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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| **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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| **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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| **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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| **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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| **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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| 40 |  |  |  |
| **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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| 40 |  |  |  |
| **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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| **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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| 26 |  |  |  |
| **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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| 30 |  |  |  |
| **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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| **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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| **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 |