4.23072 | 0.60548 | -0.69599 |
| C | -4.85735 | -0.33003 | 0.08036 |
| H | -4.59981 | -1.94276 | 1.48696 |
| H | -4.78077 | 1.29769 | -1.32128 |
| H | -5.93888 | -0.40085 | 0.08686 |
| O | -2.21886 | 1.60220 | -1.37714 |
| C | 5.34556 | -0.68776 | -0.70044 |
| H | 5.87199 | 0.13463 | -1.19000 |
| H | 5.96759 | -1.02217 | 0.13293 |
| H | 5.27146 | -1.50961 | -1.41386 |
| H | -0.23963 | 1.58749 | 1.23865 |

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| 29 |  |  |  |
| **16** |  |  |  |
| C | 0.44658 | 0.98124 | 0.51909 |
| C | 1.95094 | -0.73774 | -0.27734 |
| C | 2.99398 | 0.11218 | 0.02284 |
| C | 2.80435 | 1.37957 | 0.55421 |
| C | 1.47571 | 1.82968 | 0.81967 |
| C | -1.53734 | -0.04772 | 0.15993 |
| C | -0.56625 | -0.88658 | -0.23741 |
| H | 2.04479 | -1.71606 | -0.71433 |
| H | 3.64927 | 2.01736 | 0.76453 |
| H | 1.27791 | 2.80301 | 1.24377 |
| H | -0.63228 | -1.87510 | -0.65723 |
| N | 0.65277 | -0.26945 | -0.02093 |
| N | -0.91096 | 1.09860 | 0.65599 |
| C | -3.00768 | -0.19826 | 0.16473 |
| C | -3.66145 | -0.80387 | 1.20378 |
| C | -3.77212 | 0.33593 | -0.95507 |
| C | -5.05803 | -0.95294 | 1.19634 |
| H | -3.09185 | -1.18860 | 2.04094 |
| C | -5.20664 | 0.15130 | -0.92727 |
| C | -5.81992 | -0.47450 | 0.12332 |
| H | -5.54539 | -1.45001 | 2.02538 |
| H | -5.76246 | 0.53413 | -1.77406 |
| H | -6.89600 | -0.60305 | 0.13122 |
| O | -3.21633 | 0.94195 | -1.88608 |
| C | 4.38774 | -0.39885 | -0.17655 |
| F | 5.24387 | 0.57361 | -0.53373 |
| F | 4.45575 | -1.35196 | -1.12638 |
| F | 4.88815 | -0.95151 | 0.94955 |
| H | -1.37524 | 1.97063 | 0.83631 |

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| 36 |  |  |  |
| **17** |  |  |  |
| C | -0.15432 | 1.21991 | 0.27823 |
| C | 1.46818 | -0.48625 | -0.28018 |
| C | 2.47407 | 0.38315 | 0.08965 |
| C | 2.17933 | 1.66680 | 0.55522 |
| C | 0.82212 | 2.10179 | 0.63776 |
| C | -2.06943 | 0.09381 | -0.15989 |
| C | -1.04032 | -0.73057 | -0.42113 |
| H | 1.62051 | -1.46261 | -0.70975 |
| H | 2.97497 | 2.31621 | 0.89070 |
| H | 0.56206 | 3.09406 | 0.97873 |
| H | -1.04124 | -1.74523 | -0.78028 |
| N | 0.13643 | -0.05409 | -0.16215 |
| N | -1.52734 | 1.32154 | 0.23589 |
| C | -3.52701 | -0.10989 | -0.28367 |
| C | -4.17517 | 0.05373 | -1.47941 |
| C | -4.29129 | -0.46782 | 0.90493 |
| C | -5.55789 | -0.15830 | -1.59290 |
| H | -3.60767 | 0.33701 | -2.35735 |
| C | -5.71163 | -0.68798 | 0.74084 |
| C | -6.31601 | -0.53327 | -0.47613 |
| H | -6.03849 | -0.03828 | -2.55555 |
| H | -6.26432 | -0.97575 | 1.62647 |
| H | -7.38177 | -0.69856 | -0.58320 |
| O | -3.74824 | -0.55879 | 2.01875 |
| C | 3.88387 | -0.07367 | -0.01584 |
