**Supplementary Material**



**Figure S1.** Illustration of the compounds in the C–H BDE subset (**1**–**25**)



**Figure S2.** Illustration of the compounds in the C–H BDE subset (**26**–**50**)



**Figure S3.** Illustration of the compounds in the C–C BDE subset (**51**–**95**)



**Figure S4.** Illustration of the compounds in the O–H BDE subset (**96**–**125**)



**Figure S5.** Illustration of the compounds in the O–O BDE subset (**126**–**135**)



**Figure S6.** Illustration of the compounds in the C–O BDE subset (**136**–**160**)



**Figure S7.** Illustration of the compounds in the C–N BDE subset (**161**–**180**)



**Figure S8.** Illustration of the compounds in the N–H BDE subset (**181**–**200**)

**Table S1.** Experimental and computational dissociation energies based on Eq. (1) for 200 compounds.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Molecule | Expt. | rPM6 | | PM6 | | PM7 | | AM1 | | PM3 | | B3LYP | | B97-1 | |
| C-H | 1,3-cyclohexadiene (CHD) **1** | 74.3 | 71.4 | 58.3 | | 59.9 | | 55.9 | | 55.2 | | 70.9 | | 70.3 | |
|  | xanthene **2** | 75.5 | 75.5 | 59.6 | | 62.5 | | 56.5 | | 57.3 | | 71.9 | | 70.7 | |
|  | 1,4-CHD **3** | 76.0 | 72.4 | 58.9 | | 60.2 | | 56.5 | | 56.3 | | 71.3 | | 70.2 | |
|  | 9,10-dihydroanthracene (DHA) **4** | 76.3 | 76.6 | 60.3 | | 64.0 | | 56.6 | | 57.5 | | 74.8 | | 73.7 | |
|  | 1,3,5-cycloheptatriene **5** | 76.6 | 70.2 | 58.9 | | 59.9 | | 55.1 | | 56.5 | | 67.8 | | 67.5 | |
|  | 1,2-benzofluorene **6** | 78.7 | 82.5 | 64.9 | | 69.2 | | 61.5 | | 62.1 | | 77.0 | | 76.3 | |
|  | (Z)-9,10-diphenyl-9,10-DHA **7** | 79.4 | 72.1 | 56.6 | | 61.6 | | 51.5 | | 54.6 | | 69.5 | | 70.4 | |
|  | (E)-9,10-diphenyl-9,10-DHA **8** | 81.5 | 72.3 | 55.8 | | 59.4 | | 51.3 | | 52.9 | | 71.1 | | 70.1 | |
|  | 2-benzyl pyridine **9** | 82.0 | 81.5 | 66.6 | | 72.3 | | 62.1 | | 62.8 | | 76.9 | | 76.3 | |
|  | indene **10** | 83.0 | 83.0 | 68.4 | | 70.4 | | 67.2 | | 66.9 | | 76.5 | | 75.8 | |
|  | fluorine **11** | 83.0 | 84.4 | 68.3 | | 71.4 | | 66.3 | | 66.4 | | 78.6 | | 77.5 | |
|  | morpholin-4-yl phenyl ketone **12** | 83.3 | 80.3 | 65.8 | | 67.1 | | 65.2 | | 66.2 | | 89.3 | | 88.7 | |
|  | 1-butene **13** | 83.8 | 78.6 | 64.6 | | 66.4 | | 63.6 | | 62.9 | | 80.0 | | 79.5 | |
|  | 1,3-cyclopentadiene **14** | 83.9 | 83.8 | 69.3 | | 71.4 | | 69.3 | | 68.8 | | 79.0 | | 78.3 | |
|  | 3-benzylpyridine **15** | 84.0 | 80.6 | 64.4 | | 68.1 | | 60.6 | | 62.0 | | 79.1 | | 78.4 | |
|  | 9-anthracenylmethane **16** | 84.1 | 79.4 | 60.8 | | 65.2 | | 55.0 | | 56.0 | | 80.2 | | 80.3 | |
|  | 1-butyne **17** | 85.0 | 83.3 | 68.3 | | 69.7 | | 68.3 | | 68.4 | | 83.4 | | 82.9 | |
|  | 1-methylnaphthalene **18** | 85.1 | 85.4 | 68.1 | | 71.9 | | 64.1 | | 64.5 | | 85.4 | | 84.9 | |
|  | cumene **19** | 85.4 | 77.1 | 61.6 | | 64.7 | | 60.9 | | 59.4 | | 83.1 | | 81.9 | |
|  | ethylbenzene **20** | 85.4 | 81.3 | 65.8 | | 68.8 | | 64.3 | | 63.7 | | 84.3 | | 83.2 | |
|  | 2-butyne **21** | 87.4 | 89.4 | 74.1 | | 75.3 | | 72.9 | | 73.8 | | 85.5 | | 85.5 | |
|  | benzyl alcohol **22** | 87.5 | 83.9 | 61.3 | | 64.2 | | 62.4 | | 60.0 | | 78.4 | | 77.6 | |
|  | formaldehyde **23** | 88.0 | 73.7 | 62.8 | | 68.5 | | 74.7 | | 69.5 | | 86.2 | | 85.1 | |
|  | toluene **24** | 88.5 | 88.0 | 71.8 | | 74.5 | | 68.7 | | 69.7 | | 87.7 | | 86.7 | |
|  | benzaldehyde **25** | 88.7 | 72.8 | 64.7 | | 67.0 | | 74.8 | | 71.1 | | 88.5 | | 87.5 | |
|  | ethylamine **26** | 90.1 | 76.1 | 61.2 | | 62.0 | | 62.4 | | 63.3 | | 87.7 | | 87.1 | |
|  | piperidine **27** | 90.7 | 82.6 | 67.0 | | 68.2 | | 66.4 | | 67.7 | | 87.1 | | 86.7 | |
|  | trimethylamine **28** | 91.0 | 92.7 | 78.2 | | 80.1 | | 78.0 | | 77.7 | | 98.1 | | 97.6 | |
|  | tetrahydrofuran **29** | 92.1 | 86.8 | 72.8 | | 74.6 | | 74.6 | | 71.4 | | 92.1 | | 91.4 | |
|  | cyclohexanone **30** | 94.1 | 87.4 | 72.9 | | 75.0 | | 73.9 | | 72.3 | | 95.7 | | 95.4 | |
|  | acetic acid **31** | 95.3 | 100.0 | 84.4 | | 85.4 | | 81.2 | | 80.3 | | 95.6 | | 95.2 | |
|  | cyclopentane **32** | 95.6 | 86.3 | 71.6 | | 73.5 | | 73.7 | | 70.9 | | 92.7 | | 92.2 | |
|  | isobutene **33** | 95.7 | 80.1 | 66.3 | | 68.3 | | 66.4 | | 67.7 | | 92.1 | | 91.7 | |
|  | methanol **34** | 96.1 | 89.6 | 70.7 | | 73.6 | | 74.2 | | 71.6 | | 93.2 | | 92.4 | |
|  | norbornene **35** | 96.7 | 99.3 | 90.1 | | 93.4 | | 94.9 | | 90.9 | | 105.6 | | 104.7 | |
|  | cyclobutane **36** | 96.8 | 91.5 | 77.3 | | 79.9 | | 80.0 | | 76.9 | | 96.0 | | 95.4 | |
|  | 1-butene **37** | 98.1 | 93.0 | 78.0 | | 80.0 | | 77.9 | | 77.0 | | 99.0 | | 98.7 | |
|  | cyclohexane **38** | 99.5 | 86.5 | 72.2 | | 75.0 | | 73.9 | | 72.3 | | 95.3 | | 94.9 | |
|  | isobutane **39** | 100.2 | 94.0 | 78.8 | | 80.6 | | 78.4 | | 77.9 | | 99.1 | | 98.8 | |
|  | ethane **40** | 100.5 | 92.3 | 77.4 | | 79.6 | | 77.6 | | 76.9 | | 99.0 | | 98.1 | |
|  | oxirane **41** | 100.5 | 95.5 | 78.7 | | 81.2 | | 85.5 | | 80.7 | | 100.9 | | 100.0 | |
|  | pyridine **42** | 105.0 | 101.9 | 91.9 | | 94.5 | | 95.0 | | 91.6 | | 104.9 | | 103.9 | |
|  | methane **43** | 105.0 | 102.0 | 86.0 | | 87.9 | | 83.4 | | 84.5 | | 103.8 | | 103.0 | |
|  | cyclopropane **44** | 106.3 | 99.0 | 83.7 | | 86.1 | | 86.0 | | 83.0 | | 105.5 | | 104.9 | |
|  | ethylene **45** | 111.0 | 98.8 | 84.7 | | 87.5 | | 88.3 | | 85.6 | | 108.7 | | 107.5 | |
|  | naphthalene **46** | 111.9 | 103.6 | 91.7 | | 95.8 | | 92.5 | | 89.6 | | 110.7 | | 109.7 | |
|  | naphthalene **47** | 112.2 | 104.1 | 92.1 | | 96.3 | | 92.6 | | 90.5 | | 110.6 | | 109.8 | |
|  | benzene **48** | 113.0 | 105.0 | 93.4 | | 96.2 | | 96.3 | | 93.1 | | 111.3 | | 109.5 | |
|  | pyrrole **49** | 118.4 | 112.4 | 104.1 | | 106.9 | | 106.4 | | 105.7 | | 118.1 | | 117.2 | |
|  | acetylene **50** | 132.9 | 130.0 | 121.2 | | 124.6 | | 132.8 | | 133.8 | | 134.3 | | 132.0 | |

**Table S1.** Continued.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Molecule | Expt. | rPM6 | | PM6 | | PM7 | AM1 | PM3 | B3LYP | B97-1 |
| C-C | 1,5-hexadiene **51** | 61.5 | 59.7 | 38.3 | | 39.8 | | 36.6 | 35.3 | 48.5 | 53.9 | |
|  | bibenzyl **52** | 62.6 | 62.4 | 39.0 | | 44.2 | | 36.2 | 35.6 | 53.9 | 59.3 | |
|  | bibenzyl ketone **53** | 65.4 | 55.1 | 43.0 | | 49.4 | | 41.5 | 35.8 | 59.6 | 64.3 | |
|  | 3,3-dimethyl-1-butene **54** | 67.5 | 64.3 | 43.2 | | 44.5 | | 41.6 | 39.8 | 60.6 | 66.6 | |
|  | 2,2-diphenylpropane **55** | 69.5 | 63.7 | 41.5 | | 45.2 | | 36.3 | 37.2 | 58.5 | 64.5 | |
|  | 1,1-diphenylethane **56** | 71.3 | 68.7 | 44.8 | | 49.2 | | 41.9 | 40.9 | 60.0 | 65.8 | |
|  | 1-methylindene **57** | 72.4 | 72.9 | 50.3 | | 52.3 | | 50.5 | 48.6 | 59.7 | 65.1 | |
|  | tetralin **58** | 72.9 | 69.4 | 46.7 | | 48.8 | | 45.7 | 43.8 | 68.9 | 73.1 | |
|  | 2-methyl-1-butene **59** | 74.1 | 76.4 | 52.1 | | 53.8 | | 53.3 | 50.9 | 67.4 | 73.0 | |
|  | iso-propylbenzene **60** | 74.6 | 79.2 | 66.7 | | 70.3 | | 67.0 | 62.4 | 88.1 | 93.5 | |
|  | proline **61** | 74.6 | 56.8 | 44.0 | | 45.2 | | 52.0 | 45.7 | 74.4 | 79.0 | |
|  | cyclohexene **62** | 74.8 | 63.6 | 43.7 | | 45.1 | | 48.6 | 45.9 | 63.9 | 68.6 | |
|  | propylbenzene **63** | 74.9 | 68.7 | 45.8 | | 49.0 | | 46.2 | 44.1 | 66.2 | 71.7 | |
|  | 2-ethyl furan **64** | 75.0 | 73.3 | 50.7 | | 52.2 | | 51.4 | 49.2 | 65.4 | 70.9 | |
|  | 1-hexene **65** | 75.0 | 84.0 | 59.1 | | 61.0 | | 63.5 | 59.4 | 81.7 | 87.6 | |
|  | 1-butene **66** | 75.9 | 76.5 | 51.9 | | 53.4 | | 53.6 | 50.9 | 65.5 | 72.1 | |
|  | ethylbenzene **67** | 76.4 | 77.6 | 52.1 | | 55.3 | | 53.3 | 50.8 | 69.1 | 74.7 | |
|  | 1-butyne **68** | 76.6 | 81.1 | 55.4 | | 56.5 | | 57.9 | 55.9 | 69.7 | 75.1 | |
|  | 2-methylpiperidine **69** | 83.9 | 69.1 | 45.9 | | 46.7 | | 46.7 | 47.8 | 73.5 | 79.1 | |
|  | ethyl methyl ketone **70** | 84.3 | 72.0 | 56.1 | | 59.0 | | 59.0 | 60.2 | 77.1 | 81.8 | |
|  | acetaldehyde **71** | 84.8 | 78.3 | 56.7 | | 60.2 | | 63.7 | 56.0 | 79.1 | 83.7 | |
|  | 1-propanol **72** | 85.3 | 73.4 | 47.4 | | 50.5 | | 51.8 | 46.2 | 76.7 | 81.7 | |
|  | 1-butanol **73** | 85.4 | 74.0 | 46.9 | | 50.2 | | 51.3 | 45.8 | 77.3 | 81.7 | |
|  | ethylene glycol **74** | 85.6 | 73.3 | 43.2 | | 48.1 | | 49.7 | 42.6 | 76.6 | 81.2 | |
|  | 2-butanol **75** | 86.0 | 72.1 | 46.4 | | 48.4 | | 47.0 | 42.1 | 74.6 | 79.6 | |
|  | triphenylmethane **76** | 86.3 | 69.5 | 57.0 | | 64.4 | | 51.0 | 50.6 | 69.1 | 74.8 | |
|  | butane **77** | 86.8 | 74.7 | 52.4 | | 54.2 | | 56.2 | 52.1 | 78.5 | 84.0 | |
|  | ethanol **78** | 87.2 | 82.7 | 53.8 | | 56.8 | | 58.9 | 53.6 | 80.0 | 85.0 | |
|  | 2-propanol **79** | 87.9 | 82.5 | 53.9 | | 55.5 | | 54.9 | 50.2 | 77.2 | 82.3 | |
|  | isobutane **80** | 88.2 | 77.2 | 54.2 | | 55.6 | | 56.8 | 53.2 | 78.7 | 84.4 | |
|  | propane **81** | 88.5 | 83.9 | 58.9 | | 60.6 | | 63.3 | 59.3 | 81.6 | 87.1 | |
|  | methylcyclohexane **82** | 90.1 | 78.6 | 55.6 | | 57.5 | | 57.9 | 54.5 | 79.5 | 85.2 | |
|  | ethane **83** | 90.2 | 92.8 | 65.3 | | 67.2 | | 70.5 | 66.5 | 84.6 | 90.2 | |
|  | 2-methyloxirane **84** | 93.5 | 91.2 | 64.9 | | 66.8 | | 71.5 | 65.9 | 89.4 | 94.2 | |
|  | benzyl alcohol **85** | 98.8 | 87.0 | 65.2 | | 70.1 | | 69.2 | 63.8 | 89.2 | 93.8 | |
|  | ethylbenzene **86** | 100.0 | 87.9 | 72.7 | | 75.9 | | 74.2 | 70.4 | 92.3 | 97.4 | |
|  | 1-butene **87** | 100.0 | 85.6 | 64.1 | | 66.5 | | 69.4 | 64.6 | 91.4 | 96.5 | |
|  | propylbenzene **88** | 100.8 | 88.2 | 73.2 | | 76.5 | | 75.0 | 71.2 | 94.4 | 97.6 | |
|  | methylbenzene **89** | 102.0 | 98.6 | 80.3 | | 82.8 | | 83.1 | 79.1 | 95.8 | 100.8 | |
|  | biphenyl **90** | 114.4 | 99.6 | 92.4 | | 97.2 | | 94.2 | 89.6 | 107.7 | 111.0 | |
|  | vinylbenzene **91** | 115.2 | 97.6 | 83.8 | | 87.8 | | 89.1 | 84.1 | 107.6 | 112.2 | |
|  | 1-butyne **92** | 124.0 | 116.4 | 102.0 | | 105.1 | | 115.3 | 113.0 | 120.2 | 124.9 | |
|  | propyne **93** | 126.0 | 126.5 | 109.1 | | 111.9 | | 122.9 | 120.4 | 123.7 | 128.4 | |
|  | ethane **94** | 174.1 | 169.2 | 123.4 | | 133.5 | | 129.5 | 118.2 | 170.1 | 175.4 | |
|  | acetylene **95** | 229.5 | 233.0 | 218.6 | | 213.5 | | 227.1 | 234.9 | 225.3 | 228.2 | |
| O-H | 1-hydroxy-pyrrolidine **96** | 71.4 | 87.1 | 62.8 | | 65.5 | | 60.8 | 62.2 | 62.6 | 61.9 | |
|  | piperidinol **97** | 77 | 88.9 | 64.4 | | 67.6 | | 62.6 | 64.4 | 66.9 | 66.3 | |
|  | 7-aza-bicyclo[2.2.1]heptan-7-ol **98** | 78 | 89.8 | 65.2 | | 68.9 | | 63.3 | 63.4 | 70.9 | 70.3 | |
|  | chroman-6-ol **99** | 78.3 | 85.4 | 65.9 | | 67.3 | | 65.4 | 64.1 | 71.1 | 70.3 | |
|  | nitrous acid **100** | 78.3 | 85.8 | 59.0 | | 68.0 | | 71.9 | 59.1 | 74.6 | 72.6 | |

**Table S1.** Continued.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Molecule | Expt. | rPM6 | PM6 | | PM7 | | AM1 | PM3 | | B3LYP | | B97-1 | | |
|  | galvinol **101** | 78.7 | 89.1 | 66.6 | 68.7 | | 57.9 | | | 57.1 | | 71.3 | | 70.7 |
|  | 6-hydroxy-2H-chromene **102** | 79.2 | 90.5 | 69.0 | 71.4 | | 67.4 | | | 65.2 | | 76.8 | | 76.1 |
|  | 3-hydroxy-pyrene **103** | 80.2 | 84.7 | 60.6 | 64.4 | | 55.2 | | | 53.0 | | 72.6 | | 71.7 |
|  | hydroxyfluorene **104** | 82 | 94.0 | 72.2 | 74.6 | | 68.6 | | | 66.1 | | 81.9 | | 80.9 |
|  | 2,6-di-*tert*-butylphenol **105** | 82.8 | 91.2 | 70.7 | 71.7 | | 66.2 | | | 67.8 | | 74.9 | | 74.4 |
|  | hydroxynaphthalene **106** | 84.5 | 89.4 | 67.4 | 69.5 | | 63.5 | | | 60.6 | | 76.2 | | 75.3 |
|  | hydro-phenanthrene **107** | 84.8 | 93.4 | 71.5 | 73.9 | | 67.9 | | | 65.4 | | 80.8 | | 79.8 |
|  | 4,4’-dihydroxybiphenyl **108** | 85.5 | 94.5 | 72.5 | 74.9 | | 68.6 | | | 65.1 | | 72.7 | | 75.4 |
|  | hydroxynaphthalene **109** | 86.5 | 93.0 | 70.3 | 73.0 | | 66.6 | | | 64.3 | | 79.9 | | 78.9 |
|  | phenol **110** | 88 | 96.2 | 74.4 | 76.2 | | 71.7 | | | 69.0 | | 79.9 | | 78.9 |
|  | 1-phenyl-oxime **111** | 88.1 | 96.3 | 66.7 | 72.2 | | 67.1 | | | 67.1 | | 79.3 | | 78.5 |
|  | (Z)-benzaldoxime **112** | 88.1 | 86.4 | 56.8 | 63.7 | | 59.4 | | | 59.1 | | 74.9 | | 74.0 |
|  | hydroperoxide **113** | 88.2 | 93.5 | 76.1 | 80.3 | | 69.2 | | | 83.9 | | 81.9 | | 80.3 |
|  | 5-pyrimidinol **114** | 91.1 | 96.2 | 75.0 | 75.6 | | 71.7 | | | 70.7 | | 82.5 | | 81.7 |
|  | phenyl hydroperoxide **115** | 91.8 | 89.7 | 73.7 | 78.5 | | 67.2 | | | 83.7 | | 82.5 | | 80.8 |
|  | 1,3-cyclohexadione **116** | 92 | 87.6 | 76.8 | 75.4 | | 71.1 | | | 66.8 | | 82.5 | | 81.8 |
|  | peracetic acid **117** | 92.3 | 96.3 | 79.2 | 83.6 | | 73.7 | | | 87.6 | | 91.8 | | 90.5 |
|  | 3-hydroxypyridine **118** | 95 | 95.9 | 96.3 | 75.5 | | 71.5 | | | 69.6 | | 83.3 | | 82.5 |
|  | formoxime **119** | 98.2 | 88.0 | 59.7 | 65.4 | | 62.6 | | | 61.3 | | 73.6 | | 72.6 |
|  | benzyl alcohol **120** | 101.7 | 108.1 | 93.2 | 90.6 | | 90.4 | | | 84.2 | | 97.0 | | 96.3 |
|  | nitric acid **121** | 104 | 118.7 | 105.6 | 103.0 | | 106.2 | | | 101.2 | | 97.0 | | 95.8 |
|  | methanol **122** | 104.2 | 106.6 | 95.4 | 92.1 | | 92.4 | | | 86.1 | | 97.4 | | 97.3 |
|  | 2-propanol **123** | 105.7 | 111.3 | 96.9 | 93.8 | | 93.9 | | | 88.4 | | 98.7 | | 97.9 |
|  | acetic acid **124** | 105.8 | 120.5 | 106.9 | 104.7 | | 104.3 | | | 97.6 | | 103.1 | | 102.4 |
|  | water **125** | 119.3 | 125.3 | 115.3 | 112.3 | | 105.4 | | | 101.4 | | 113.7 | | 113.1 |
| O-O | chroline peroxide **126** | 17.9 | 30.4 | 33.8 | 27.3 | | 26.4 | | | 13.3 | | 10.9 | | 13.2 |
|  | di-*tert*-butyl peroxide **127** | 38.2 | 17.6 | 25.2 | 23.8 | | 7.0 | | | 14.1 | | 27.6 | | 30.5 |
|  | pernytric acid **128** | 39.0 | 35.0 | 42.6 | 38.2 | | 24.5 | | | 35.9 | | 33.7 | | 36.7 |
|  | peroxynitric acid **129** | 40.6 | 31.3 | 35.2 | 31.3 | | 20.1 | | | 30.6 | | 32.4 | | 35.5 |
|  | *tert*-butyl hydroperoxide **130** | 43.0 | 32.1 | 36.5 | 31.8 | | 20.7 | | | 28.5 | | 37.1 | | 40.2 |
|  | fluoride hydroperoxide **131** | 46.1 | 46.8 | 53.7 | 46.6 | | 26.8 | | | 36.6 | | 32.5 | | 35.3 |
|  | methyl hydroperoxide **132** | 46.7 | 28.6 | 33.6 | 29.2 | | 17.7 | | | 25.6 | | 37.3 | | 40.3 |
|  | bis(trifluoromethyl)peroxide **133** | 47.5 | 21.6 | 32.6 | 34.8 | | 20.4 | | | 27.1 | | 35.6 | | 37.9 |
|  | fluorine peroxide **134** | 47.7 | 60.7 | 76.1 | 59.7 | | 19.4 | | | 31.9 | | 16.7 | | 18.9 |
|  | hydroperoxide **135** | 51.0 | 43.6 | 46.1 | 40.4 | | 31.4 | | | 42.1 | | 45.4 | | 48.8 |
| O-C | piperidinol **136** | 47.0 | 47.2 | 33.6 | 35.7 | | 29.5 | | | 32.2 | | 33.1 | | 38.0 |
|  | allyl phenyl ether **137** | 49.8 | 41.5 | 33.2 | 34.9 | | 25.1 | | | 22.5 | | 39.9 | | 44.0 |
|  | 1-methoxynaphthalene **138** | 57.5 | 51.2 | 39.4 | 47.2 | | 35.9 | | | 31.0 | | 50.1 | | 54.4 |
|  | methyl nitrile **139** | 58.9 | 54.4 | 31.2 | 37.7 | | 45.4 | | | 28.8 | | 51.5 | | 55.5 |
|  | 1-methoxynaphthalene **140** | 61.0 | 54.7 | 42.0 | 50.2 | | 38.8 | | | 34.8 | | 53.1 | | 57.4 |
|  | anisole **141** | 64.2 | 58.0 | 46.3 | 47.3 | | 44.1 | | | 39.6 | | 54.2 | | 58.4 |
|  | ethyl vinyl ether **142** | 65.2 | 52.7 | 42.8 | 40.8 | | 34.0 | | | 28.2 | | 54.7 | | 58.7 |
|  | phenyl vinyl ether **143** | 76.6 | 61.0 | 61.5 | 62.0 | | 48.8 | | | 46.9 | | 69.7 | | 73.5 |
|  | phenyl vinyl ether **144** | 79.1 | 58.1 | 51.9 | 54.9 | | 46.7 | | | 45.2 | | 70.4 | | 74.4 |
|  | diphenyl ether **145** | 79.4 | 58.1 | 59.2 | 64.1 | | 49.7 | | | 49.4 | | 70.2 | | 74.1 |
|  | methyl nitrate **146** | 81.0 | 85.5 | 82.0 | 76.7 | | 79.3 | | | 73.6 | | 74.0 | | 77.8 |
|  | dimethylether **147** | 83.2 | 70.0 | 68.8 | 64.3 | | 67.4 | | | 60.2 | | 74.5 | | 78.8 |
|  | methyl acetate **148** | 84.3 | 83.0 | 79.5 | 75.6 | | 76.8 | | | 78.3 | | 77.6 | | 84.0 |
|  | tropylium phenoxide **149** | 91.6 | 63.1 | 64.0 | 68.5 | | 52.9 | | | 52.3 | | 79.9 | | 84.0 |
|  | piperidinol **150** | 92.0 | 87.5 | 84.3 | 78.6 | | 81.3 | | | 77.0 | | 85.9 | | 90.3 |

**Table S1.** Continued.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Molecule | Expt. | rPM6 | | PM6 | | PM7 | AM1 | | PM3 | | | B3LYP | B97-1 | |
|  | ethanol **151** | 94.0 | 80.1 | 79.6 | | 74.2 | | | 73.2 | | 69.3 | 86.6 | | | 90.8 | |
|  | cyclohexanol **152** | 95.8 | 80.0 | 79.8 | | 74.7 | | | 68.2 | | 65.5 | 86.8 | | | 91.0 | |
|  | pyridinol **153** | 95.9 | 90.7 | 103.7 | | 100.4 | | | 89.5 | | 89.3 | 108.5 | | | 112.4 | |
|  | methyl acetate **154** | 100.5 | 61.4 | 73.9 | | 71.0 | | | 68.9 | | 59.1 | 88.9 | | | 93.2 | |
|  | ethyl vinyl ether **155** | 101.6 | 70.8 | 75.0 | | 72.9 | | | 69.9 | | 64.2 | 89.2 | | | 93.1 | |
|  | formic acid **156** | 109.9 | 78.0 | 84.3 | | 80.4 | | | 83.2 | | 78.1 | 99.1 | | | 102.9 | |
|  | 2-naphtol **157** | 112.3 | 91.3 | 100.0 | | 97.6 | | | 87.2 | | 87.4 | 105.5 | | | 109.1 | |
|  | 1-naphtol **158** | 112.5 | 91.2 | 100.3 | | 98.5 | | | 86.9 | | 87.0 | 105.3 | | | 109.4 | |
|  | phenol **159** | 113.1 | 91.9 | 102.1 | | 98.6 | | | 91.3 | | 91.0 | 102.3 | | | 106.2 | |
|  | carbon dioxide **160** | 127.2 | 96.5 | 127.8 | | 122.9 | | | 130.8 | | 122.3 | 126.7 | | | 129.2 | |
| N-C | nitroso-trichloromethane **161** | 29.9 | 23.5 | 22.2 | | 30.7 | | | 4.6 | | 14.9 | 22.5 | | | 26.7 | |
|  | nitroso-tert-butane **162** | 39.9 | 38.3 | 21.9 | | 23.4 | | | 6.1 | | 11.7 | 30.7 | | | 35.1 | |
|  | nitrosomethane **163** | 41.1 | 63.8 | 38.1 | | 39.4 | | | 28.8 | | 31.8 | 35.1 | | | 39.3 | |
|  | phenylnitromethane **164** | 49.0 | 34.4 | 15.6 | | 21.3 | | | 1.0 | | 22.0 | 39.6 | | | 44.0 | |
|  | azomethane **165** | 52.5 | 54.1 | 40.0 | | 41.4 | | | 32.1 | | 40.3 | 44.8 | | | 49.6 | |
|  | nitrosobenzene **166** | 54.2 | 64.3 | 49.7 | | 51.9 | | | 40.5 | | 43.9 | 50.5 | | | 54.0 | |
|  | *N,N,N',N'*-tetramethylethylenediamine **167** | 55.6 | 41.9 | 34.0 | | 34.5 | | | 30.6 | | 35.6 | 60.8 | | | 66.1 | |
|  | nitrofuran **168** | 70.4 | 50.6 | 44.7 | | 52.7 | | | 35.3 | | 62.8 | 69.6 | | | 73.0 | |
|  | nitrobenzene **169** | 70.7 | 51.3 | 40.5 | | 46.5 | | | 27.6 | | 51.2 | 65.9 | | | 69.4 | |
|  | methyl hydrazine **170** | 70.7 | 63.8 | 45.8 | | 43.8 | | | 38.8 | | 45.3 | 58.2 | | | 63.0 | |
|  | benzylamine **171** | 72.6 | 69.7 | 54.0 | | 53.7 | | | 50.4 | | 47.0 | 65.5 | | | 70.4 | |
|  | trimethylamine **172** | 79.3 | 65.0 | 52.6 | | 51.8 | | | 51.5 | | 49.3 | 69.7 | | | 74.7 | |
|  | methyl azide **173** | 80.1 | 77.3 | 62.7 | | 60.7 | | | 50.8 | | 54.8 | 64.7 | | | 69.3 | |
|  | methylamine **174** | 85.7 | 84.8 | 67.1 | | 66.0 | | | 68.3 | | 61.9 | 79.1 | | | 84.1 | |
|  | cyclohexylamine **175** | 88.2 | 71.3 | 59.3 | | 57.8 | | | 53.8 | | 50.5 | 77.7 | | | 82.7 | |
|  | carboxamide **176** | 99.1 | 74.0 | 73.7 | | 74.4 | | | 69.7 | | 61.2 | 92.8 | | | 96.8 | |
|  | formamide **177** | 101.4 | 80.9 | 74.7 | | 76.8 | | | 74.6 | | 61.9 | 96.0 | | | 99.9 | |
|  | methyl isocyanide **178** | 101.6 | 98.0 | 80.0 | | 32.1 | | | 87.4 | | 92.3 | 97.8 | | | 102.6 | |
|  | aniline **179** | 103.2 | 94.1 | 88.8 | | 88.7 | | | 84.8 | | 79.8 | 93.3 | | | 97.8 | |
|  | 2-naphthylamine **180** | 108.9 | 94.0 | 87.1 | | 88.2 | | | 81.0 | | 76.3 | 93.6 | | | 98.1 | |
| N-H | phenylhydroxylamine **181** | 69.8 | 72.3 | 64.7 | | 65.6 | | | 58.2 | | 62.8 | 70.4 | | | 69.4 | |
|  | difluoroammonia **182** | 75.7 | 74.7 | 76.9 | | 70.6 | | | 61.0 | | 67.7 | 70.7 | | | 69.3 | |
|  | aminopyridine **183** | 87.0 | 82.4 | 83.6 | | 85.5 | | | 77.5 | | 73.2 | 93.7 | | | 92.7 | |
|  | diphenylamine **184** | 87.2 | 72.4 | 70.9 | | 72.5 | | | 64.7 | | 63.3 | 81.6 | | | 80.5 | |
|  | phthalimide **185** | 89.1 | 108.5 | 112.1 | | 110.8 | | | 103.2 | | 91.2 | 116.9 | | | 115.9 | |
|  | n-methyl-phenylamine **186** | 89.3 | 72.0 | 71.3 | | 72.0 | | | 68.6 | | 65.4 | 85.4 | | | 84.5 | |
|  | aniline **187** | 89.7 | 79.5 | 78.4 | | 80.0 | | | 73.7 | | 70.6 | 82.9 | | | 82.1 | |
|  | indole **188** | 90.8 | 80.1 | 81.9 | | 83.7 | | | 73.6 | | 73.6 | 89.6 | | | 88.6 | |
|  | carbazole **189** | 93.6 | 78.6 | 79.6 | | 82.1 | | | 71.9 | | 72.3 | 87.2 | | | 86.2 | |
|  | hydrazoic acid **190** | 93.8 | 81.5 | 81.6 | | 79.8 | | | 71.1 | | 71.4 | 85.7 | | | 84.7 | |
|  | pyrrole **191** | 97.0 | 82.6 | 84.3 | | 85.2 | | | 76.7 | | 78.9 | 93.2 | | | 92.2 | |
|  | 2-quinolone **192** | 101.0 | 91.2 | 90.4 | | 90.6 | | | 81.1 | | 74.6 | 97.2 | | | 96.3 | |
|  | methylamine **193** | 101.6 | 81.1 | 82.3 | | 81.3 | | | 82.1 | | 75.0 | 95.9 | | | 95.1 | |
|  | oxazolidin-2-one **194** | 105.8 | 84.6 | 88.9 | | 87.9 | | | 86.1 | | 78.6 | 101.8 | | | 100.7 | |
|  | n-methylacetamide **195** | 106.5 | 84.3 | 88.9 | | 86.9 | | | 87.0 | | 75.5 | 103.5 | | | 102.1 | |
|  | benzamide **196** | 107.0 | 91.0 | 97.9 | | 96.8 | | | 95.2 | | 83.4 | 93.7 | | | 105.7 | |
|  | pyrrolidone **197** | 107.0 | 87.6 | 92.6 | | 91.1 | | | 88.4 | | 78.9 | 104.6 | | | 103.5 | |
|  | ammonia **198** | 108.2 | 91.7 | 91.8 | | 91.2 | | | 89.2 | | 82.1 | 104.4 | | | 103.9 | |
|  | formamide **199** | 108.5 | 95.4 | 98.4 | | 97.1 | | | 95.7 | | 83.0 | 93.9 | | | 112.1 | |
|  | urea **200** | 111.0 | 91.3 | 95.9 | | 95.0 | | | 93.0 | | 81.5 | 104.3 | | | 103.5 | |

**Cartesian coordinates optimized at the B97-1/TZVP level**

(1) C-H BDE (**1**-**50**)

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C -3.404083 1.440644 1.002173

C -4.179974 0.362146 0.381018

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H -1.678482 -1.504989 -0.807289

H -4.142474 -1.538494 -0.543957

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H -3.929495 2.191524 1.584772

H -5.261796 0.450937 0.348214

H -1.334953 0.883148 -1.063990

**1•** = -232.680322

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C -2.033320 1.475224 0.868846

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H -1.730381 -1.739660 0.571158

H -1.723414 -1.121681 -1.048611

H -4.134539 -1.610088 -0.318949

H -1.481341 2.348122 1.205395

H -3.971907 2.402056 1.212984

H -5.268605 0.415777 0.447483

**2** = -576.448205

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C -2.992542 2.792839 4.653861

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C -0.776241 3.025597 3.669413

C -0.275321 2.220817 4.699400

C -1.103819 1.706635 5.691378

C 0.130488 3.580740 2.594516

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C -1.994306 4.620191 1.694229

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H -4.048311 3.033927 4.608675

H 0.787947 1.997703 4.716152

H -0.690151 1.085705 6.478134

H 0.925094 4.180449 3.056703

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H -0.098275 6.255813 -1.249048

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O -2.751098 4.078098 2.706537

**2•** = -575.835175

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C -0.784406 3.102642 3.682887

C -0.258225 2.310442 4.732048

C -1.082890 1.767514 5.704286

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H 1.074535 3.541022 2.640198

H -2.538373 6.564817 -1.037518

H -0.068252 6.302303 -1.180719

H 1.137330 4.971043 0.521508

O -2.786547 4.069214 2.697918

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C 2.350932 -2.068898 -3.728431

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C 0.939960 -1.585135 -3.940695

C 0.876195 -0.217062 -4.568638

C 1.954838 0.490987 -4.901352

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H 0.388997 -2.306206 -4.562859

H 3.905645 0.002175 -5.647763

H -0.114631 0.192514 -4.749905

H 1.836908 1.473565 -5.351891

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H 4.420402 -1.770442 -3.879914

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C 2.334775 -2.102993 -3.865820

C 3.381838 0.036627 -4.652398

C 1.038086 -1.604867 -4.156422

C 0.895591 -0.295870 -4.685777

C 1.978762 0.498184 -4.926568

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H 0.163400 -2.218098 -3.972693

H 3.984205 0.096486 -5.577756

H -0.100338 0.080661 -4.901148

H 1.845295 1.497510 -5.329768

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H 4.435057 -1.754380 -3.854257