| C | 4.26687 | -1.33444 | 0.44120 |
| C | 4.85755 | 0.75290 | -0.57639 |
| C | 5.58451 | -1.75822 | 0.33935 |
| H | 3.52594 | -1.97807 | 0.90234 |
| C | 6.17560 | 0.33161 | -0.67744 |
| H | 4.57046 | 1.72906 | -0.95083 |
| C | 6.54447 | -0.92664 | -0.22075 |
| H | 5.86379 | -2.73918 | 0.70839 |
| H | 6.91684 | 0.98707 | -1.12176 |
| H | 7.57451 | -1.25643 | -0.29957 |
| H | -2.03424 | 2.00913 | 0.76475 |

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| 36 |  |  |  |
| **18** |  |  |  |
| C | -0.78003 | 0.97920 | 0.18098 |
| C | -0.90275 | 3.39637 | 0.10319 |
| C | -2.26986 | 3.27416 | 0.02004 |
| C | -2.90771 | 2.04390 | 0.01559 |
| C | -2.15187 | 0.82489 | 0.11842 |
| C | 1.46506 | 0.71148 | 0.16744 |
| C | 1.20923 | 2.03110 | 0.15743 |
| H | -0.34216 | 4.31586 | 0.09552 |
| H | -2.85721 | 4.18301 | -0.03542 |
| H | -3.98695 | 1.99560 | -0.01128 |
| H | 1.88367 | 2.86957 | 0.14461 |
| N | -0.16291 | 2.20582 | 0.16841 |
| N | 0.23511 | 0.05781 | 0.21721 |
| C | 2.74602 | -0.02383 | 0.17425 |
| C | 3.41008 | -0.29545 | 1.34057 |
| C | 3.30056 | -0.48263 | -1.09390 |
| C | 4.63365 | -0.98431 | 1.33836 |
| H | 2.99078 | 0.03724 | 2.28220 |
| C | 4.56702 | -1.18090 | -1.05035 |
| C | 5.20427 | -1.41995 | 0.13607 |
| H | 5.14076 | -1.17277 | 2.27601 |
| H | 4.97675 | -1.50236 | -1.99968 |
| H | 6.15134 | -1.94651 | 0.15243 |
| O | 2.70410 | -0.29505 | -2.16673 |
| C | -2.78211 | -0.49735 | 0.08720 |
| C | -3.92845 | -0.71673 | -0.69145 |
| C | -2.29890 | -1.57900 | 0.83957 |
| C | -4.54454 | -1.95593 | -0.73099 |
| H | -4.32273 | 0.09516 | -1.29149 |
| C | -2.91620 | -2.82032 | 0.79592 |
| H | -1.46498 | -1.43186 | 1.51720 |
| C | -4.04096 | -3.02104 | 0.00729 |
| H | -5.42321 | -2.09515 | -1.35185 |
| H | -2.52513 | -3.63260 | 1.39946 |
| H | -4.52434 | -3.99061 | -0.02537 |
| H | 0.09021 | -0.91157 | -0.01157 |

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| 40 |  |  |  |
| **19** |  |  |  |
| C | 1.02724 | 1.11052 | 0.72505 |
| C | -0.66763 | -0.45136 | -0.01371 |
| C | -1.63720 | 0.44465 | 0.38784 |
| C | -1.28660 | 1.67198 | 0.95764 |
| C | 0.08865 | 2.01287 | 1.13006 |
| C | 2.89153 | -0.04573 | 0.16445 |
| C | 1.82762 | -0.79520 | -0.17230 |
| H | -0.85793 | -1.37385 | -0.53737 |
| H | -2.05594 | 2.34261 | 1.31221 |
| H | 0.39072 | 2.94806 | 1.58048 |
| H | 1.78495 | -1.77319 | -0.61993 |
| N | 0.68121 | -0.10333 | 0.16858 |
| N | 2.40516 | 1.12240 | 0.76303 |
| C | 4.33883 | -0.31246 | 0.04151 |
| C | 5.01447 | -1.05384 | 0.97467 |
| C | 5.06438 | 0.25326 | -1.08904 |
| C | 6.38616 | -1.31798 | 0.84010 |
| H | 4.47669 | -1.45706 | 1.82395 |
| C | 6.47398 | -0.05343 | -1.19562 |