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C -2.184772 3.055942 3.332374

C -0.920097 3.655237 3.234199

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C -0.992314 4.185219 5.600134

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C -1.206216 3.851188 0.746947

C -2.470768 3.251753 0.845106

C -3.388634 3.407272 -0.196177

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H -2.770201 3.565990 6.649165

H -3.824978 2.577025 4.638038

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H -1.538535 5.320712 -2.308265

H 0.092254 5.067198 -0.461200

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H 0.298211 2.706852 1.751511

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C -0.820471 3.907661 5.691637

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H -1.492038 4.702917 0.313177

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H -2.430644 2.494332 -1.629983

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**8•** -1001.834923

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H -1.356539 -2.232736 -0.249588

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H -0.064964 0.138134 2.303569

**9•** -517.832570

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C -2.440361 0.143151 -0.000112

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C 0.956971 -1.410195 0.000075

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C -0.735145 -0.451198 0.000345

C -1.650930 -1.503397 0.000071

C -3.015890 -1.209941 -0.000231

C 0.735192 -0.451400 0.000490

C 1.184275 0.886128 0.000243

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H -1.315428 -2.535743 -0.000041

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**11•** -500.609003

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H -4.400653 0.820444 0.029389

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H 0.759820 -1.326420 1.269329

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**13** -157.104466

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H 1.959491 0.932742 -0.856916

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H 0.669806 -1.227345 0.904298

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H 0.505946 -1.459682 -0.000532

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H 0.000095 -1.876843 0.879048

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H -2.212217 -0.608721 -0.000820

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**15** -518.451560

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H 2.556413 2.231599 0.057245

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H -4.618010 0.947190 0.069517

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H -2.426992 -2.747076 -0.019735

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**16•** -577.987297

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H -0.534691 -1.243523 0.016650