| C | 7.10550 | -0.81597 | -0.25226 |
| H | 6.88836 | -1.92268 | 1.58458 |
| H | 6.99646 | 0.35274 | -2.05276 |
| H | 8.16306 | -1.03492 | -0.34336 |
| O | 4.49903 | 0.98913 | -1.91556 |
| C | -3.06427 | 0.08164 | 0.19716 |
| C | -3.54077 | -1.19084 | 0.52603 |
| C | -3.97354 | 0.99766 | -0.31679 |
| C | -4.86736 | -1.53034 | 0.34633 |
| H | -2.85862 | -1.91867 | 0.95129 |
| C | -5.31351 | 0.67280 | -0.50312 |
| H | -3.62802 | 1.98628 | -0.59747 |
| C | -5.76491 | -0.59864 | -0.17080 |
| H | -5.23645 | -2.51422 | 0.61112 |
| H | -5.98364 | 1.41626 | -0.91403 |
| O | -7.05103 | -1.02250 | -0.31226 |
| C | -8.00292 | -0.11510 | -0.82065 |
| H | -7.74806 | 0.20666 | -1.83498 |
| H | -8.94911 | -0.65097 | -0.84290 |
| H | -8.10212 | 0.76386 | -0.17649 |
| H | 2.93310 | 1.97568 | 0.81771 |

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| 42 |  |  |  |
| **20** |  |  |  |
| C | 1.75591 | 1.16719 | -0.71513 |
| C | 0.00611 | -0.35672 | -0.02840 |
| C | -0.92891 | 0.57881 | -0.42881 |
| C | -0.53542 | 1.80373 | -0.96942 |
| C | 0.85114 | 2.10503 | -1.12268 |
| C | 3.57735 | -0.05394 | -0.15347 |
| C | 2.48729 | -0.77462 | 0.16274 |
| H | -0.21910 | -1.28068 | 0.47788 |
| H | -1.27905 | 2.50446 | -1.32065 |
| H | 1.18735 | 3.03615 | -1.55626 |
| H | 2.40899 | -1.75557 | 0.59862 |
| N | 1.36704 | -0.04052 | -0.17782 |
| N | 3.13001 | 1.13748 | -0.73264 |
| C | 5.01505 | -0.36257 | -0.01534 |
| C | 5.68574 | -1.09601 | -0.95793 |
| C | 5.73552 | 0.15148 | 1.14278 |
| C | 7.04843 | -1.39834 | -0.81003 |
| H | 5.15179 | -1.46283 | -1.82595 |
| C | 7.13534 | -0.19321 | 1.26152 |
| C | 7.76256 | -0.94486 | 0.30649 |
| H | 7.54701 | -1.99476 | -1.56350 |
| H | 7.65416 | 0.17537 | 2.13762 |
| H | 8.81277 | -1.19281 | 0.40732 |
| O | 5.17453 | 0.87483 | 1.98287 |
| C | -2.36894 | 0.25555 | -0.27305 |
| C | -2.86320 | -1.00604 | -0.60960 |
| C | -3.26243 | 1.20889 | 0.21748 |
| C | -4.20579 | -1.30577 | -0.45999 |
| H | -2.18718 | -1.75006 | -1.01486 |
| C | -4.60717 | 0.91503 | 0.36682 |
| H | -2.89048 | 2.18593 | 0.50284 |
| C | -5.08854 | -0.34742 | 0.02929 |
| H | -4.59023 | -2.28221 | -0.72831 |
| H | -5.28787 | 1.66176 | 0.75439 |
| C | -6.51878 | -0.71792 | 0.17069 |
| O | -6.97783 | -1.79721 | -0.10773 |
| O | -7.27109 | 0.28724 | 0.64965 |
| C | -8.65975 | 0.00009 | 0.81224 |
| H | -9.10446 | 0.91175 | 1.20219 |
| H | -9.10931 | -0.26609 | -0.14383 |
| H | -8.80026 | -0.82336 | 1.51169 |
| H | 3.69239 | 1.96509 | -0.82131 |

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| 40 |  |  |  |
| **21** |  |  |  |
| C | 0.14030 | 1.43783 | 0.16819 |
| C | 0.70443 | 3.78817 | 0.00822 |