C -0.466074 0.876414 -0.056551

C -1.191559 2.080625 -0.149517

C -2.563175 2.039728 -0.239986

H -7.448379 -3.730323 -0.084491

H -5.018348 -3.818979 -0.050653

H -7.327953 0.552553 -0.351388

H -8.638146 -1.542963 -0.244399

H -5.212861 1.719798 -0.374714

H 0.615075 0.900447 0.027424

H -0.670364 3.031905 -0.143507

H -3.138052 2.958698 -0.302431

C -2.561558 -2.894701 -0.289097

H -1.481891 -2.935466 -0.323057

H -3.068239 -3.847902 -0.344914

**17** -155.877908

C -1.961154 -0.263638 -0.000084

H -2.959365 -0.631169 0.000414

C -0.832889 0.158609 -0.000036

C 0.544876 0.648898 0.000020

H 0.692940 1.289324 0.877486

C 1.587205 -0.484944 0.000016

H 1.473053 -1.116396 -0.884288

H 2.598330 -0.068742 -0.000494

H 1.473697 -1.116005 0.884661

H 0.693111 1.289440 -0.877277

**17•** -155.245494

C -1.971920 -0.230643 0.000008

H -2.984395 -0.556415 0.000204

C -0.808178 0.150261 -0.000059

C 0.499060 0.568491 -0.000086

H 0.692832 1.638198 0.000389

C 1.670040 -0.366821 -0.000018

H 1.348404 -1.409511 -0.002455

H 2.306027 -0.198235 -0.878504

H 2.303125 -0.201766 0.881299

**18** -425.028879

C -2.317291 1.171801 -0.000021

C -0.971346 1.456045 0.000126

C 0.000531 0.417349 0.000055

C -0.459358 -0.940278 -0.000163

C -1.856702 -1.198440 -0.000307

C -2.767196 -0.169212 -0.000241

H -3.041625 1.978997 0.000035

H -0.644401 2.489289 0.000295

C 1.409201 0.681055 0.000198

C 0.489002 -1.998584 -0.000223

H -2.193467 -2.230389 -0.000474

H -3.831139 -0.379142 -0.000350

C 1.832843 -1.723818 -0.000070

C 2.286446 -0.382715 0.000138

H 0.131747 -3.023422 -0.000407

H 2.556925 -2.531319 -0.000113

H 3.354545 -0.189855 0.000250

C 1.930785 2.100342 0.000407

H 1.591469 2.651694 -0.883518

H 1.591315 2.651514 0.884384

H 3.023136 2.101363 0.000504

**18•** -424.393331

C -2.377082 1.071778 0.000738

C -1.044367 1.436564 0.001146

C -0.015520 0.469818 0.000332

C -0.387959 -0.910554 -0.000382

C -1.763503 -1.257465 -0.000956

C -2.741973 -0.288443 -0.000449

H -3.145698 1.837518 0.001366

H -0.791580 2.490270 0.002164

C 1.406130 0.825693 0.000045

C 0.618081 -1.919617 -0.000163

H -2.033292 -2.309447 -0.001675

H -3.790021 -0.568961 -0.000774

C 1.959191 -1.576537 0.000727

C 2.348858 -0.238435 0.000752

H 0.314394 -2.961677 -0.000606

H 2.716741 -2.353618 0.001374

H 3.404817 0.013268 0.000884

C 1.863565 2.139864 -0.001634

H 1.203500 2.996418 -0.001496

H 2.928609 2.340227 -0.002180

**19** -349.999391

H -1.793309 -1.514698 -0.004261

C 2.132584 -1.077173 -0.001601

C 2.651499 0.216037 0.000510

C 1.778473 1.304692 0.002216

C 0.399995 1.099559 0.002016

C -0.137087 -0.195258 -0.000149

C 0.751222 -1.276564 -0.002251

H 2.801355 -1.931957 -0.002726

H 3.724584 0.375742 0.000648

H 2.172723 2.315947 0.003444

H -0.263469 1.959323 0.002878

H 0.355535 -2.288422 -0.004199

C -1.641736 -0.429168 -0.001318

C -2.309193 0.135474 -1.268828

H -1.858846 -0.284176 -2.172792

H -3.378387 -0.099893 -1.277705

H -2.207517 1.224644 -1.318466

C -2.309926 0.127763 1.269335

H -1.856326 -0.293416 2.170988

H -2.213401 1.217240 1.323584

H -3.377926 -0.112503 1.279024

**19•** -349.368603

C -1.503223 -2.935421 -4.710834

C -1.368022 -4.239382 -4.222890

C -0.138633 -4.642686 -3.691076

C 0.934442 -3.765776 -3.644299

C 0.826650 -2.431378 -4.132680

C -0.436815 -2.050080 -4.670045

H -2.451918 -2.609903 -5.126155

H -2.204873 -4.928452 -4.256706

H -0.019958 -5.652460 -3.310614

H 1.874129 -4.109337 -3.227566

H -0.574144 -1.046221 -5.054878

C 1.928040 -1.523220 -4.085773

C 1.793104 -0.126469 -4.626092

H 1.018648 0.445998 -4.097335

H 2.730821 0.424487 -4.531527

H 1.511909 -0.122120 -5.687741

C 3.246775 -1.947229 -3.501178

H 3.142833 -2.303585 -2.467915

H 3.702396 -2.770237 -4.069509

H 3.958880 -1.119762 -3.495236

**20** -310.715978

H -2.189120 0.880481 -1.190611

C 1.636254 1.204193 0.096608

C 2.322997 -0.001322 0.239158

C 1.634332 -1.205580 0.095374

C 0.268659 -1.201254 -0.186408

C -0.434466 0.001282 -0.329341

C 0.270543 1.202656 -0.185175

H 2.165302 2.146155 0.200025

H 3.386139 -0.002187 0.455281

H 2.161739 -2.148577 0.197775

H -0.259119 -2.143931 -0.302953

H -0.255660 2.146337 -0.300794

C -1.925695 0.001713 -0.592493

C -2.758671 -0.001211 0.702040

H -2.537977 0.880917 1.310495

H -3.829980 -0.001437 0.479081

H -2.536883 -0.885485 1.307002

H -2.188157 -0.875136 -1.193875

**20•** -310.083141

C 1.334794 1.365097 0.000136

C 2.298800 0.350442 -0.000001

C 1.887903 -0.989431 -0.000204

C 0.541359 -1.309631 -0.000078

C -0.461752 -0.296682 0.000132

C -0.017177 1.057025 0.000077

H 1.647417 2.404641 0.000164

H 3.354511 0.598928 -0.000240

H 2.629605 -1.781877 -0.000316

H 0.230606 -2.350374 0.000076

H -0.747879 1.858723 -0.000171

C -1.831748 -0.647917 0.000473

C -2.960394 0.333246 -0.000232

H -2.934861 0.986910 -0.883061

H -3.925227 -0.177373 0.004354

H -2.930083 0.994137 0.876947

H -2.074795 -1.706605 0.000432

**21** -155.887477

C -2.063133 -0.000131 -0.000059

H -2.456655 -0.450635 0.916577

H -2.456289 -0.569014 -0.848493

H -2.456824 1.018875 -0.068408

C -0.602987 0.000151 0.000260

C 0.602934 0.000523 -0.000200

C 2.063146 -0.000153 0.000013

H 2.456391 -0.567174 -0.849629

H 2.457496 1.018727 -0.065806

H 2.456115 -0.453120 0.915677

**21•** -155.250861

C -1.970756 -0.000305 0.000619

H -2.360177 -0.004012 1.025800

H -2.366616 -0.885670 -0.507646

H -2.368300 0.887656 -0.501686

C -0.516040 0.000893 -0.004288

C 0.711053 0.000125 -0.001397

C 2.079563 -0.000244 0.001556

H 2.635841 -0.930939 0.002371

H 2.636336 0.930151 0.002223

**22** -346.646100

C 1.381181 -1.341595 0.042615

C 2.307382 -0.303228 -0.054036

C 1.859873 1.017262 -0.087980

C 0.494942 1.293064 -0.023922

C -0.437926 0.256753 0.082945

C 0.016526 -1.064618 0.116152

H 1.722146 -2.371824 0.061562

H 3.368836 -0.521069 -0.110465

H 2.571863 1.831816 -0.173071

H 0.152068 2.323621 -0.065366

H -0.706538 -1.869538 0.180130

C -1.909480 0.577599 0.214878

H -2.146817 0.726952 1.279784

H -2.120767 1.522612 -0.305504

O -2.689265 -0.487092 -0.320562

H -3.601651 -0.357256 -0.046485

**22•** -346.022114

C 1.343103 -1.345184 -0.000243

C 2.277566 -0.301814 -0.000833

C 1.825160 1.024824 -0.000269

C 0.470335 1.307492 0.000935

C -0.493712 0.259348 0.001057

C -0.017497 -1.082860 0.001104

H 1.686931 -2.374899 -0.000601

H 3.340214 -0.517805 -0.001952

H 2.541921 1.839926 -0.000477

H 0.130894 2.339377 0.002221

H -0.734328 -1.895768 0.000779

C -1.865292 0.566765 -0.001074

H -2.229721 1.588891 -0.002596

O -2.787655 -0.436284 0.000404

H -3.672652 -0.060873 -0.004660

**23** -114.480460

C 0.000007 0.527856 0.000000

H 0.942640 1.112164 0.000000

H -0.942732 1.111953 0.000000

O 0.000007 -0.673907 0.000000

**23•** -113.844512

C -0.061694 0.584364 0.000000

H 0.863719 1.222299 0.000000

O -0.061694 -0.591060 0.000000

**24** -271.433978

H -2.823373 1.018826 -0.005456

C -0.197751 -1.199557 -0.000075

C 1.195221 -1.206956 0.000003

C 1.903079 -0.003937 0.000139

C 1.204741 1.201705 -0.000005

C -0.191033 1.203603 -0.000116

C -0.913205 0.005854 -0.000202

H -0.739865 -2.141248 -0.000118

H 1.729723 -2.151501 -0.000139

H 2.987919 -0.008117 0.000300

H 1.744969 2.142911 -0.000014

H -0.726769 2.148450 -0.000053

C -2.423421 0.002099 0.000122

H -2.818949 -0.508133 0.884614

H -2.819438 -0.518053 -0.878328

**24•** -270.795560

C -0.251776 -1.217739 0.000933

C 1.132476 -1.211199 -0.000250

C 1.837496 -0.000203 -0.000900

C 1.132448 1.211057 0.000193

C -0.251598 1.218198 0.000841

C -0.994649 0.000163 0.000785

H -0.791734 -2.159733 0.001126

H 1.675132 -2.151122 -0.000473

H 2.922039 -0.000019 -0.002166

H 1.675562 2.150715 0.000560

H -0.791773 2.160082 0.001101

C -2.399737 -0.000190 -0.000973

H -2.958645 0.928259 -0.004506

H -2.958538 -0.928701 0.000584

**25** -345.469825

C 2.216927 -0.241931 -0.000126

C 1.729340 1.064911 -0.000127

C 0.354469 1.287529 0.000029

C -0.533035 0.205712 0.000184

C -0.037745 -1.105929 0.000182

C 1.333553 -1.326734 0.000033

H 3.287996 -0.418159 -0.000235

H 2.418089 1.903314 -0.000237

H -0.036895 2.301869 0.000044

H -0.743505 -1.930649 0.000314

H 1.720994 -2.340310 0.000025

C -1.994427 0.464534 0.000395

O -2.848757 -0.393305 -0.000428

H -2.271123 1.541826 0.000080

**25•** -344.830129

C 2.175684 -0.257782 -0.000471

C 1.707109 1.056282 -0.000353

C 0.336196 1.302187 0.000106

C -0.563427 0.230937 0.000828

C -0.090199 -1.091743 0.000708

C 1.278858 -1.330715 -0.000012

H 3.243752 -0.449498 -0.000981

H 2.408254 1.883691 -0.000770

H -0.050565 2.315790 0.000021

H -0.802380 -1.910043 0.001171

H 1.652160 -2.349424 -0.000137

C -2.020305 0.514607 0.001279

O -2.924339 -0.254144 -0.001476

**26** -135.078126

N -1.209624 -0.320471 -0.117514

H -2.074073 0.209943 -0.077540

H -1.246634 -1.000238 0.636659

C -0.048940 0.562641 0.053886

H -0.064115 1.132023 0.998668

C 1.247779 -0.239297 -0.027443

H 1.304160 -0.779329 -0.976469

H 2.119621 0.416510 0.056549

H 1.305578 -0.973561 0.783970

H -0.070208 1.297877 -0.757897

**26•** -134.439047

N -1.221767 -0.231043 -0.104526

H -2.085429 0.243433 0.121777

H -1.206075 -1.160552 0.297431

C -0.059659 0.521360 0.120422

H -0.138238 1.566404 -0.163352

C 1.252333 -0.176815 -0.016704

H 1.450431 -0.519800 -1.047026

H 2.072103 0.485334 0.272617

H 1.303535 -1.064792 0.627924

**27** -251.741345

C 0.009265 1.459254 0.222282

C 1.269286 0.704174 -0.229281

C 1.212248 -0.766054 0.223126

C -1.222101 -0.749992 0.223985

C -1.259755 0.719663 -0.230148

H 2.072737 -1.323577 -0.160008

H 1.344456 0.740381 -1.324739

H 2.171183 1.185075 0.167612

H 0.009630 1.535099 1.318277

H 0.015814 2.484268 -0.163216

H -2.090420 -1.296642 -0.157123

H -1.281316 -0.789545 1.320128

H -1.333176 0.755823 -1.325719

H -2.155749 1.212912 0.165098

N -0.009753 -1.471467 -0.176284

H -0.011135 -1.597253 -1.185207

H 1.272588 -0.808544 1.319103

**27•** -251.102794

C 1.179523 0.815929 0.271864

C 1.330262 -0.655708 -0.152741

C 0.091220 -1.443238 0.153278

C -1.325987 0.558413 0.185249

C -0.130929 1.391974 -0.283616

H 0.111247 -2.524263 0.049485

H 1.547264 -0.680233 -1.237698

H 2.190628 -1.116197 0.343515

H 1.167265 0.880077 1.367285

H 2.034816 1.403082 -0.078631

H -2.248073 0.908846 -0.288382

H -1.440053 0.680168 1.276169

H -0.098629 1.389477 -1.380156

H -0.268914 2.429723 0.037827

N -1.132275 -0.849738 -0.168503

H -1.934160 -1.426734 0.045898

**28** -292.196104

N 0.000817 -0.000753 0.008538

C 0.116627 1.397904 0.438003

H 1.169656 1.683855 0.373036

H -0.169685 1.510825 1.501586

C -0.694488 2.362706 -0.428760

H -0.549534 3.392319 -0.086581

H -0.375101 2.292803 -1.471835

H -1.766826 2.151836 -0.389740

C -1.267563 -0.599933 0.440859

H -1.216686 -0.910561 1.502268

H -2.040011 0.171560 0.384912

C -1.705422 -1.778580 -0.430408

H -2.667678 -2.168531 -0.083661

H -1.812150 -1.460491 -1.470761

H -0.987751 -2.603168 -0.401893

C 1.154307 -0.800966 0.436461

H 0.874450 -1.855598 0.369267

H 1.395181 -0.611520 1.500470

C 2.396232 -0.580681 -0.429225

H 2.755759 0.451024 -0.382626

H 3.211879 -1.228006 -0.091830

H 2.174617 -0.813779 -1.473954

**28•** -291.540226

N -1.485658 2.027119 -0.138950

C -0.635548 2.496679 -1.240972

H -0.696178 1.745008 -2.034694

H 0.426699 2.543364 -0.931956

C -1.077118 3.844483 -1.811294

H -0.439036 4.123625 -2.655592

H -2.111413 3.786360 -2.160436

H -1.014277 4.649924 -1.073966

C -1.205168 2.729668 1.118461

H -0.298013 2.321545 1.604623

H -0.980738 3.771465 0.876553

C -2.379911 2.708329 2.098029

H -2.131952 3.280873 2.997410

H -3.265955 3.151223 1.635948

H -2.636463 1.694059 2.416458

C -1.387880 0.572383 0.020247

H -1.904541 0.306310 0.956249

H -0.336602 0.247948 0.164376

C -2.004500 -0.177807 -1.107131

H -2.892515 0.215185 -1.589244

H -1.679484 -1.183995 -1.344869

**29** -232.330201

C 1.183452 -0.459720 0.000000

O 0.002031 -1.260207 -0.000001

C -1.182017 -0.463381 0.000000

C -0.775009 1.026163 0.000001

C 0.771706 1.028387 0.000000

H 1.776403 -0.716357 0.884934

H 1.776403 -0.716356 -0.884935

H -1.774016 -0.721754 -0.885000

H -1.774016 -0.721755 0.884999

H -1.170601 1.540606 -0.877984

H -1.170601 1.540604 0.877986

H 1.165694 1.543988 -0.877964

H 1.165694 1.543988 0.877965

**29•** -231.684135

C 1.252062 0.128068 -0.069024

O 0.526101 -1.065339 0.230832

C -0.822313 -0.855434 -0.183391

C -1.121137 0.628246 0.115275

C 0.239365 1.226711 -0.038573

H 2.052505 0.234615 0.674827

H 1.738840 0.044586 -1.060075

H -0.928135 -1.053107 -1.261398

H -1.452302 -1.556797 0.366555

H -1.869284 1.054088 -0.563202

H -1.507438 0.751253 1.139840

H 0.469142 2.282523 -0.088926

**30** -309.743206

C -1.015025 -1.265469 -0.282906

C 0.392434 -1.285842 0.347967

C 1.160146 -0.000122 0.066379

C 0.392860 1.285811 0.348064

C -1.014318 1.265565 -0.283002

C -1.790638 0.000292 0.106321

H 0.294792 -1.373418 1.439596

H 0.988738 -2.131084 -0.002304

H -0.918168 -1.308655 -1.374828

H -1.564643 -2.162615 0.019017

H 0.294089 1.373036 1.439526

H 0.989304 2.131137 -0.001773

H -1.563843 2.162879 0.018601

H -0.917748 1.308621 -1.374964

H -1.973197 0.000114 1.189231

H -2.772623 0.000511 -0.378153

O 2.298819 -0.000242 -0.348860

**30•** -309.090918

C -1.056461 -1.284764 -0.231219

C 0.363954 -1.284342 0.395302

C 1.114875 -0.000439 0.069788

C 0.365446 1.283930 0.396044

C -1.054407 1.285618 -0.231841

C -1.775395 0.000971 0.011967

H 0.267908 -1.346139 1.486827

H 0.956452 -2.135443 0.053551

H -0.943851 -1.452991 -1.317299

H -1.629343 -2.136034 0.148196

H 0.268406 1.345389 1.487487

H 0.958564 2.134874 0.054956

H -1.626879 2.137914 0.145809

H -0.940417 1.452047 -1.318001

H -2.850732 0.001599 0.155338

O 2.223977 -0.000883 -0.419639

**31** -229.039750

C 1.394937 -0.122240 -0.000078

H 1.674022 -0.699010 0.885455

H 1.921655 0.829857 -0.007091

H 1.672756 -0.712151 -0.877167

C -0.091435 0.127087 -0.000195

O -0.629842 1.205131 0.000032

O -0.790137 -1.036251 -0.000043

H -1.729615 -0.798813 0.000534

**31•** -228.387679

C 1.376294 -0.282772 -0.000351

H 1.663396 -1.326215 -0.001517

H 2.124802 0.497329 0.002964

C -0.014466 0.110092 0.000128

O -0.410825 1.261752 -0.000243

O -0.863851 -0.954553 0.000217

H -1.761760 -0.592621 0.000093

**32** -196.408372

C 0.193318 1.277785 0.129585

C -1.126228 0.571698 -0.243216

C -0.914282 -0.867265 0.253338

C 0.541895 -1.167973 -0.150821

C 1.295150 0.183180 0.011106

H 0.396746 2.146803 -0.501828

H 0.134778 1.640351 1.161327

H -1.259254 0.567840 -1.332005

H -2.004885 1.056179 0.192255

H -1.018581 -0.900022 1.344889

H -1.629156 -1.580694 -0.166593

H 0.988448 -1.971333 0.441315

H 0.568795 -1.488782 -1.197889

H 1.930830 0.176920 0.900932

H 1.953158 0.368190 -0.842352

**32•** -195.761163

C -1.234358 0.435821 0.119960

C -0.738101 -0.989538 -0.222918

C 0.737682 -0.989417 0.224361

C 1.234373 0.434838 -0.122507

C 0.000704 1.277101 0.001009

H -2.050812 0.770801 -0.532541

H -1.639434 0.465006 1.146281

H -0.795751 -1.146161 -1.305969

H -1.328479 -1.775107 0.256048

H 0.794821 -1.142381 1.308029

H 1.327710 -1.776948 -0.251806

H 2.054378 0.769987 0.525344

H 1.634201 0.461033 -1.151054

H 0.001565 2.360934 0.006231

**33** -158.315223

C 0.739754 -1.260198 0.096101

H 1.771988 -1.274745 -0.268199

H 0.244361 -2.169172 -0.259835

H 0.771868 -1.304222 1.191099

C -0.000293 -0.000005 -0.374514

H -0.000577 0.000011 -1.473077

C -1.461595 -0.010251 0.096260

H -1.516221 -0.010828 1.191292

H -2.002065 0.871044 -0.263863

H -1.989744 -0.898854 -0.264180

C 0.721988 1.270451 0.096103

H 1.753758 1.299750 -0.268624

H 0.213581 2.172379 -0.259403

H 0.753930 1.314656 1.191097

**33•** -157.657442

C 1.271187 -0.682678 0.101996

H 2.172453 -0.169719 -0.247405

H 1.288299 -1.703023 -0.293009

H 1.317865 -0.739961 1.194416

C 0.000054 0.060247 -0.348334

H 0.000001 0.053246 -1.455308

C -1.273242 -0.679061 0.101963

H -1.318846 -0.738880 1.194323

H -2.173153 -0.162152 -0.245141

H -1.294913 -1.698513 -0.295271

C 0.002292 1.483143 0.103271

H 0.932996 2.032980 0.196655

H -0.926450 2.036120 0.197361

**34** -115.673209

C -0.665029 -0.019874 0.000003

H -1.032060 -0.543349 0.893276

H -1.031911 -0.544197 -0.892844

H -1.082611 0.988391 -0.000497

O 0.749621 0.121908 0.000001

H 1.139791 -0.756865 0.000041

**34•** -115.025589

C -0.683929 -0.027848 0.065169

H -1.233721 0.888608 -0.099644

H -1.122066 -0.992268 -0.173470

O 0.670222 0.125346 -0.023182

H 1.097587 -0.732015 0.067553

**35** -272.572984

C -0.086786 1.129427 0.324649

C -0.086801 -1.129435 0.324633

C -0.034652 -0.000016 1.382731

C 1.187993 0.781752 -0.520122

C 1.187992 -0.781750 -0.520137

C -1.279427 0.669351 -0.505101

C -1.279436 -0.669328 -0.505110

H -0.119795 2.156793 0.688645

H 0.888247 -0.000026 1.972351

H -0.902414 -0.000014 2.046017

H 2.085777 1.176628 -0.035244

H 1.136631 1.205363 -1.525229

H 1.136604 -1.205336 -1.525252

H 2.085776 -1.176643 -0.035280

H -1.922146 1.324725 -1.081926

H -1.922169 -1.324684 -1.081941

H -0.119809 -2.156808 0.688598

**35•** -271.905763

C -0.139325 1.133358 0.056286

C -0.036138 -1.004584 0.579140

C -0.033993 0.298119 1.371995

C 1.157558 0.632808 -0.686642

C 1.228857 -0.894005 -0.287331

C -1.324070 0.433551 -0.605496

C -1.252422 -0.870488 -0.284467

H -0.211218 2.218293 0.150458

H 0.890599 0.483273 1.926444

H -0.903007 0.420109 2.020143

H 2.036355 1.174493 -0.324863

H 1.090621 0.778198 -1.766819

H 1.205999 -1.556932 -1.153430

H 2.133800 -1.106106 0.288139

H -2.001361 0.899548 -1.313798

H -1.844597 -1.683434 -0.687189

**36** -157.095205

C -0.048587 1.101264 -0.000153

C 1.101268 0.048582 -0.000056

C 0.048585 -1.101266 -0.000074

C -1.101265 -0.048584 0.000269

H -0.076757 1.742491 0.883738

H -0.076954 1.741937 -0.884439

H 1.742130 0.076874 0.884095

H 1.742295 0.076853 -0.884088

H 0.076990 -1.742343 0.883917

H 0.076725 -1.742073 -0.884269

H -1.741812 -0.076819 0.884650

H -1.742616 -0.076902 -0.883526

**36•** -156.442869

C -1.104457 -0.062287 -0.001178

C 0.000001 1.049072 0.001399

C 1.104457 -0.062289 -0.001178

C -0.000001 -1.081675 0.001473

H -1.761539 -0.065124 0.879771

H -1.755616 -0.065161 -0.886623

H 0.000001 1.681799 0.890930

H 0.000002 1.687753 -0.883871

H 1.761541 -0.065127 0.879770

H 1.755614 -0.065164 -0.886624

H -0.000002 -2.165897 0.003553

**37** -157.104467

C 1.862144 0.019097 -0.275966

H 1.962233 0.936370 -0.850652

H 2.736081 -0.621605 -0.221002

C 0.721822 -0.299647 0.333516

H 0.668125 -1.231886 0.897076

C -0.538441 0.521019 0.306504

H -0.362665 1.442659 -0.258977

H -0.790598 0.822710 1.331939

C -1.730757 -0.244727 -0.291961

H -1.928387 -1.164939 0.267129

H -2.639391 0.363811 -0.266427

H -1.533999 -0.521573 -1.331645

**37•** -156.446890

C 1.796312 -0.045633 -0.266762

H 1.872451 0.649745 -1.098780

H 2.687646 -0.612504 -0.019122

C 0.663479 -0.192525 0.417013

H 0.624339 -0.904132 1.240594

C -0.619649 0.549883 0.134152

H -0.434778 1.276221 -0.676774

H -0.895563 1.151527 1.011148

C -1.755655 -0.352426 -0.223791

H -1.581308 -1.242906 -0.817291

H -2.779708 -0.073750 -0.003448

**38** -235.700020

C -1.381459 0.493456 -0.229557

C -1.118101 -0.949176 0.229599

C 0.263184 -1.442454 -0.229647

C 1.381419 -0.493485 0.229679

C 1.118149 0.949135 -0.229562

C -0.263173 1.442494 0.229488

H 0.447859 -2.454684 0.146851

H -1.169408 -0.993127 1.326053

H -1.902051 -1.615534 -0.146933

H -1.445321 0.515770 -1.325956

H -2.350190 0.839625 0.147452

H 1.444946 -0.515796 1.326101

H 2.350252 -0.839659 -0.147051

H 1.902039 1.615518 0.147055

H 1.169624 0.993029 -1.326009

H -0.275572 1.509445 1.325900

H -0.447835 2.454598 -0.147370

H 0.275550 -1.509000 -1.326089

**38•** -235.048428

C -1.269298 0.710397 -0.243842

C -1.287648 -0.780527 0.157510

C 0.002794 -1.462497 -0.165287

C 1.290860 -0.775901 0.156699

C 1.266471 0.715376 -0.242752

C -0.003039 1.410200 0.270776

H 0.004966 -2.523818 -0.395373

H -1.476662 -0.836237 1.247154

H -2.128770 -1.296587 -0.317810

H -1.302384 0.786933 -1.337973

H -2.165679 1.210485 0.139164

H 1.481877 -0.832300 1.245864

H 2.133438 -1.287678 -0.320772

H 2.160299 1.218853 0.141773

H 1.300771 0.793809 -1.336722

H -0.003744 1.401511 1.369931

H -0.004960 2.462743 -0.033859

**39** -158.315223

C 0.739754 -1.260198 0.096101

H 1.771988 -1.274745 -0.268199

H 0.244361 -2.169172 -0.259835

H 0.771868 -1.304222 1.191099

C -0.000293 -0.000005 -0.374514

H -0.000577 0.000011 -1.473077

C -1.461595 -0.010251 0.096260

H -1.516221 -0.010828 1.191292

H -2.002065 0.871044 -0.263863

H -1.989744 -0.898854 -0.264180

C 0.721988 1.270451 0.096103

H 1.753758 1.299750 -0.268624

H 0.213581 2.172379 -0.259403

H 0.753930 1.314656 1.191097

**39•** -157.668788

C 0.740464 -1.289214 0.015254

H 1.737812 -1.244456 -0.435499

H 0.198074 -2.128677 -0.432972

H 0.888342 -1.543678 1.080883

C -0.000106 0.000001 -0.152008

C -1.486895 0.003455 0.015255

H -1.780886 0.004171 1.080998

H -1.942886 0.892212 -0.434197

H -1.946999 -0.883206 -0.434144

C 0.746451 1.285759 0.015253

H 1.743534 1.236391 -0.435595

H 0.207919 2.127752 -0.432879

H 0.895606 1.539482 1.080881

**40** -79.746456

H 1.164733 -0.703674 0.736727

C 0.765225 0.000006 0.000007

H 1.164778 0.989874 0.240911

H 1.164746 -0.286337 -0.977706

C -0.765254 -0.000007 -0.000004

H -1.164599 0.284993 0.978141

H -1.164633 0.704667 -0.735817

H -1.164848 -0.989517 -0.242273

**40•** -79.089764

C 0.793882 -0.000010 0.019942

H 1.351503 0.927245 -0.044188

H 1.351713 -0.927107 -0.044211

C -0.693551 -0.000034 0.001822

H -1.106461 0.886572 0.493967

H -1.092253 0.001772 -1.027174

H -1.106487 -0.888220 0.491017

**41** -153.733025

C -0.701026 1.422383 -0.000000

C 0.768991 1.420330 0.000000

O 0.038150 2.648651 -0.000000

H -1.238466 1.207958 -0.919254

H -1.238466 1.207958 0.919254

H 1.306528 1.200147 -0.918383

H 1.306528 1.200147 0.918383

**41•** -153.073314

C -0.733813 1.390358 -0.010791

C 0.717293 1.436637 -0.065735

O 0.060972 2.631295 -0.024990

H -1.336192 1.251921 -0.905904

H -1.226066 1.185965 0.935864

H 1.427148 1.198995 -0.855975

**42** -248.195500

C -2.197455 -0.660467 -0.073237

C -0.802712 -0.665329 -0.073303

C -0.135103 0.557187 -0.073416

C -0.890022 1.727816 -0.073597

C -2.280697 1.621321 -0.073617

N -2.935338 0.455033 -0.073366

H 0.949298 0.596714 -0.073804

H -2.751051 -1.595932 -0.073090

H -0.259648 -1.603885 -0.073168

H -0.416832 2.703467 -0.073745

H -2.900987 2.513959 -0.073664

**42•** -247.529620

C -2.200878 -0.682080 -0.073228

C -0.810415 -0.669080 -0.073329

C -0.143612 0.561415 -0.073538

C -0.882622 1.745931 -0.073640

C -2.264906 1.583397 -0.073508

N -2.902126 0.469908 -0.073311

H 0.941925 0.596644 -0.073592

H -2.766683 -1.608106 -0.073066

H -0.259628 -1.602786 -0.073263

H -0.410165 2.720168 -0.073813

**43** -40.465726

C -0.000003 0.000000 0.000000

H 0.080976 1.088153 -0.004512

H 0.485716 -0.404563 -0.889409

H 0.486242 -0.397213 0.892429

H -1.052918 -0.286375 0.001492

**43•** -39.801286

C 0.000000 0.001480 0.000000

H 0.461764 -0.285142 -0.934113

H 0.461764 -0.285142 0.934113

H -0.923527 0.561406 0.000000

**44** -117.807523

C 0.000000 0.872348 0.000000

C 0.755489 -0.436169 0.000000

C -0.755525 -0.436211 0.000000

H 0.000056 1.463408 0.908266

H 0.000056 1.463408 -0.908266

H 1.267393 -0.731626 0.908273

H 1.267393 -0.731626 -0.908273

H -1.267341 -0.731687 -0.908296

H -1.267341 -0.731687 0.908296

**44•** -117.139979

C -0.772445 0.363642 -0.031632

C 0.772446 0.363641 -0.031632

C 0.000000 -0.871770 0.171173

H -1.253090 0.830611 0.825345

H -1.304434 0.510058 -0.969572

H 1.253091 0.830610 0.825344

H 1.304435 0.510054 -0.969573

H -0.000003 -1.814407 -0.358998

**45** -78.532418

C 0.000000 -0.664249 0.000000

H -0.923479 -1.236208 0.000000

H 0.923501 -1.236186 0.000000

C 0.000000 0.664249 0.000000

H 0.923479 1.236208 0.000000

H -0.923501 1.236186 0.000000

**45•** -77.860817

C -0.587372 0.029186 0.000520

H -1.032630 1.029589 -0.001012

H -1.287703 -0.803955 -0.001295

C 0.707075 -0.143911 -0.000079

H 1.602117 0.462714 -0.000341

**46** -385.742507

C 2.430575 -0.708718 0.000012

C 1.244861 -1.402513 0.000009

C -0.000174 -0.714497 -0.000015

C 0.000247 0.714579 -0.000026

C 1.245218 1.402413 -0.000003

C 2.430867 0.708416 0.000010

H -1.240819 -2.488018 -0.000055

H 3.375997 -1.240695 0.000007

H 1.240358 -2.488199 0.000017

C -1.245204 -1.402366 -0.000014

C -1.244940 1.402463 -0.000013

H 1.240972 2.488044 0.000022

H 3.376328 1.240276 0.000013

C -2.430598 0.708743 0.000022

C -2.430850 -0.708533 0.000010

H -1.240547 2.488174 -0.000053

H -3.375957 1.240813 0.000078

H -3.376346 -1.240310 0.000023

**46•** -385.067419

C 2.408478 -0.624203 0.000067

C 1.255877 -1.373682 0.000232

C -0.017946 -0.744314 0.000140

C -0.086372 0.687596 -0.000131

C 1.126733 1.428482 -0.000293

C 2.343999 0.790315 -0.000198

H -1.203542 -2.579666 0.000497

H 3.375990 -1.114941 0.000145

H 1.303201 -2.458070 0.000442

C -1.236833 -1.494153 0.000310

C -1.357015 1.328647 -0.000223

H 1.075734 2.512973 -0.000496

H 3.262157 1.367668 -0.000319

C -2.526216 0.593949 -0.000061

C -2.397257 -0.796061 0.000207

H -1.397605 2.414360 -0.000437

H -3.496615 1.078217 -0.000129

**47** -385.742507

C 2.430575 -0.708718 0.000012

C 1.244861 -1.402513 0.000009

C -0.000174 -0.714497 -0.000015

C 0.000247 0.714579 -0.000026

C 1.245218 1.402413 -0.000003

C 2.430867 0.708416 0.000010

H -1.240819 -2.488018 -0.000055

H 3.375997 -1.240695 0.000007

H 1.240358 -2.488199 0.000017

C -1.245204 -1.402366 -0.000014

C -1.244940 1.402463 -0.000013

H 1.240972 2.488044 0.000022

H 3.376328 1.240276 0.000013

C -2.430598 0.708743 0.000022

C -2.430850 -0.708533 0.000010

H -1.240547 2.488174 -0.000053

H -3.375957 1.240813 0.000078

H -3.376346 -1.240310 0.000023

**47•** -385.067172

C 2.395184 -0.730206 0.000022

C 1.191635 -1.393472 0.000194

C -0.036157 -0.677460 0.000115

C 0.014737 0.760701 -0.000138

C 1.274573 1.418620 -0.000312

C 2.437452 0.686604 -0.000233

H -1.331933 -2.409800 0.000491

H 3.323060 -1.291658 0.000086

H 1.161188 -2.478851 0.000393

C -1.303400 -1.324954 0.000294

C -1.226638 1.410586 -0.000199

H 1.296879 2.502365 -0.000508

H 3.396820 1.191982 -0.000360

C -2.446787 0.821909 -0.000033

C -2.474490 -0.604391 0.000224

H -3.369858 1.391928 -0.000078

H -3.432812 -1.113587 0.000367

**48** -232.145801

C 0.707178 -1.202820 -0.000001

C -0.688174 -1.213789 -0.000008

C -1.395390 -0.010978 0.000005

C -0.707169 1.202826 -0.000001

C 0.688165 1.213795 -0.000008

C 1.395390 0.010967 0.000008

H 1.257128 -2.138332 0.000007

H -1.223341 -2.157837 -0.000007

H -2.480534 -0.019497 0.000018

H -1.257141 2.138325 0.000001

H 1.223352 2.157830 0.000001

H 2.480535 0.019511 0.000004

**48•** -231.470872

C 1.224468 0.771735 -0.000001

C 1.212441 -0.631986 0.000003

C 0.000001 -1.324154 -0.000001

C -1.212443 -0.631981 -0.000001

C -1.224469 0.771732 0.000005

C 0.000002 1.396690 -0.000002

H 2.158246 1.324337 -0.000006

H 2.152135 -1.176041 0.000001

H -0.000005 -2.408814 -0.000002

H -2.152132 -1.176044 -0.000005

H -2.158241 1.324343 -0.000002

**49** -210.089451

C 0.328664 -1.124403 -0.000057

C -0.985073 -0.709712 -0.000016

C -0.981115 0.715080 -0.000044

C 0.334874 1.122540 0.000119

N 1.121908 -0.003040 -0.000012

H 2.127681 -0.005767 0.000122

H 0.758891 -2.113112 -0.000141

H -1.851084 -1.354073 -0.000053

H -1.843474 1.364328 -0.000085

H 0.770531 2.108878 0.000228

**49•** -209.402335

C 0.693086 -0.884782 0.000002

C -0.682658 -0.929965 -0.000086

C -1.183165 0.417083 0.000037

C -0.063207 1.200475 0.000125

N 1.067394 0.448917 -0.000059

H 2.010027 0.800338 0.000081

H 1.431298 -1.671162 0.000014

H -1.285414 -1.826292 -0.000170

H -2.212004 0.737828 0.000022

**50** -77.300088

C 0.000000 0.000000 0.600609

H 0.000000 0.000000 1.665060

C 0.000000 0.000000 -0.600609

H 0.000000 0.000000 -1.665060

**50•** -76.589371

C 0.000000 0.000000 0.474297

H 0.000000 0.000000 1.540575

C 0.000000 0.000000 -0.731059

(2) C-C BDE (**51**-**95**)