| C | -0.64205 | 4.05540 | -0.04812 |
| C | -1.60332 | 3.05594 | 0.00116 |
| C | -1.21465 | 1.67822 | 0.13217 |
| C | 2.21914 | 0.54394 | 0.13426 |
| C | 2.34687 | 1.88109 | 0.08182 |
| H | 1.49978 | 4.51305 | -0.03921 |
| H | -0.94905 | 5.09171 | -0.12644 |
| H | -2.65339 | 3.31159 | -0.00530 |
| H | 3.23203 | 2.49144 | 0.03303 |
| N | 1.08318 | 2.43999 | 0.10648 |
| N | 0.85466 | 0.26401 | 0.22906 |
| C | 3.24053 | -0.52229 | 0.15254 |
| C | 3.83864 | -0.92282 | 1.31800 |
| C | 3.60142 | -1.17270 | -1.10158 |
| C | 4.81887 | -1.92731 | 1.32549 |
| H | 3.55952 | -0.44703 | 2.25011 |
| C | 4.62252 | -2.19633 | -1.04908 |
| C | 5.20550 | -2.55546 | 0.13469 |
| H | 5.28305 | -2.21220 | 2.26109 |
| H | 4.89458 | -2.65927 | -1.98939 |
| H | 5.96716 | -3.32609 | 0.15839 |
| O | 3.04379 | -0.87215 | -2.16989 |
| C | -2.19591 | 0.58391 | 0.16040 |
| C | -3.34773 | 0.63911 | -0.62502 |
| C | -2.04591 | -0.54022 | 0.98772 |
| C | -4.30004 | -0.37296 | -0.60998 |
| H | -3.49901 | 1.48754 | -1.28262 |
| C | -2.98128 | -1.55629 | 1.00808 |
| H | -1.20101 | -0.59841 | 1.66535 |
| C | -4.11733 | -1.48353 | 0.20552 |
| H | -5.17116 | -0.28282 | -1.24566 |
| H | -2.86164 | -2.41392 | 1.65982 |
| O | -4.98352 | -2.53165 | 0.29452 |
| C | -6.15482 | -2.49785 | -0.48918 |
| H | -6.69527 | -3.41464 | -0.26485 |
| H | -6.78282 | -1.63865 | -0.23428 |
| H | -5.92145 | -2.47053 | -1.55796 |
| H | 0.44058 | -0.62449 | 0.00031 |

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| 42 |  |  |  |
| **22** |  |  |  |
| C | -1.03395 | 1.60538 | -0.08417 |
| C | -2.00003 | 3.81676 | -0.00570 |
| C | -0.72827 | 4.32244 | 0.05614 |
| C | 0.39437 | 3.49670 | 0.03592 |
| C | 0.29767 | 2.08692 | -0.06646 |
| C | -2.89769 | 0.36387 | -0.00079 |
| C | -3.27472 | 1.66140 | -0.01201 |
| H | -2.91914 | 4.37906 | 0.00448 |
| H | -0.60110 | 5.39659 | 0.10862 |
| H | 1.37491 | 3.95254 | 0.05179 |
| H | -4.24540 | 2.12334 | 0.02210 |
| N | -2.11088 | 2.42852 | -0.06535 |
| N | -1.51913 | 0.34514 | -0.05249 |
| C | -3.69645 | -0.87316 | 0.01899 |
| C | -5.02483 | -0.86107 | -0.32400 |
| C | -3.06341 | -2.12746 | 0.40303 |
| C | -5.80320 | -2.02662 | -0.27373 |
| H | -5.49140 | 0.06331 | -0.64555 |
| C | -3.89860 | -3.29914 | 0.43726 |
| C | -5.22946 | -3.24121 | 0.11186 |
| H | -6.85117 | -1.97969 | -0.54187 |
| H | -3.41842 | -4.22418 | 0.73132 |
| H | -5.83838 | -4.13721 | 0.14502 |
| O | -1.84435 | -2.19066 | 0.68438 |
| C | 1.44004 | 1.20097 | -0.09812 |
| C | 2.65657 | 1.58424 | 0.51089 |
| C | 1.42361 | -0.04746 | -0.76041 |
| C | 3.76484 | 0.76931 | 0.48300 |
| H | 2.71071 | 2.52325 | 1.04889 |
| C | 2.53683 | -0.85854 | -0.79072 |
| H | 0.55140 | -0.35624 | -1.32315 |
| C | 3.72527 | -0.47151 | -0.16597 |
| H | 4.67603 | 1.08123 | 0.97722 |
| H | 2.51085 | -1.80508 | -1.31670 |
| C | 4.88161 | -1.37690 | -0.22874 |
| O | 4.89379 | -2.45208 | -0.78198 |
| O | 5.96732 | -0.88519 | 0.40734 |
| C | 7.12353 | -1.71726 | 0.38621 |
| H | 7.44894 | -1.89810 | -0.63810 |
| H | 7.88757 | -1.17444 | 0.93715 |
| H | 6.91738 | -2.67477 | 0.86419 |
| H | -0.99907 | -0.50777 | 0.12683 |

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| 29 |  |  |  |
| **23** |  |  |  |
| C | 1.43798 | 0.26099 | 0.96078 |
| C | 2.84444 | -0.41132 | -0.89191 |
| C | 3.92467 | -0.17668 | -0.07625 |
| C | 3.81981 | 0.26771 | 1.23179 |
| C | 2.51373 | 0.48583 | 1.77113 |
| C | -0.59798 | 0.05855 | -0.00840 |
| C | 0.32433 | -0.28562 | -0.92267 |
| H | 2.89226 | -0.74699 | -1.91288 |
| H | 4.70367 | 0.44062 | 1.82577 |
| H | 2.37217 | 0.81541 | 2.79014 |
| H | 0.20294 | -0.60994 | -1.94146 |
| N | 1.57458 | -0.16985 | -0.34114 |
| N | 0.08383 | 0.36432 | 1.17216 |
| C | -2.07360 | 0.09854 | -0.08738 |
| C | -2.82858 | -1.01392 | 0.15330 |
| C | -2.72581 | 1.36390 | -0.39772 |
| C | -4.23874 | -1.00005 | 0.07404 |
| H | -2.33134 | -1.94594 | 0.39928 |
| C | -4.16776 | 1.34767 | -0.48375 |
| C | -4.88232 | 0.20478 | -0.25240 |
| H | -4.65169 | 2.28317 | -0.73578 |
| H | -5.96490 | 0.22139 | -0.31978 |
| O | -2.07398 | 2.40913 | -0.55806 |
| Cl | 5.50970 | -0.46247 | -0.75693 |
| C | -5.01170 | -2.25614 | 0.31842 |
| H | -4.77630 | -3.01339 | -0.43532 |
| H | -4.76064 | -2.69195 | 1.28899 |
| H | -6.08707 | -2.08277 | 0.29292 |
| H | -0.31185 | 0.89258 | 1.92927 |

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| 32 |  |  |  |
| **24** |  |  |  |
| C | -0.77317 | -0.43020 | 1.04173 |
| C | -2.25325 | 0.30712 | -0.72394 |
| C | -3.30959 | -0.00137 | 0.10678 |
| C | -3.13883 | -0.52166 | 1.38126 |
| C | -1.81550 | -0.73825 | 1.87175 |
| C | 1.22544 | -0.10085 | 0.03100 |
| C | 0.26627 | 0.26746 | -0.83428 |
| H | -2.33406 | 0.68580 | -1.72739 |
| H | -3.99437 | -0.75972 | 1.99467 |
| H | -1.63136 | -1.12981 | 2.86123 |
| H | 0.34610 | 0.65407 | -1.83520 |
| N | -0.96168 | 0.07288 | -0.22663 |
| N | 0.58412 | -0.50686 | 1.20411 |
| C | 2.69887 | -0.09197 | -0.08975 |
| C | 3.42919 | 1.02246 | 0.20965 |
| C | 3.37527 | -1.31202 | -0.50943 |
| C | 4.83680 | 1.05510 | 0.09320 |
| H | 2.91419 | 1.92024 | 0.53406 |
| C | 4.81351 | -1.24812 | -0.63026 |
| C | 5.50309 | -0.10454 | -0.33526 |
| H | 5.31528 | -2.14878 | -0.96176 |
| H | 6.58343 | -0.08510 | -0.43131 |
| O | 2.74709 | -2.36008 | -0.73203 |
| C | -4.69118 | 0.31072 | -0.37971 |