**51(A-B)** -234.462238

C 2.996517 -0.202094 0.150605

H 3.032208 -1.286596 0.215301

H 3.916012 0.332037 0.366429

C 1.877597 0.439250 -0.181084

H 1.888790 1.528364 -0.231023

C 0.559859 -0.217510 -0.487261

H 0.673746 -1.307135 -0.456400

H 0.248707 0.042587 -1.507248

C -0.559859 0.217510 0.487261

H -0.673746 1.307135 0.456400

H -0.248707 -0.042587 1.507248

C -1.877597 -0.439250 0.181084

H -1.888790 -1.528364 0.231023

C -2.996517 0.202094 -0.150605

H -3.032208 1.286596 -0.215301

H -3.916012 -0.332037 -0.366429

**51(A•)** -117.188169

C 1.228030 -0.196240 -0.000028

H 1.295866 -1.279653 -0.000380

H 2.155850 0.363034 -0.000025

C 0.000072 0.442724 0.000094

H 0.000079 1.531700 0.000086

C -1.228140 -0.196304 0.000032

H -1.295896 -1.279687 0.000459

H -2.155674 0.363526 -0.000733

**51(B•)** -117.188169

C 1.228030 -0.196240 -0.000028

H 1.295866 -1.279653 -0.000380

H 2.155850 0.363034 -0.000025

C 0.000072 0.442724 0.000094

H 0.000079 1.531700 0.000086

C -1.228140 -0.196304 0.000032

H -1.295896 -1.279687 0.000459

H -2.155674 0.363526 -0.000733

**52(A-B)** -541.685777

C -4.662801 -0.001089 -0.229263

C -3.974216 -1.205296 -0.084233

C -2.611777 -1.201209 0.211825

C -1.911629 0.001427 0.368576

C -2.616170 1.202643 0.221894

C -3.978783 1.204318 -0.074076

H -5.723748 -0.002162 -0.456190

H -4.499170 -2.148516 -0.197029

H -2.084991 -2.144369 0.330187

H -2.092663 2.146619 0.348064

H -4.506954 2.146647 -0.178829

C -0.424966 0.001975 0.648683

H -0.158367 -0.874731 1.248682

H -0.157467 0.882945 1.241866

C 0.424975 -0.003607 -0.648664

H 0.157882 -0.884932 -1.241537

H 0.157999 0.872750 -1.248963

C 1.911634 -0.002198 -0.368551

C 2.614651 -1.202905 -0.210432

C 2.613283 1.200944 -0.223257

C 3.977216 -1.203486 0.085564

H 2.089947 -2.147373 -0.327675

C 3.975781 1.206124 0.072728

H 2.087645 2.143568 -0.350590

C 4.662797 0.002511 0.229226

H 4.504230 -2.145422 0.199288

H 4.501933 2.149714 0.176497

H 5.723750 0.004349 0.456121

**52(A•)** -270.795564

C -1.837785 0.000214 0.000023

C -1.132641 -1.210901 0.000083

C 0.251542 -1.218190 0.000011

C 0.994929 -0.000267 -0.000073

C 0.251776 1.217796 -0.000071

C -1.132395 1.211170 -0.000025

H -2.922311 0.000166 0.000034

H -1.675518 -2.150696 0.000071

H 0.791348 -2.160282 -0.000233

H 0.791940 2.159671 -0.000097

H -1.675059 2.151092 -0.000083

C 2.399859 0.000073 0.000097

H 2.959372 -0.928051 -0.000745

H 2.958513 0.928726 0.000784

**52(B•)** -270.795564

C -1.837785 0.000214 0.000023

C -1.132641 -1.210901 0.000083

C 0.251542 -1.218190 0.000011

C 0.994929 -0.000267 -0.000073

C 0.251776 1.217796 -0.000071

C -1.132395 1.211170 -0.000025

H -2.922311 0.000166 0.000034

H -1.675518 -2.150696 0.000071

H 0.791348 -2.160282 -0.000233

H 0.791940 2.159671 -0.000097

H -1.675059 2.151092 -0.000083

C 2.399859 0.000073 0.000097

H 2.959372 -0.928051 -0.000745

H 2.958513 0.928726 0.000784

**53(A-B)** -655.009928

C -5.014991 -0.852210 0.068525

C -4.144853 -1.173041 -0.974101

C -2.929913 -0.504524 -1.105226

C -2.564956 0.495718 -0.196411

C -3.443306 0.808215 0.846174

C -4.660941 0.141019 0.979634

H -5.961721 -1.372605 0.168829

H -4.412200 -1.947290 -1.685793

H -2.254228 -0.767859 -1.912287

H -3.175200 1.582971 1.559291

H -5.331088 0.398750 1.793280

C -1.247088 1.217884 -0.324442

H -1.103523 1.583592 -1.351776

H -1.230011 2.109358 0.311910

C 0.000283 0.371628 -0.016233

O 0.003277 -0.832651 -0.058601

C 1.242793 1.201476 0.349026

H 1.082269 1.524233 1.388226

H 1.235150 2.119585 -0.248902

C 2.562432 0.484816 0.211669

C 2.911324 -0.554967 1.081666

C 3.459922 0.842948 -0.799335

C 4.128616 -1.217716 0.943407

H 2.221735 -0.853427 1.864480

C 4.680093 0.181729 -0.939870

H 3.205067 1.648865 -1.482145

C 5.017808 -0.851304 -0.067613

H 4.382945 -2.022860 1.624952

H 5.364977 0.475204 -1.728771

H 5.966278 -1.367343 -0.173707

**53(A•)** -270.795564

C -1.837710 -0.000033 -0.000147

C -1.132530 -1.211109 0.000093

C 0.251612 -1.217923 0.000159

C 0.994793 0.000070 0.000098

C 0.251649 1.218070 0.000127

C -1.132529 1.211062 -0.000133

H -2.922240 -0.000043 -0.000301

H -1.675434 -2.150873 0.000103

H 0.791667 -2.159853 -0.000077

H 0.791716 2.159984 0.000366

H -1.675411 2.150850 0.000068

C 2.399899 -0.000083 -0.000077

H 2.959133 -0.928415 -0.000981

H 2.959466 0.928030 0.000095

**54(B•)** -384.111869

C -2.662119 -0.051503 0.143065

O -2.516012 0.351323 1.240622

C -1.610992 -0.299534 -0.956919

H -1.873254 0.401549 -1.757406

H -1.816238 -1.299003 -1.351484

C -0.176923 -0.146606 -0.513535

C 0.422859 1.116954 -0.462354

C 0.563455 -1.262333 -0.107679

C 1.736996 1.260829 -0.022749

H -0.141156 1.993111 -0.769098

C 1.878532 -1.120265 0.332186

H 0.109908 -2.248937 -0.138898

C 2.469015 0.142136 0.375864

H 2.189935 2.246316 0.007811

H 2.441442 -1.995512 0.639340

H 3.492517 0.253819 0.717478

**54(A-B)** -235.672904

C -1.117260 -0.464026 1.260673

H -1.200599 -1.555302 1.290863

H -0.605179 -0.138749 2.171096

H -2.130577 -0.048430 1.268747

C -0.352251 0.001384 -0.000102

C -1.121369 -0.469386 -1.256283

C -0.258658 1.535713 -0.003475

C 1.010440 -0.665557 -0.000767

C 2.206163 -0.079310 -0.000345

H -0.612314 -0.148255 -2.169887

H -2.134675 -0.053748 -1.262977

H -1.204886 -1.560785 -1.281357

H 0.265742 1.901662 -0.891431

H -1.262274 1.972065 -0.002848

H 0.268286 1.905508 0.881387

H 0.969967 -1.756141 -0.001337

H 3.116561 -0.669754 -0.000553

H 2.327562 0.999022 0.000089

**54(A•)** -39.801298

C -0.001093 -0.000036 0.002453

H 0.553889 -0.927877 -0.004891

H 0.533928 0.939488 -0.004890

H -1.081256 -0.011396 -0.004935

**54(B•)** -195.765457

C -0.398122 -0.032424 0.002437

C -1.665438 -0.837868 -0.001206

C -0.567346 1.458786 0.000425

C 0.845594 -0.666949 0.001533

C 2.098388 -0.084015 -0.001138

H -2.283512 -0.601041 -0.878344

H -2.282858 -0.610414 0.878840

H -1.466373 -1.912250 -0.007048

H -1.108475 1.786402 -0.897530

H -1.170572 1.781129 0.859409

H 0.380273 1.997099 0.035167

H 0.818488 -1.756516 0.002095

H 2.989804 -0.699465 -0.001326

H 2.244775 0.989871 -0.003572

**55(A-B)** -580.962495

C -0.000197 1.172275 -0.000305

C -1.259981 0.283781 -0.032449

C 1.260160 0.284499 0.032921

C -0.044607 2.086878 -1.247982

C -1.362412 -0.728832 -0.999497

C 1.364263 -0.725674 1.002267

C -2.340304 0.467209 0.836711

C 2.338998 0.465897 -0.838522

C -2.500656 -1.523153 -1.096698

C 2.502761 -1.519713 1.099489

C -3.484678 -0.330081 0.744272

C 3.483552 -0.331037 -0.746073

C -3.571339 -1.327216 -0.222198

C 3.571900 -1.325816 0.222687

H -0.977156 2.657231 -1.245184

H 0.785239 2.800079 -1.246740

H -0.008491 1.510937 -2.176180

H -0.531425 -0.906634 -1.675411

H 0.534303 -0.901898 1.679865

H -2.302156 1.234780 1.600863

H 2.299219 1.231474 -1.604527

H -2.550891 -2.300365 -1.852689

H 2.554267 -2.295073 1.857288

H -4.306799 -0.167199 1.434038

H 4.304543 -0.169947 -1.437605

H -4.458732 -1.947332 -0.293945

H 4.459475 -1.945670 0.294520

C 0.043181 2.088525 1.246123

H 0.975034 2.659984 1.242484

H -0.787698 2.800491 1.243632

H 0.007425 1.513888 2.175127

**55(A•)** -541.058238

C 0.013000 1.022095 -0.034425

C -1.275290 0.336240 -0.035565

C 1.272362 0.311159 0.010273

C 0.039698 2.526537 -0.126488

C -1.458663 -0.899732 -0.701675

C 1.381077 -1.009884 0.521428

C -2.411080 0.900506 0.592494

C 2.480247 0.938878 -0.393833

C -2.696287 -1.531051 -0.728237

C 2.605013 -1.659085 0.595938

C -3.643708 0.258445 0.575187

C 3.700407 0.279162 -0.323434

C -3.797607 -0.961712 -0.085472

C 3.775623 -1.025895 0.167883

H -0.954826 2.957975 -0.014783

H 0.701098 2.973510 0.624004

H 0.409920 2.849498 -1.109893

H -0.623691 -1.341815 -1.232955

H 0.494640 -1.508188 0.894880

H -2.315149 1.837436 1.129963

H 2.453592 1.948707 -0.786080

H -2.805807 -2.468939 -1.263530

H 2.651244 -2.663720 1.004356

H -4.489278 0.710983 1.083359

H 4.601118 0.785898 -0.655371

H -4.761924 -1.458016 -0.104736

H 4.730331 -1.537323 0.226334

**55(B•)** -39.801329

C -0.000001 0.000021 0.000367

H 0.941280 0.532389 -0.000735

H -0.931777 0.548844 -0.000735

H -0.009500 -1.081358 -0.000735

**56(A-B)** -541.682694

C -2.749201 -1.419302 -0.938706

C -1.590704 -0.673642 -1.132045

C -1.270717 0.403735 -0.292172

C -2.152106 0.711076 0.748531

C -3.315439 -0.037361 0.948666

C -3.619065 -1.103718 0.107335

H -2.975888 -2.246330 -1.603978

H -0.915592 -0.931180 -1.943646

H -1.942772 1.542893 1.412169

H -3.984729 0.220518 1.763322

H -4.523488 -1.683036 0.260821

C 0.023662 1.175049 -0.547508

H 0.069377 1.352085 -1.629114

C 1.259990 0.349053 -0.189460

C 2.337079 0.269949 -1.078557

C 1.364046 -0.308816 1.042712

C 3.490763 -0.442777 -0.748643

H 2.272502 0.770991 -2.040865

C 2.514850 -1.019177 1.377108

H 0.531720 -0.276098 1.739374

C 3.583696 -1.089245 0.482192

H 4.313255 -0.494552 -1.454947

H 2.575710 -1.524900 2.335558

H 4.477779 -1.646638 0.741303

C 0.085100 2.553350 0.137082

H 0.994453 3.077138 -0.168339

H -0.776608 3.169077 -0.137564

H 0.112557 2.460986 1.226698

**56(A•)** -501.776430

C -2.860241 -1.405259 -0.402447

C -1.564684 -0.905481 -0.395841

C -1.301080 0.438611 -0.023626

C -2.421649 1.249036 0.301912

C -3.711027 0.739967 0.301070

C -3.941610 -0.595488 -0.044343

H -3.032725 -2.434098 -0.702211

H -0.752553 -1.540297 -0.727000

H -2.252840 2.287420 0.571503

H -4.543528 1.383285 0.567150

H -4.950121 -0.994516 -0.049258

C 0.000541 1.040842 -0.005555

H 0.000397 2.128873 -0.006983

C 1.301660 0.438873 0.016917

C 2.424712 1.248996 -0.301280

C 1.562078 -0.905857 0.389342

C 3.713596 0.738787 -0.293077

H 2.257961 2.288022 -0.569917

C 2.856951 -1.406846 0.402797

H 0.747656 -1.539908 0.715715

C 3.940971 -0.597432 0.052227

H 4.548248 1.381924 -0.552791

H 3.027018 -2.436105 0.702485

H 4.949183 -0.997096 0.062718

**56(B•)** -39.801327

C -0.000005 0.000155 -0.000389

H 0.930123 0.551635 0.000778

H -0.943390 0.528641 0.000778

H 0.013295 -1.081204 0.000777

**57(A-B)** -386.904307

C 0.334457 0.929598 0.016023

C -0.105983 -0.389850 -0.220131

C 0.801493 -1.438404 -0.260038

C 2.161097 -1.164531 -0.063334

C 2.597789 0.142350 0.167176

C 1.688469 1.202391 0.209225

C -0.839857 1.809813 0.006915

C -1.947140 1.081660 -0.223367

H 0.472744 -2.457709 -0.441370

H 2.882404 -1.974695 -0.090974

H 3.655285 0.334984 0.316445

H 2.033003 2.216058 0.389129

H -0.801168 2.881457 0.163811

H -2.959915 1.462758 -0.282002

C -1.613736 -0.387363 -0.396020

H -1.862190 -0.693815 -1.423474

C -2.367878 -1.309755 0.579542

H -2.079210 -2.353901 0.430063

H -2.144565 -1.037181 1.614491

H -3.448649 -1.233410 0.427931

**57(A•)** -346.999125

C -0.257853 0.714839 -0.002379

C -0.257966 -0.714860 -0.002088

C 0.939832 -1.416934 -0.000564

C 2.147608 -0.696610 0.001043

C 2.147551 0.696700 0.001142

C 0.939416 1.416946 -0.000431

C -1.646966 1.141311 -0.000155

C -2.459469 -0.000047 0.001612

H 0.951560 -2.502654 -0.001385

H 3.090552 -1.233097 0.002323

H 3.090234 1.233568 0.002526

H 0.951623 2.502683 -0.000540

H -1.987868 2.168842 0.001359

H -3.540965 -0.000287 0.003394

C -1.646651 -1.141392 0.000406

H -1.988146 -2.168763 0.000815

**57(B•)** -39.801327

C 0.000000 -0.000152 0.000220

H 0.936812 -0.540214 -0.000440

H -0.936849 -0.540149 -0.000440

H 0.000037 1.081278 -0.000439

**58(A-A)** -388.106031

C -2.386870 -0.683353 -0.345375

C -2.385800 0.683551 0.347103

C -1.158542 1.494940 -0.084214

C 0.136746 -0.701780 0.023190

C 0.137129 0.702541 -0.024275

C 1.362415 -1.381860 0.044337

C 1.363363 1.381835 -0.044322

C 2.573135 -0.698023 0.022091

C 2.573635 0.697095 -0.021464

H -3.299968 -1.239184 -0.108670

H -2.375353 -0.537737 -1.433155

H -2.370840 0.537975 1.434818

H -3.299612 1.239446 0.113220

H -1.060605 2.397345 0.529205

H -1.307294 1.843719 -1.115788

H 1.359953 -2.468433 0.078107

H 1.361947 2.468412 -0.077622

H 3.509226 -1.246730 0.037999

H 3.510072 1.245221 -0.036337

C -1.158631 -1.494682 0.082579

H -1.060958 -2.395536 -0.533137

H -1.306042 -1.846079 1.113454

**58(A• •A)** -387.989473

C -2.637502 1.024312 -1.037552

C -2.552028 -0.185561 -0.172637

C -1.510746 -0.080346 0.974810

C 0.688270 -1.025200 0.021149

C -0.081252 0.089090 0.510688

C 2.022558 -0.770740 -0.422149

C 0.509788 1.348155 0.543564

C 2.574764 0.495269 -0.384132

C 1.819978 1.568419 0.104430

H -3.569541 1.293077 -1.521315

H -1.740887 1.560491 -1.328086

H -2.304108 -1.067389 -0.787810

H -3.533528 -0.399803 0.267163

H -1.596755 -0.972871 1.604287

H -1.778934 0.773523 1.604851

H 2.608197 -1.607334 -0.791545

H -0.068252 2.185133 0.925266

H 3.591772 0.654872 -0.727164

H 2.245955 2.565084 0.146299

C 0.189491 -2.337709 -0.023381

H 0.812542 -3.144223 -0.392448

H -0.806388 -2.594696 0.311765

**59(A-B)** -196.392230

C 1.917171 0.080842 -0.386514

H 1.908378 1.172291 -0.454754

H 2.905046 -0.218078 -0.024128

H 1.789984 -0.321461 -1.396022

C 0.815920 -0.442703 0.552852

C -0.590337 -0.118100 0.093219

C -0.964095 1.343223 0.033346

C -1.457516 -1.079545 -0.235043

H 0.970530 -0.013427 1.552416

H 0.915147 -1.527684 0.657812

H -2.012523 1.475727 -0.242644

H -0.798958 1.826543 1.003955

H -0.351073 1.882927 -0.696990

H -1.185906 -2.129828 -0.185950

H -2.467481 -0.849308 -0.560853

**59(A•)** -156.474456

C 0.746555 1.225518 0.000133

C 0.092231 -0.004026 -0.000047

C -1.426331 -0.026309 0.000067

C 0.796993 -1.196138 0.000012

H 0.196433 2.159921 -0.000715

H 1.829521 1.281909 0.000102

H -1.810025 -1.048591 -0.003256

H -1.822737 0.482591 0.883905

H -1.822629 0.487875 -0.880833

H 1.881827 -1.203281 -0.000151

H 0.290929 -2.154696 -0.000050

**59(B•)** -39.801300

C 0.000676 0.000017 -0.000914

H -0.540593 -0.935748 0.001825

H -0.544486 0.933440 0.001825

H 1.081020 0.002207 0.001836

**60(A-B)** -349.999400

C 0.400385 1.099151 0.012249

C 1.778557 1.304319 0.019732

C 2.651816 0.215845 0.005798

C 2.132411 -1.076799 -0.016102

C 0.751051 -1.276041 -0.023218

C -0.137499 -0.195360 -0.008762

H -0.262352 1.959619 0.022611

H 2.172168 2.315751 0.036469

H 3.724970 0.375377 0.011562

H 2.800448 -1.932173 -0.027393

H 0.355944 -2.288198 -0.039996

C -1.642390 -0.429640 -0.011538

H -1.794029 -1.515618 -0.042044

C -2.315209 0.168111 -1.261043

H -1.865808 -0.224924 -2.177199

H -3.383661 -0.070097 -1.272964

H -2.216590 1.258226 -1.279946

C -2.303893 0.095534 1.276620

H -3.373149 -0.139587 1.283426

H -1.848712 -0.351490 2.164790

H -2.200595 1.182389 1.358265

**60(A•)** -231.470868

C -1.224491 -0.771582 -0.000004

C -1.212535 0.631984 0.000018

C -0.000020 1.324155 -0.000006

C 1.212556 0.631932 -0.000005

C 1.224511 -0.771536 0.000027

C -0.000015 -1.396970 -0.000013

H -2.158182 -1.324030 -0.000032

H -2.152211 1.175743 0.000000

H 0.000044 2.408687 -0.000013

H 2.152170 1.175796 -0.000037

H 2.158142 -1.324089 -0.000021

**60(B•)** -118.379357

C -0.000001 0.534719 -0.043612

H 0.000093 1.610950 0.099188

C 1.297539 -0.198306 0.002614

H 2.143347 0.451642 -0.237427

H 1.493361 -0.627592 1.000855

H 1.306771 -1.043912 -0.697892

C -1.297570 -0.198266 0.002641

H -1.491572 -0.630765 0.999844

H -2.143693 0.452502 -0.233913

H -1.308112 -1.041705 -0.700508

**61(A-B)** -401.028053

C 2.081008 -0.651754 -0.360424

H 2.462003 -0.362336 -1.347027

H 2.699879 -1.474916 0.002981

C 2.055576 0.570851 0.584652

C 0.687237 1.236261 0.295238

H 2.893978 1.252361 0.418788

H 2.101883 0.235528 1.625077

H 0.786869 2.164831 -0.270483

H 0.153421 1.471564 1.219101

C -0.084832 0.161265 -0.562717

H -0.132996 0.503160 -1.599922

N 0.685381 -1.086446 -0.505786

H 0.406041 -1.607720 0.320513

C -1.521376 0.020088 -0.107128

O -2.448976 0.651049 -0.546316

O -1.660567 -0.866998 0.911119

H -2.598082 -0.870017 1.155320

**61(A•)** -211.812919

C 1.017075 0.717214 -0.121052

H 1.321134 1.044546 -1.123295

H 1.737492 1.127463 0.593995

C -0.431777 1.152497 0.193499

C -1.273990 -0.095647 -0.160812

H -0.726883 2.045004 -0.362658

H -0.531225 1.366796 1.261479

H -1.542882 -0.082128 -1.231363

H -2.208616 -0.145642 0.404724

C -0.325150 -1.208566 0.176333

H -0.536895 -2.260732 0.014213

N 0.975521 -0.751947 -0.067605

H 1.742272 -1.224669 0.388329

**61(B•)** -189.089087

C 0.133292 0.420690 0.000996

O 1.157413 -0.173750 -0.000410

O -1.117064 -0.017431 -0.000738

H -1.122540 -0.994693 0.003204

**62(A-A)** -234.495129

C 0.697939 -1.191047 -0.321255

C 1.497479 0.047821 0.111248

C 0.664170 1.305851 0.058568

C -0.666001 1.304760 -0.058862

C -1.497695 0.045874 -0.110527

C -0.696053 -1.192291 0.320697

H 1.883671 -0.089678 1.131821

H 2.382682 0.168034 -0.524820

H 0.589108 -1.186644 -1.413092

H 1.244259 -2.103248 -0.060522

H -1.197158 2.252504 -0.116058

H -2.382031 0.165011 0.526947

H -1.885496 -0.092140 -1.130420

H -0.586936 -1.188861 1.412581

H -1.240861 -2.105267 0.059413

H 1.193725 2.254493 0.114941

**62(A• •A)** -234.385762

C 1.824372 -0.528342 0.342197

C 0.346789 -0.662567 -0.062691

C -0.468066 0.564935 0.229376

C -1.856270 0.637875 0.143889

C -2.707652 -0.386369 -0.222239

C 2.565081 0.540402 -0.385693

H 0.290441 -0.898553 -1.136832

H -0.090144 -1.528874 0.451345

H 1.890231 -0.356349 1.428289

H 2.323402 -1.499038 0.184791

H -2.307894 1.598150 0.387402

H -3.779161 -0.232155 -0.262735