| F | -5.60638 | -0.55810 | 0.08287 |
| F | -4.77920 | 0.29677 | -1.72417 |
| F | -5.09918 | 1.53727 | 0.01229 |
| C | 5.58194 | 2.31271 | 0.40574 |
| H | 5.33783 | 2.67884 | 1.40632 |
| H | 6.66067 | 2.17000 | 0.35070 |
| H | 5.31360 | 3.11017 | -0.29363 |
| H | 1.02444 | -1.02020 | 1.94647 |

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| 46 |  |  |  |
| **25** |  |  |  |
| C | -0.18937 | 0.17404 | -0.20410 |
| C | 1.39559 | -1.65564 | -0.20931 |
| C | 2.41756 | -0.73178 | -0.09737 |
| C | 2.14362 | 0.63058 | -0.03688 |
| C | 0.80173 | 1.13398 | -0.11618 |
| C | -2.12149 | -0.99701 | -0.21583 |
| C | -1.10588 | -1.87848 | -0.24226 |
| H | 1.52050 | -2.71911 | -0.32525 |
| H | 2.96120 | 1.33086 | 0.05740 |
| H | -1.11954 | -2.95431 | -0.26425 |
| N | 0.08155 | -1.16938 | -0.23731 |
| N | -1.55551 | 0.27586 | -0.22444 |
| C | -3.58289 | -1.20745 | -0.21740 |
| C | -4.28283 | -1.37196 | -1.38305 |
| C | -4.29146 | -1.22212 | 1.05703 |
| C | -5.67042 | -1.58491 | -1.37431 |
| H | -3.75567 | -1.35006 | -2.32895 |
| C | -5.71917 | -1.45323 | 1.01952 |
| C | -6.37801 | -1.62647 | -0.16642 |
| H | -6.19394 | -1.72449 | -2.31145 |
| H | -6.23191 | -1.47874 | 1.97283 |
| H | -7.44827 | -1.79618 | -0.17830 |
| O | -3.69666 | -1.02937 | 2.12980 |
| C | 0.49048 | 2.56221 | -0.02686 |
| C | 1.26857 | 3.40985 | 0.77663 |
| C | -0.56369 | 3.14697 | -0.74611 |
| C | 0.99313 | 4.76321 | 0.87098 |
| H | 2.08452 | 2.99041 | 1.35357 |
| C | -0.83886 | 4.50275 | -0.64764 |
| H | -1.13780 | 2.54536 | -1.44241 |
| C | -0.06655 | 5.32177 | 0.16490 |
| H | 1.60723 | 5.38877 | 1.51007 |
| H | -1.65278 | 4.92570 | -1.22700 |
| H | -0.28057 | 6.38159 | 0.24064 |
| C | 3.81979 | -1.21950 | -0.04911 |
| C | 4.17403 | -2.30221 | 0.75586 |
| C | 4.81412 | -0.60481 | -0.81016 |
| C | 5.48428 | -2.75720 | 0.79996 |
| H | 3.41679 | -2.77563 | 1.37098 |
| C | 6.12487 | -1.05752 | -0.76584 |
| H | 4.55042 | 0.22564 | -1.45531 |
| C | 6.46540 | -2.13639 | 0.03901 |
| H | 5.74117 | -3.59492 | 1.43923 |
| H | 6.88248 | -0.56925 | -1.36920 |
| H | 7.48969 | -2.49074 | 0.07352 |
| H | -2.03783 | 1.12263 | 0.02730 |

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| 52 |  |  |  |
| **26** |  |  |  |
| C | -1.32564 | 3.28490 | 0.20771 |
| C | -3.30241 | 2.30126 | -0.77155 |
| C | -3.82559 | 3.56711 | -0.88163 |
| C | -3.14008 | 4.69985 | -0.45699 |
| C | -1.83832 | 4.54517 | 0.11141 |
| C | -0.05554 | 1.43328 | 0.48543 |
| C | -1.22921 | 1.03238 | -0.04281 |
| H | -3.78739 | 1.40071 | -1.10574 |
| H | -4.81092 | 3.66509 | -1.32215 |
| H | -3.57839 | 5.68201 | -0.55757 |
| H | -1.26177 | 5.39062 | 0.46039 |
| N | -2.02029 | 2.16494 | -0.20689 |
| N | -0.12451 | 2.82009 | 0.69520 |
| C | 1.14165 | 0.66208 | 0.87510 |
| C | 1.24750 | 0.06583 | 2.10262 |
| C | 2.25125 | 0.57243 | -0.06705 |
| C | 2.39317 | -0.66490 | 2.44888 |
| H | 0.43366 | 0.15241 | 2.81210 |
| C | 3.42871 | -0.20847 | 0.31478 |
| C | 3.46133 | -0.79718 | 1.55474 |
| H | 2.44949 | -1.13974 | 3.42064 |
| H | 4.32436 | -1.37588 | 1.86059 |
| O | 2.20831 | 1.15990 | -1.15929 |
| C | -1.71191 | -0.33322 | -0.38934 |
| H | -2.16297 | -0.32305 | -1.38641 |
| H | -0.85157 | -1.00031 | -0.46063 |
| C | -2.71907 | -0.90947 | 0.62460 |
| H | -2.23560 | -0.96554 | 1.60355 |
| H | -3.56078 | -0.22249 | 0.73876 |
| C | -3.22059 | -2.27155 | 0.21898 |
| C | -4.39018 | -2.41131 | -0.52423 |
| C | -2.50562 | -3.42146 | 0.54768 |
| C | -4.83370 | -3.66276 | -0.93058 |
| H | -4.96743 | -1.52863 | -0.78269 |
| C | -2.94408 | -4.67525 | 0.14516 |
| H | -1.59521 | -3.33432 | 1.13342 |
| C | -4.11074 | -4.79984 | -0.59750 |
| H | -5.74938 | -3.74967 | -1.50531 |
| H | -2.37531 | -5.55835 | 0.41554 |
| H | -4.45675 | -5.77846 | -0.91102 |
| C | 4.53210 | -0.29824 | -0.69471 |
| H | 4.10190 | -0.65461 | -1.63645 |
| H | 4.86747 | 0.71743 | -0.92823 |
| C | 5.73120 | -1.16155 | -0.30650 |
| H | 6.20273 | -0.77753 | 0.60302 |
| H | 5.39027 | -2.17892 | -0.08040 |
| C | 6.74992 | -1.22427 | -1.40483 |
| H | 6.39874 | -1.62020 | -2.35660 |
| C | 8.01112 | -0.83315 | -1.29831 |
| H | 8.70101 | -0.90183 | -2.13165 |
| H | 8.40678 | -0.42830 | -0.37133 |
| H | 0.69269 | 3.40517 | 0.71796 |

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| --- | --- | --- | --- |
| 26 |  |  |  |
| **27** |  |  |  |
| C | 2.86974 | -0.68913 | -0.00001 |
| C | 4.12482 | 1.37845 | 0.00011 |
| C | 5.27683 | 0.63269 | 0.00009 |
| C | 5.25439 | -0.76260 | 0.00001 |
| C | 4.01965 | -1.45331 | -0.00003 |
| C | 0.76816 | 0.12188 | 0.00001 |
| C | 1.61434 | 1.18051 | 0.00008 |
| H | 4.06492 | 2.45463 | 0.00017 |
| H | 6.22386 | 1.15819 | 0.00012 |
| H | 6.18197 | -1.31853 | -0.00001 |
| H | 3.95601 | -2.53174 | -0.00009 |
| H | 1.42121 | 2.23699 | 0.00013 |
| N | 2.90747 | 0.68197 | 0.00006 |
| N | 1.55560 | -1.02413 | -0.00004 |
| C | -0.69836 | 0.04643 | -0.00001 |
| C | -1.46811 | 1.17148 | 0.00002 |
| C | -1.37259 | -1.25039 | -0.00004 |
| C | -2.87662 | 1.14360 | -0.00000 |
| C | -2.81417 | -1.23241 | -0.00006 |
| C | -3.54528 | -0.06727 | -0.00004 |
| O | -0.76165 | -2.33506 | -0.00006 |
| F | -0.91447 | 2.38870 | 0.00005 |
| F | -3.54831 | 2.28125 | 0.00002 |
| F | -4.87350 | -0.08987 | -0.00006 |
| F | -3.44867 | -2.39034 | -0.00010 |
| H | 1.15157 | -1.95114 | -0.00009 |