H -2.341134 -1.373512 -0.482208

H 2.121421 1.060629 -1.227584

H 3.592540 0.772346 -0.129022

H 0.074776 1.461751 0.517522

**63(A-B)** -234.495129-349.999719

C 3.742347 0.000203 -0.233087

H 4.017391 0.884972 0.350800

H 4.017378 -0.882623 0.353735

H 4.350620 -0.001321 -1.142297

C 2.246972 -0.000402 -0.565420

H 2.000614 -0.877577 -1.175100

H 2.000218 0.876009 -1.176009

C 1.357570 0.000077 0.694046

C -0.121354 0.000005 0.373760

C -0.819804 1.201600 0.201609

C -0.819816 -1.201572 0.201718

C -2.173026 1.204615 -0.134588

C -2.173048 -1.204564 -0.134478

C -2.855038 0.000019 -0.304981

H 1.600849 0.879679 1.301919

H 1.600902 -0.879091 1.302534

H -0.298147 2.145274 0.337467

H -0.298196 -2.145256 0.337662

H -2.695876 2.147557 -0.259261

H -2.695907 -2.147510 -0.259085

H -3.908674 0.000006 -0.563845

**63(A•)** -234.495129-270.795559

C 2.399278 0.000030 -0.000105

C 0.994723 0.000011 0.000645

C 0.251672 1.218167 0.000547

C 0.251738 -1.218180 0.000547

C -1.132298 1.211007 -0.000173

C -1.132248 -1.211015 -0.000168

C -1.837627 -0.000018 -0.000315

H 2.958762 0.928087 -0.002144

H 2.958794 -0.928007 -0.002127

H 0.791874 2.160086 -0.000030

H 0.791955 -2.160092 -0.000045

H -1.675355 2.150791 -0.000612

H -1.675290 -2.150812 -0.000617

H -2.922171 -0.000065 -0.000292

**63(B•)** -234.495129-79.089780

C 0.694005 0.000023 0.002141

H 1.106060 0.888246 0.492273

H 1.106105 -0.886828 0.494793

H 1.094284 -0.001488 -1.025871

C -0.794073 -0.000003 0.017004

H -1.352977 -0.927297 -0.038037

H -1.353065 0.927246 -0.038029

**64(A-B)** -308.532696

C -2.040401 -0.432991 0.000215

C -1.827494 0.907292 -0.000164

C -0.400287 1.083670 -0.000123

C 0.147125 -0.164904 0.000012

O -0.850616 -1.100742 -0.000012

H -2.925069 -1.048510 0.000408

H -2.582439 1.678327 -0.000296

H 0.137829 2.018778 -0.000232

C 1.545749 -0.688546 0.000045

H 1.682882 -1.335364 0.876037

H 1.682901 -1.335422 -0.875900

C 2.604520 0.418107 0.000021

H 2.512900 1.053873 0.885446

H 3.607742 -0.015352 0.000035

H 2.512907 1.053831 -0.885435

**64(A•)** -268.618308

C -1.330894 -0.729048 0.000167

C -1.469318 0.636139 -0.000092

C -0.164903 1.171570 0.000050

C 0.729926 0.080089 0.000390

O -0.021431 -1.086651 -0.000277

H -2.042586 -1.538918 0.000693

H -2.402974 1.177884 -0.001630

H 0.123013 2.211548 0.001404

C 2.101738 -0.006334 0.000057

H 2.697525 0.895903 -0.001942

H 2.597175 -0.967705 0.000257

**64(B•)** -39.801327

C -0.000006 0.000161 0.000157

H -0.941209 0.532512 -0.000315

H 0.932419 0.547767 -0.000315

H 0.008826 -1.081242 -0.000314

**65(A-B)** -235.671419

C -3.018993 -0.377708 -0.172084

H -3.130894 -1.049331 0.685602

H -3.929184 0.224960 -0.244444

H -2.957118 -0.997944 -1.072435

C -1.774338 0.503825 -0.022855

H -1.877221 1.135295 0.868835

H -1.706109 1.189085 -0.877154

C -0.475770 -0.305423 0.079356

H -0.542631 -0.992911 0.933030

H -0.361973 -0.933315 -0.813180

C 0.776571 0.577792 0.235363

H 0.863613 1.252426 -0.624623

H 0.647114 1.212712 1.123398

C 2.042439 -0.220116 0.380754

H 2.077357 -0.904699 1.228976

C 3.090304 -0.158073 -0.438864

H 3.974692 -0.766450 -0.280439

H 3.101077 0.508384 -1.297595

**65(A•)** -39.801327

C 0.000000 0.000154 -0.000335

H 0.936835 0.540181 0.000670

H -0.936835 0.540181 0.000670

H 0.000000 -1.081282 0.000670

**65(B•)** -195.730388

C -2.472063 -0.197316 0.063243

H -3.009298 0.124715 -0.822713

H -2.879217 -1.031969 0.622554

C -1.131050 0.364352 0.381656

H -1.132510 1.453307 0.236756

H -0.876742 0.182218 1.431126

C 0.007866 -0.231275 -0.504748

H 0.053320 -1.315678 -0.360272

H -0.249965 -0.057123 -1.557154

C 1.344240 0.386043 -0.202855

H 1.418224 1.461924 -0.364270

C 2.409054 -0.272742 0.250912

H 3.346794 0.233027 0.456417

H 2.381110 -1.344801 0.428304

**66(A-B)** -157.104466

C 1.861058 0.018361 -0.277373

H 1.959491 0.932741 -0.856916

H 2.735488 -0.621553 -0.220847

C 0.722107 -0.297988 0.335910

H 0.669806 -1.227345 0.904299

C -0.538916 0.521599 0.306689

H -0.363187 1.443023 -0.259151

H -0.792620 0.823741 1.331573

C -1.729603 -0.245843 -0.292718

H -1.927064 -1.165724 0.266949

H -2.638934 0.361784 -0.269173

H -1.530859 -0.523443 -1.331781

**66(A•)** -117.188169

C 1.227993 0.196245 0.000105

H 1.295711 1.279672 0.000315

H 2.155928 -0.362860 -0.000018

C 0.000082 -0.442791 -0.000155

H -0.000004 -1.531774 -0.000097

C -1.228091 0.196323 -0.000096

H -1.295845 1.279739 -0.000447

H -2.155691 -0.363439 0.001126

**66(B•)** -39.801327

C -0.000007 -0.000166 0.000177

H 0.929568 -0.552576 -0.000355

H -0.943970 -0.527607 -0.000355

H 0.014440 1.081179 -0.000355

**67(A-B)** -310.715984

C 2.323551 0.003930 0.238797

C 1.638485 -1.202662 0.098243

C 0.272707 -1.203347 -0.183473

C -0.434569 -0.003656 -0.329362

C 0.266834 1.200051 -0.187855

C 1.632442 1.206699 0.093866

H 3.386833 0.007082 0.454604

H 2.168284 -2.144077 0.203394

H -0.251847 -2.148442 -0.296446

H -0.262124 2.142179 -0.304761

H 2.157969 2.150963 0.195097

C -1.925732 -0.006836 -0.592490

H -2.188420 -0.890778 -1.183755

H -2.188855 0.866388 -1.199384

C -2.759378 0.004744 0.701920

H -3.830232 0.002383 0.476534

H -2.538549 -0.872935 1.316543

H -2.539100 0.893699 1.300299

**67(A•)** -270.795563

C 1.837587 0.000085 -0.000054

C 1.132577 -1.211095 -0.000072

C -0.251544 -1.218047 0.000009

C -0.994718 -0.000062 0.000061

C -0.251811 1.218060 0.000169

C 1.132340 1.211164 0.000031

H 2.922115 0.000293 -0.000226

H 1.675518 -2.150854 -0.000078

H -0.791617 -2.159980 0.000420

H -0.792086 2.159865 0.000325

H 1.675161 2.151006 -0.000063

C -2.399711 -0.000129 -0.000198

H -2.958752 -0.928556 0.000915

H -2.958663 0.928366 -0.000962

**67(B•)** -39.801328

C -0.000007 -0.000168 -0.000334

H -0.947099 -0.521985 0.000667

H 0.926268 -0.558083 0.000667

H 0.020872 1.081075 0.000667

**68(A-B)** -155.877906

C 1.586874 -0.485263 0.000002

H 1.472507 -1.116547 0.884336

H 2.598018 -0.069136 0.000281

H 1.472967 -1.116179 -0.884651

C 0.545121 0.649027 0.000014

H 0.693404 1.289481 -0.877306

H 0.693157 1.289108 0.877652

C -0.832922 0.159262 -0.000082

C -1.960907 -0.263887 -0.000021

H -2.959044 -0.631565 0.000205

**68(A•)** -79.089760

C 0.693251 -0.000024 -0.001787

H 1.106692 -0.887409 -0.492205

H 1.093224 0.000196 1.026658

H 1.106484 0.887342 -0.492459

C -0.794096 -0.000016 -0.020230

H -1.350551 0.927534 0.045044

H -1.350781 -0.927427 0.045062

**68(B•)** -76.588890

C -0.000107 0.731070 0.000000

C -0.000107 -0.474374 0.000000

H 0.001282 -1.540178 0.000000

**69(A-B)** -291.030290

N 0.310974 -1.164535 -0.241660

C 0.988609 0.010015 0.321123

C 0.257820 1.273685 -0.156507

C -1.234122 1.231753 0.207126

C -1.879790 -0.067415 -0.295577

C -1.083355 -1.281623 0.190319

H 0.734147 2.157465 0.282847

H -1.751947 2.104038 -0.205706

H -1.341447 1.288846 1.298882

H -2.916793 -0.141945 0.049587

H -1.894735 -0.072324 -1.391659

H -1.175553 -1.350055 1.291906

H -1.499322 -2.202338 -0.230605

H 0.823619 -2.005094 0.005869

H 0.940138 -0.002158 1.429374

H 0.371336 1.345086 -1.245586

C 2.457833 0.004375 -0.097155

H 2.541893 0.029852 -1.187673

H 2.981805 0.871497 0.315507

H 2.968073 -0.895863 0.262907

**69(A•)** -251.102804

N -1.134966 -0.846833 -0.168017

C 0.087725 -1.444184 0.151001

C 1.329098 -0.659074 -0.151657

C 1.181376 0.813624 0.271466

C -0.127467 1.392621 -0.284219

C -1.324656 0.561319 0.185623

H 2.187673 -1.120248 0.347114

H 2.037982 1.398902 -0.078893

H 1.169639 0.878101 1.366679

H -0.262703 2.430580 0.037173

H -0.095918 1.389663 -1.380656

H -1.437596 0.684091 1.276452

H -2.246389 0.914393 -0.286793

H -1.937973 -1.422362 0.047372

H 0.104917 -2.525286 0.050057

H 1.548670 -0.685839 -1.235667

**69(B•)** -39.801300

C -0.000813 -0.000047 -0.001751

H 0.530532 0.941480 0.003494

H 0.555373 -0.927003 0.003495

H -1.081024 -0.014196 0.003518

**70(A-B)** -232.358184

C 1.886453 -0.510338 0.035038

H 2.040740 -0.920975 1.039600

H 2.675377 0.211812 -0.175949

H 1.941627 -1.347579 -0.667159

C 0.528671 0.171885 -0.020918

C -0.686292 -0.750057 -0.061442

H -0.569749 -1.498308 0.733724

H -0.626163 -1.319083 -0.999707

C -2.022870 -0.020883 0.050021

H -2.135412 0.709861 -0.753647

H -2.853491 -0.729510 -0.004681

H -2.094005 0.522251 0.995428

O 0.423163 1.378486 -0.022975

**70(A•)** -39.801327

C -0.000005 0.000165 0.000160

H 0.929745 0.552278 -0.000321

H -0.943799 0.527917 -0.000321

H 0.014087 -1.081185 -0.000320

**70(B•)** -192.426366

C 0.951454 -0.502715 -0.001588

C -0.553403 -0.732181 0.000606

H -0.761927 -1.360820 0.873886

H -0.764853 -1.363984 -0.869579

C -1.390752 0.552096 -0.000271

H -1.177202 1.156704 -0.884656

H -2.456564 0.308362 0.002368

H -1.173547 1.160372 0.880660

O 1.536288 0.524521 0.000606

**71(A-B)** -153.779338

C -1.170046 -0.147985 -0.000098

H -1.163285 -1.238435 -0.004358

H -1.708277 0.229571 -0.877047

H -1.705030 0.222203 0.882172

C 0.234991 0.397010 -0.000062

H 0.309557 1.507662 0.000022

O 1.234671 -0.276894 0.000021

**71(A•)** -113.844511

C -0.062085 0.584358 0.000000

H 0.869196 1.214954 0.000000

O -0.062085 -0.590138 0.000000

**71(B•)** -39.801327

C 0.000006 0.000168 -0.000270

H -0.930415 0.551153 0.000540

H 0.943169 0.529036 0.000540

H -0.012792 -1.081194 0.000540

**72(A-B)** -194.245696

C -1.898799 0.146141 -0.000281

H -2.034957 0.777093 0.884563

H -2.699671 -0.598063 -0.001583

H -2.033341 0.778614 -0.884273

C -0.523441 -0.528281 0.000324

H -0.417887 -1.172266 0.880066

H -0.417404 -1.172506 -0.879203

C 0.615276 0.480860 0.000343

H 0.536315 1.126101 0.889294

H 0.535762 1.126719 -0.888076

O 1.850375 -0.232906 -0.000331

H 2.569964 0.405234 -0.000449

**72(A•)** -79.089760

C -0.693233 0.000020 -0.001789

H -1.106690 0.888088 -0.490987

H -1.093010 -0.001458 1.026720

H -1.106710 -0.886670 -0.493496

C 0.794086 0.000002 -0.020301

H 1.350734 0.927424 0.045139

H 1.350561 -0.927520 0.045168

**72(B•)** -115.025591

C -0.683484 -0.028201 -0.064563

H -1.238789 0.885689 0.098272

H -1.117213 -0.994905 0.171807

O 0.669193 0.125869 0.023178

H 1.103362 -0.728530 -0.068123

**73(A-B)** -233.529123

C 1.443403 0.518978 0.230640

H 2.056921 1.347251 -0.153046

H 1.487562 0.547827 1.330522

O 1.926258 -0.731881 -0.260375

H 2.822323 -0.859951 0.063880

C -2.404827 -0.147607 -0.133231

H -2.788984 0.840635 0.142421

H -3.075157 -0.897131 0.297631

H -2.465990 -0.234174 -1.223193

C -0.965287 -0.340905 0.354106

H -0.612870 -1.342192 0.088311

H -0.938148 -0.281847 1.450091

C 0.001747 0.697919 -0.226761

H -0.322318 1.706674 0.060569

H -0.023617 0.657648 -1.322712

**73(A•)** -118.373187

C -1.217764 0.285695 -0.000677

H -1.258998 0.929576 0.882459

H -2.106229 -0.353990 0.000373

H -1.258727 0.926515 -0.886010

C 0.072130 -0.573860 0.000918

H 0.052031 -1.228689 -0.878531

H 0.051592 -1.225646 0.882672

C 1.319224 0.241857 -0.000120

H 1.736845 0.619704 0.927012

H 1.741942 0.610378 -0.928698

**73(B•)** -115.025580

C -0.684157 0.028051 0.065515

H -1.120888 0.992119 -0.176167

H -1.232467 -0.889265 -0.097721

O 0.670060 -0.125331 -0.023933

H 1.097821 0.731492 0.072258

**74(A-B)** -230.180567

C -0.733372 0.566848 0.271962

H -1.276055 1.450982 -0.072661

H -0.699401 0.592774 1.371034

O -1.448822 -0.565905 -0.190872

H -0.899149 -1.333204 0.008470

C 0.687087 0.600282 -0.267228

H 1.196174 1.508917 0.084384

H 0.660100 0.608699 -1.364798

O 1.339739 -0.576507 0.216059

H 2.168703 -0.691652 -0.256330

**74(A•)** -115.025562

C 0.684211 -0.028244 -0.067128

H 1.233781 0.887798 0.099402

H 1.121526 -0.990664 0.180797

O -0.670010 0.125253 0.024698

H -1.100493 -0.729696 -0.075013

**74(B•)** -115.025562

C 0.684211 -0.028244 -0.067128

H 1.233781 0.887798 0.099402

H 1.121526 -0.990664 0.180797

O -0.670010 0.125253 0.024698

H -1.100493 -0.729696 -0.075013

**75(A-B)** -233.535063

C -2.070960 -0.029955 0.112453

H -2.215151 -0.034055 1.198348

H -2.910595 -0.567856 -0.337248

H -2.105723 1.007174 -0.227880

C -0.737457 -0.680440 -0.267143

H -0.625207 -0.698616 -1.357997

H -0.718529 -1.722313 0.073382

C 0.479437 0.033628 0.321620

H 0.356904 0.081663 1.416503

C 1.788977 -0.689167 0.001581

H 1.929814 -0.759330 -1.081226

H 2.646918 -0.153831 0.423459

H 1.790701 -1.699877 0.421509

O 0.481659 1.363691 -0.211830

H 1.237607 1.833113 0.154726

**75(A•)** -79.089760

C -0.693233 -0.000035 0.001789

H -1.106679 -0.888482 0.490290

H -1.093010 0.002292 -1.026719

H -1.106720 0.886274 0.494192

C 0.794086 -0.000003 0.020301

H 1.350527 0.927543 -0.045161

H 1.350767 -0.927402 -0.045144

**75(B•)** -154.318113

C -0.091796 -0.505168 -0.099383

H -0.232096 -1.526830 0.250991

C 1.229494 0.163646 0.010849

H 1.303286 0.999593 -0.693383

H 1.412150 0.571853 1.018705

H 2.030519 -0.545667 -0.212123

O -1.169724 0.340447 0.023134

H -1.982259 -0.173388 -0.018059

**76(A-B)** -733.366669

C 0.000903 -0.002031 -0.751092

H 0.001231 -0.000215 -1.848037

C -0.427356 1.406516 -0.327947

C -1.224914 1.645642 0.795396

C 0.014442 2.504292 -1.078484

C -1.564095 2.948714 1.164684

H -1.592354 0.809247 1.380615

C -0.326362 3.804949 -0.715635

H 0.635847 2.335526 -1.953769

C -1.117146 4.032431 0.411683

H -2.184853 3.113733 2.039553

H 0.023140 4.640703 -1.313325

H -1.385683 5.044506 0.695914

C -1.006356 -1.078245 -0.333464

C -2.193435 -1.212798 -1.066317

C -0.802629 -1.920441 0.763595

C -3.152866 -2.157230 -0.710945

H -2.367575 -0.565156 -1.921249

C -1.764757 -2.866049 1.124909

H 0.116067 -1.845169 1.335429

C -2.942194 -2.988188 0.390721

H -4.063685 -2.246729 -1.294277

H -1.587491 -3.511147 1.979523

H -3.687254 -3.726104 0.669251

C 1.435531 -0.332443 -0.329949

C 2.187938 -1.218124 -1.112286

C 2.020603 0.197903 0.824347

C 3.486284 -1.569941 -0.750155

H 1.748418 -1.638709 -2.012671

C 3.319724 -0.156225 1.192552

H 1.462404 0.899280 1.435516

C 4.057244 -1.040562 0.407938

H 4.053012 -2.254768 -1.372800

H 3.756394 0.266897 2.091573

H 5.069033 -1.310922 0.691436

**76(A•)** -501.776430

C 0.000509 -1.037278 0.003772

H 0.000715 -2.125187 0.004371

C 1.302241 -0.436322 -0.017674

C 1.565830 0.908491 -0.388283

C 2.423497 -1.249190 0.299781

C 2.861811 1.406573 -0.400066

H 0.753185 1.544966 -0.714865

C 3.713602 -0.741966 0.292863

H 2.255099 -2.288375 0.566991

C 3.944096 0.594173 -0.050058

H 3.034262 2.436117 -0.697760

H 4.546813 -1.387516 0.551661

H 4.953306 0.991641 -0.059379

C -1.301693 -0.436027 0.022006

C -2.421439 -1.249166 -0.300050

C -1.567758 0.908059 0.392625

C -3.711833 -0.742831 -0.298269

H -2.250867 -2.287843 -0.567910

C -2.864223 1.405161 0.399827

H -0.756831 1.545117 0.722601

C -3.944680 0.592861 0.044759

H -4.543335 -1.388788 -0.561549

H -3.038172 2.434425 0.697810

H -4.953924 0.990218 0.050626

**76(B•)** -231.470868

C 0.000185 1.397023 -0.000036

C -1.224450 0.771637 -0.000024

C 1.224620 0.771433 0.000049

C -1.212648 -0.631824 -0.000008

H -2.157992 1.324318 0.000104

C 1.212471 -0.632120 -0.000083

H 2.158398 1.323745 0.000183

C -0.000137 -1.324109 0.000102

H -2.152318 -1.175605 -0.000134

H 2.152037 -1.176047 -0.000207

H -0.000367 -2.408640 0.000052

**77(A-B)** -158.313550

C -1.963154 0.121714 0.000069

H -2.104913 0.750870 0.885919

H -2.750128 -0.639346 -0.000864

H -2.104360 0.752508 -0.884692

C -0.567077 -0.518092 -0.000082

H -0.461746 -1.165830 -0.879992

H -0.461647 -1.166155 0.879577

C 0.567079 0.518097 -0.000078

H 0.461635 1.165963 0.879726

H 0.461770 1.166033 -0.879843

C 1.963152 -0.121717 0.000073

H 2.104845 -0.751399 -0.885418

H 2.750131 0.639337 0.000505

H 2.104412 -0.751992 0.885193

**77(A•)** -79.089760

C -0.693233 0.000035 -0.001789

H -1.106679 0.888482 -0.490290

H -1.093010 -0.002292 1.026719

H -1.106720 -0.886274 -0.494192

C 0.794086 0.000003 -0.020301

H 1.350527 -0.927543 0.045161

H 1.350767 0.927402 0.045144

**77(B•)** -79.089760

C -0.794086 -0.000002 0.020300

H -1.350567 0.927516 -0.045167

H -1.350727 -0.927429 -0.045136

C 0.693233 -0.000018 0.001789

H 1.106688 -0.888046 0.491063

H 1.093011 0.001366 -1.026720

H 1.106710 0.886712 0.493421

**78(A-B)** -154.962433

C -1.225771 -0.223188 -0.000006

H -1.293207 -0.859487 -0.886521

H -2.074860 0.467735 -0.000926

H -1.293931 -0.858016 0.887496

C 0.084649 0.548376 -0.000008

H 0.137368 1.194084 0.889002

H 0.137427 1.194105 -0.888981

O 1.155735 -0.396910 0.000006

H 1.988054 0.085735 -0.000036

**78(A•)** -115.025591

C -0.683491 0.028203 0.064570

H -1.238808 -0.885680 -0.098275

H -1.117190 0.994907 -0.171833

O 0.669197 -0.125870 -0.023182

H 1.103371 0.728518 0.068148

**78(B•)** -39.801327

C -0.000005 0.000168 0.000265

H 0.931898 0.548641 -0.000529

H -0.941738 0.531577 -0.000529

H 0.009870 -1.081224 -0.000529

**79(A-B)** -194.250685

C 1.269021 -0.681531 -0.083220

H 1.304177 -1.692084 0.335943

H 2.159386 -0.138074 0.243976

H 1.299646 -0.757914 -1.174516

C -0.000019 0.049238 0.351753

H -0.000111 0.135688 1.447655

C -1.268465 -0.682554 -0.083376

H -1.303055 -1.693035 0.336024

H -2.159324 -0.139680 0.243476

H -1.298767 -0.759202 -1.174661

O -0.000215 1.364591 -0.230313

H -0.003449 2.016655 0.473664

**79(A•)** -39.801327

C 0.000005 -0.000168 0.000265

H -0.931898 -0.548641 -0.000529

H 0.941738 -0.531577 -0.000529

H -0.009870 1.081224 -0.000529

**79(B•)** -154.318122

C 0.091778 -0.505185 -0.098600

H 0.233050 -1.527441 0.249303

C -1.229611 0.163573 0.010687

H -2.030803 -0.547826 -0.204669

H -1.408863 0.578791 1.016242

H -1.306672 0.994759 -0.698972

O 1.169765 0.340596 0.023139

H 1.982162 -0.173374 -0.019533

**80(A-B)** -158.315228

C -1.270265 -0.723063 0.096031

H -1.318141 -0.749719 1.191045

H -2.172206 -0.218125 -0.264637

H -1.296605 -1.756591 -0.263975

C 1.261426 -0.738367 0.096033

H 1.275313 -1.772108 -0.264061

H 2.169414 -0.244320 -0.264543

H 1.308914 -0.765692 1.191048

C 0.000002 -0.000116 -0.373873

H 0.000013 -0.000013 -1.472465

C 0.008838 1.461445 0.096047

H 0.897334 1.990019 -0.264083

H 0.008736 1.516217 1.191039

H -0.872779 2.000938 -0.264795

**80(A•)** -118.379365

C -1.297288 -0.198339 -0.002511

H -1.309550 -1.036749 0.706746

H -2.144449 0.453605 0.226751

H -1.488034 -0.638495 -0.996950

C 1.297288 -0.198339 -0.002511

H 1.488034 -0.638494 -0.996950

H 2.144448 0.453605 0.226752

H 1.309549 -1.036749 0.706745

C 0.000000 0.535230 0.042178

H 0.000000 1.611963 -0.096029

**80(B•)** -39.801327

C 0.000004 -0.000159 -0.000269

H 0.943207 -0.528975 0.000538

H -0.930335 -0.551279 0.000538

H -0.012895 1.081208 0.000538

**81(A-B)** -119.030077

C 1.276571 -0.260254 0.000015

H 1.320120 -0.905294 0.884252

H 2.174630 0.364982 -0.001396

H 1.318458 -0.907161 -0.882931

C 0.000000 0.587603 0.000039

H 0.000000 1.246388 0.876557

H 0.000000 1.245987 -0.876818

C -1.276571 -0.260254 0.000015

H -1.320118 -0.905297 0.884251

H -2.174630 0.364982 -0.001393

H -1.318459 -0.907158 -0.882933

**81(A•)** -39.801327

C 0.000005 0.000168 -0.000265

H -0.931898 0.548641 0.000529

H 0.941738 0.531577 0.000529

H -0.009870 -1.081224 0.000529

**81(B•)** -79.089760

C 0.794086 0.000002 0.020301

H 1.350730 0.927426 -0.045138

H 1.350565 -0.927517 -0.045169

C -0.693233 0.000018 0.001789

H -1.106691 0.888045 0.491064

H -1.093010 -0.001365 -1.026720

H -1.106708 -0.886714 0.493418

**82(A-B)** -274.985722

C 1.905148 0.001193 0.287970

C 1.196206 -1.266691 -0.210386

C -0.293144 -1.263469 0.167819

C -1.019231 -0.000847 -0.331220

C -0.295280 1.262508 0.168036

C 1.193760 1.267853 -0.210634

H -0.786381 -2.157498 -0.232146

H 1.290407 -1.326546 -1.303190

H 1.685207 -2.159709 0.194483

H 1.913833 0.000858 1.386434

H 2.952364 0.001994 -0.034266

H -0.966837 -0.000432 -1.430565

H -0.790183 2.155873 -0.231301

H -0.391392 1.314856 1.262228

H 1.287642 1.327214 -1.303485

H 1.681960 2.161570 0.193720

H -0.389448 -1.316627 1.261976

C -2.496951 -0.000652 0.075694

H -3.014752 0.884992 -0.307306

H -3.015969 -0.885494 -0.307400

H -2.599492 -0.000428 1.167140

**82(A•)** -235.048437

C 0.004859 1.412020 0.268569

C 1.270142 0.708147 -0.243298

C 1.285635 -0.782505 0.159461

C -0.004904 -1.463623 -0.165277

C -1.291113 -0.774335 0.159238

C -1.265116 0.716184 -0.243006

H 2.127648 -1.299174 -0.313204

H 1.304592 0.783621 -1.337393

H 2.167471 1.206282 0.139825

H 0.004980 1.408038 1.367622

H 0.008076 2.463087 -0.040764

H -0.008132 -2.519599 -0.417559

H -2.136257 -1.284698 -0.314660

H -1.478075 -0.828708 1.249104

H -1.299489 0.792383 -1.337065

H -2.158850 1.220654 0.140374

H 1.471014 -0.837214 1.249607

**82(B•)** -39.801327

C 0.000005 -0.000166 -0.000300

H -0.933637 -0.545684 0.000599

H 0.940033 -0.534582 0.000599

H -0.006424 1.081262 0.000599

**83(A-B)** -79.746460

C -0.766006 -0.000004 -0.000006

H -1.163820 0.303176 0.973103

H -1.163811 -0.994324 -0.223984

H -1.163830 0.691151 -0.749089

C 0.766006 0.000004 0.000006

H 1.163830 -0.691108 0.749129

H 1.163820 -0.303231 -0.973086

H 1.163811 0.994337 0.223927

**83(A•)** -39.801336

C -0.000006 -0.000002 0.000681

H 0.438572 0.988509 -0.001363

H 0.636820 -0.874046 -0.001363

H -1.075358 -0.114453 -0.001363

**83(B•)** -39.801336

C -0.000006 -0.000002 0.000681

H 0.438572 0.988509 -0.001363

H 0.636820 -0.874046 -0.001363

H -1.075358 -0.114453 -0.001363

**84(A-B)** -193.024915

C -1.042531 0.617876 -0.057933

C 0.152660 -0.043892 0.488841

O -0.829403 -0.786478 -0.246417

H -1.867973 0.879855 0.601152

H -0.945738 1.226046 -0.955967

H 0.152553 -0.267326 1.556434

C 1.510101 0.100253 -0.148018

H 2.079154 0.900377 0.337034

H 2.082230 -0.827943 -0.053323

H 1.413619 0.335387 -1.211325

**84(A•)** -153.073303

C -0.795659 0.195541 0.017685

C 0.598393 0.564314 -0.160120

O 0.327597 -0.758354 0.031544

H -1.294516 0.290644 0.979608

H -1.441257 0.112901 -0.852158

H 1.298595 1.104156 0.474810

**84(B•)** -39.801327

C -0.000001 0.000157 0.000200

H -0.937313 0.539344 -0.000400

H 0.936364 0.540993 -0.000400

H 0.000955 -1.081280 -0.000399

**85(A-B)** -346.646098

C -2.307390 -0.303128 -0.054174

C -1.381271 -1.341556 0.042670

C -0.016607 -1.064656 0.116377

C 0.437944 0.256690 0.083155

C -0.494845 1.293055 -0.023912

C -1.859788 1.017334 -0.088152

H -3.368833 -0.520890 -0.110742

H -1.722296 -2.371744 0.061641

H 0.706378 -1.869613 0.180472

H -0.151896 2.323564 -0.065382

H -2.571705 1.831908 -0.173409

C 1.909506 0.577372 0.215290

H 2.146938 0.725761 1.280313

H 2.120822 1.522833 -0.304263

O 2.689210 -0.486892 -0.321148

H 3.601611 -0.357352 -0.046978

**85(A•)** -231.470868

C -0.000443 -1.324115 0.000002

C 1.212371 -0.632242 -0.000025

C 1.224816 0.771172 0.000029

C 0.000434 1.396947 0.000001

C -1.224263 0.771888 -0.000033

C -1.212807 -0.631642 0.000020

H -0.000693 -2.408656 -0.000006

H 2.151810 -1.176417 -0.000025

H 2.158610 1.323429 0.000017

H -2.157739 1.324691 0.000001

H -2.152640 -1.175103 0.000049

**85(B•)** -115.025572

C -0.684532 0.028312 0.067071

H -1.232884 -0.888956 -0.098554

H -1.121294 0.991143 -0.181280

O 0.670135 -0.125247 -0.024872

H 1.100293 0.729916 0.076379

**86(A-B)** -310.716006

C 2.324894 0.004294 0.237926

C 1.639390 -1.202564 0.098503

C 0.273087 -1.203672 -0.181981

C -0.434851 -0.004022 -0.328420

C 0.266960 1.199944 -0.187126

C 1.633170 1.207066 0.093209

H 3.388407 0.007536 0.453162

H 2.169311 -2.144064 0.203576

H -0.251167 -2.149178 -0.294007

H -0.262074 2.142297 -0.303276

H 2.158359 2.151677 0.194086

C -1.925811 -0.007953 -0.592211

H -2.187558 -0.893056 -1.182366

H -2.188953 0.863567 -1.201760

C -2.761611 0.005790 0.700411

H -3.832102 0.002379 0.473095

H -2.541975 -0.870401 1.317631

H -2.543624 0.895943 1.297993

**86(A•)** -231.470899

C -0.000383 -1.323505 0.000004

C 1.213078 -0.632486 -0.000014

C 1.225192 0.771573 -0.000007

C 0.000406 1.396741 0.000017

C -1.224717 0.772182 -0.000004

C -1.213478 -0.631901 -0.000005

H -0.000697 -2.408442 0.000050

H 2.152440 -1.177382 0.000013

H 2.160166 1.322630 0.000009

H -2.159350 1.323816 -0.000014

H -2.153153 -1.176240 -0.000008

**86(B•)** -79.089771

C -0.793943 0.000011 -0.018877

H -1.351740 -0.927410 0.041833

H -1.351820 0.927374 0.041829

C 0.693518 0.000007 -0.001925

H 1.092712 -0.000105 1.026834

H 1.106629 -0.887228 -0.492914

H 1.106768 0.887261 -0.492768

**87(A-B)** -155.877906

C 1.586874 -0.485263 0.000002

H 1.472507 -1.116547 0.884336

H 2.598018 -0.069136 0.000281

H 1.472967 -1.116179 -0.884651

C 0.545121 0.649027 0.000014

H 0.693404 1.289481 -0.877306

H 0.693157 1.289108 0.877652

C -0.832922 0.159262 -0.000082

C -1.960907 -0.263887 -0.000021

H -2.959044 -0.631565 0.000205

**87(A•)** -79.089760

C 0.693251 -0.000024 -0.001787

H 1.106692 -0.887409 -0.492205

H 1.093224 0.000196 1.026658

H 1.106484 0.887342 -0.492459

C -0.794096 -0.000016 -0.020230

H -1.350551 0.927534 0.045044

H -1.350781 -0.927427 0.045062

**87(B•)** -76.588890

C -0.000107 0.731070 0.000000

C -0.000107 -0.474374 0.000000

H 0.001282 -1.540178 0.000000

**88(A-B)** -349.999719

C 3.742347 0.000203 -0.233087

H 4.017391 0.884972 0.350800

H 4.017378 -0.882623 0.353735

H 4.350620 -0.001321 -1.142297

C 2.246972 -0.000402 -0.565420

H 2.000614 -0.877577 -1.175100

H 2.000218 0.876009 -1.176009

C 1.357570 0.000077 0.694046

H 1.600849 0.879679 1.301919

H 1.600902 -0.879091 1.302534

C -0.121354 0.000005 0.373760

C -0.819804 1.201600 0.201609

C -0.819816 -1.201572 0.201718

C -2.173026 1.204615 -0.134588

C -2.173048 -1.204564 -0.134478

C -2.855038 0.000019 -0.304981

H -0.298147 2.145274 0.337467

H -0.298196 -2.145256 0.337662

H -2.695876 2.147557 -0.259261

H -2.695907 -2.147510 -0.259085

H -3.908674 0.000006 -0.563845

**88(A•)** -118.373188

C 1.217971 0.285789 0.001707

H 1.258270 0.931618 -0.879985

H 1.257855 0.924174 0.888804

H 2.107266 -0.352883 -0.000836

C -0.072234 -0.574306 -0.002317

H -0.052656 -1.231212 0.875344

H -0.051467 -1.223341 -0.886004

C -1.317488 0.243346 0.000353

H -1.738007 0.623229 -0.924792

H -1.750752 0.599444 0.929005

**88(B•)** -231.470875

C -0.000080 1.396838 0.000043

C 1.224380 0.771776 -0.000026

C -1.224472 0.771650 -0.000018

C 1.212495 -0.631931 -0.000092

C -1.212415 -0.632048 -0.000087

C 0.000077 -1.324180 0.000040

H 2.158455 1.324022 0.000218

H -2.158570 1.323857 0.000187

H 2.152430 -1.175730 0.000000

H -2.152317 -1.175900 -0.000016

H 0.000087 -2.408880 0.000447

**89(A-B)** -271.433022

C -0.912489 0.000220 -0.011898

C -0.194582 -1.201633 -0.009039

C 1.199883 -1.204577 0.002203

C 1.902794 -0.000084 0.008505

C 1.200033 1.204418 0.002205

C -0.194572 1.201867 -0.009068

H -0.732956 -2.144596 -0.017522

H 1.737230 -2.146839 0.001834

H 2.987104 -0.000206 0.013552

H 1.737459 2.146647 0.001900

H -0.732735 2.144920 -0.017494

C -2.424967 -0.000071 0.009763

H -2.826585 -0.882685 -0.495324

H -2.799141 -0.007502 1.039804

H -2.826979 0.889421 -0.482771

**89(A•)** -231.470868

C -0.000444 -1.396947 0.000009

C 1.224301 -0.771826 -0.000049

C 1.212813 0.631608 0.000029

C 0.000381 1.324111 0.000004

C -1.212360 0.632276 -0.000038

C -1.224784 -0.771234 0.000036

H 2.157725 -1.324714 -0.000012

H 2.152577 1.175189 0.000056

H 0.000743 2.408650 0.000024

H -2.151860 1.176340 -0.000058

H -2.158633 -1.323395 0.000038

**89(B•)** -39.801328

C -0.000014 -0.000173 0.000288

H 0.922014 -0.565092 -0.000575

H -0.951047 -0.514753 -0.000576

H 0.029114 1.080881 -0.000575

**90(A-B)** -463.118708

C 2.876384 -1.199941 -0.000558

C 1.484027 -1.198120 -0.000564

C 0.747630 0.000108 -0.000004

C 1.484241 1.198259 0.000554

C 2.876563 1.199844 0.000563

C 3.584926 -0.000123 0.000005

H 3.407819 -2.145946 -0.001010

H 0.975704 -2.154007 -0.001041

H 0.976081 2.154218 0.001022

H 3.408206 2.145731 0.001013

H 4.669521 -0.000182 -0.000001

C -0.747629 0.000109 -0.000002

C -1.484239 1.198264 -0.000555

C -1.484029 -1.198118 0.000561

C -2.876563 1.199842 -0.000560

H -0.976083 2.154225 -0.001022

C -2.876386 -1.199943 0.000562

H -0.975707 -2.154006 0.001046

C -3.584924 -0.000121 -0.000002

H -3.408209 2.145728 -0.001009

H -3.407821 -2.145946 0.001014

H -4.669519 -0.000180 -0.000002

**90(A•)** -231.470868

C 1.212546 0.631970 -0.000002

C 1.224478 -0.771594 0.000035

C 0.000000 -1.396970 -0.000022

C -1.224521 -0.771523 -0.000005

C -1.212547 0.631944 0.000029

C 0.000035 1.324158 -0.000007

H 2.152227 1.175719 -0.000044

H 2.158164 -1.324057 -0.000024

H -2.158154 -1.324070 -0.000045

H -2.152163 1.175811 0.000010

H -0.000017 2.408689 -0.000061

**90(B•)** -231.470868

C 1.212546 0.631970 -0.000002

C 1.224478 -0.771594 0.000035

C 0.000000 -1.396970 -0.000022

C -1.224521 -0.771523 -0.000005

C -1.212547 0.631944 0.000029

C 0.000035 1.324158 -0.000007

H 2.152227 1.175719 -0.000044

H 2.158164 -1.324057 -0.000024

H -2.158154 -1.324070 -0.000045

H -2.152163 1.175811 0.000010

H -0.000017 2.408689 -0.000061

**91(A-B)** -309.510629

C 2.263230 0.260906 0.001162

C 1.361411 1.327967 -0.000750

C -0.008913 1.091926 -0.002161

C -0.514361 -0.219374 -0.001365

C 0.405504 -1.280376 0.000168

C 1.779130 -1.045695 0.001656

H 3.331791 0.449278 0.002095

H 1.730300 2.348779 -0.001290

H -0.690914 1.935699 -0.004155

H 0.034435 -2.301344 0.000275

H 2.469847 -1.882759 0.002927

C -1.954711 -0.528972 -0.002671

H -2.184756 -1.593428 -0.008842

C -2.974428 0.335357 0.003405

H -3.999367 -0.017976 0.001632

H -2.832512 1.411317 0.010692

**91(A•)** -231.470881

C -0.000382 1.324124 -0.000064

C -1.212452 0.631662 0.000026

C -1.223956 -0.771624 0.000037

C 0.000392 -1.397416 -0.000098

C 1.224366 -0.771075 0.000017

C 1.212131 0.632222 0.000106

H -0.000675 2.409341 -0.000309

H -2.152898 1.175334 0.000086

H -2.158332 -1.324746 0.000099

H 2.159030 -1.323693 -0.000090

H 2.152288 1.176408 0.000075

**91(B•)** -77.860818

C 0.707050 0.143470 -0.000012

H 1.602131 -0.462422 0.000043

C -0.587191 -0.029221 0.000008

H -1.035408 -1.028399 -0.000023

H -1.285873 0.805326 0.000010

**92(A-B)** -155.877906

C 1.586874 -0.485263 0.000002

H 1.472507 -1.116547 0.884336

H 2.598018 -0.069136 0.000281

H 1.472967 -1.116179 -0.884651

C 0.545121 0.649027 0.000014

H 0.693404 1.289481 -0.877306

H 0.693157 1.289108 0.877652

C -0.832922 0.159262 -0.000082

C -1.960907 -0.263887 -0.000021

H -2.959044 -0.631565 0.000205

**92(A•)** -39.801328

C -0.000012 0.000176 -0.000142

H -0.950017 0.516645 0.000284

H 0.923147 0.563228 0.000284

H 0.026941 -1.080932 0.000284

**92(B•)** -115.956829

C 1.252508 -0.000144 0.000747

H 1.806789 -0.931644 -0.000176

H 1.807356 0.931007 -0.000178

C -0.114798 0.000311 -0.001858

C -1.339522 0.000164 0.001663

H -2.403274 -0.001348 -0.002958

**93(A-B)** -116.595056

C -1.240480 -0.000050 -0.000094

H -1.629110 -0.832644 -0.593803

H -1.629468 0.930367 -0.424090

H -1.629423 -0.098130 1.017704

C 0.218411 0.000192 0.000081

C 1.422394 -0.000018 0.000251

H 2.486056 -0.000334 -0.001243

**93(A•)** -39.801328

C -0.000011 0.000171 -0.000291

H -0.947528 0.521206 0.000582

H 0.925835 0.558826 0.000582

H 0.021759 -1.081055 0.000582

**93(B•)** -76.588878

C -0.018236 -0.737528 0.000000

C -0.018236 0.482573 0.000000

H 0.218830 1.529735 0.000000

**94(A-B)** -78.532421

C 0.000000 0.664608 0.000000

H -0.925344 1.233515 0.000000

H 0.925226 1.233723 0.000000

C 0.000000 -0.664608 0.000000

H 0.925344 -1.233515 0.000000

H -0.925226 -1.233723 0.000000

**94(A•)** -39.126369

C 0.000000 -0.102975 0.000000

H -1.000002 0.308936 0.000000

H 1.000002 0.308915 0.000000

**94(B•)** -39.126369

C 0.000000 0.102975 0.000000

H 1.000002 -0.308936 0.000000

H -1.000002 -0.308915 0.000000

acetylene

-77.300090

C 0.000000 0.000000 0.600623

H 0.000000 0.000000 1.664594

C 0.000000 0.000000 -0.600623

H 0.000000 0.000000 -1.664594

-38.468083

C 0.000000 0.000000 -0.161158

H 0.000000 0.000000 0.966945

-38.468083

C 0.000000 0.000000 -0.161158

H 0.000000 0.000000 0.966945

(3) O-H BDE (**96**-**125**)

H = -0.500215

**96** = -518.816941

N -0.336942 -0.735608 -0.456637

C 0.967940 1.163771 -0.059762

C 1.052230 -0.374286 -0.073422

C -1.302906 0.326012 -0.045714

C 2.026505 -0.837295 -1.169316

H 3.037218 -0.482890 -0.952067

H 2.040667 -1.930773 -1.210810

H 1.719941 -0.458759 -2.147436

C 1.533416 -0.895423 1.295772

H 1.617493 -1.983272 1.266963

H 2.515316 -0.465542 1.507543

H 0.857026 -0.631055 2.109065

O 1.896570 1.902424 0.154880

C -0.465359 1.580355 -0.358872

H -0.518900 1.829800 -1.425957

H -0.752362 2.464989 0.212405

C -2.555741 0.207363 -0.920144

H -3.091534 -0.719716 -0.695882

H -3.238114 1.042126 -0.733669

H -2.282841 0.204485 -1.978707

C -1.703135 0.294914 1.444072

H -2.506938 1.015701 1.621267

H -2.062435 -0.697830 1.721810

H -0.872845 0.560734 2.102400

O -0.714249 -2.009855 0.075214

H -0.879360 -2.531760 -0.716904

**96•** = -518.218017

N -0.324568 -0.809914 -0.101995

C 0.943252 1.155748 -0.093239

C 1.086484 -0.369801 -0.022907

C -1.346761 0.278640 -0.023411

C 1.874349 -0.897682 -1.234611

H 2.907431 -0.546735 -1.184622

H 1.859327 -1.990180 -1.220200

H 1.431675 -0.557778 -2.174908

C 1.741580 -0.813991 1.294745

H 1.754667 -1.905014 1.338893

H 2.763765 -0.432378 1.338787

H 1.192513 -0.438021 2.161787

O 1.851634 1.936004 0.043556

C -0.510402 1.523537 -0.374893

H -0.585375 1.760889 -1.443108

H -0.791984 2.418632 0.183023

C -2.466814 -0.011244 -1.026767

H -2.947228 -0.962087 -0.787809

H -3.218052 0.782647 -0.989679

H -2.071298 -0.071472 -2.044436

C -1.905647 0.348515 1.409969

H -2.695544 1.102903 1.469117

H -2.323355 -0.620816 1.691155

H -1.126547 0.613683 2.130943

O -0.648417 -2.031905 0.040409

**97** = -326.918267

C 1.756686 0.000701 -0.118949

C 0.899191 -1.259821 -0.303419

C -0.333185 -1.215294 0.612149

C -0.334044 1.214891 0.612299

C 0.897631 1.260346 -0.303279

H -0.987034 -2.074231 0.440029

H 0.565896 -1.333099 -1.344362

H 1.480169 -2.163040 -0.085119

H 2.192182 0.000474 0.890663

H 2.595884 0.001209 -0.822656

H -0.988372 2.073593 0.440810

H -0.023220 1.246050 1.664532

H 0.564976 1.333511 -1.344457

H 1.478056 2.163971 -0.084930

H -0.023437 -1.246628 1.664687

N -1.153051 -0.000477 0.475761

O -1.683539 -0.000516 -0.877857

H -2.633110 0.000717 -0.719470

**97•** = -326.312773

C 1.754964 0.000654 -0.045499

C 0.923795 -1.267560 -0.299445

C -0.376453 -1.240136 0.522617

C -0.377002 1.239710 0.523079

C 0.922344 1.267966 -0.299658

H -1.041096 -2.066902 0.270944

H 0.660983 -1.335643 -1.361194

H 1.497222 -2.165377 -0.045968

H 2.108195 0.000664 0.994762

H 2.646556 0.001048 -0.680314

H -1.042323 2.066411 0.273003

H -0.147489 1.278121 1.595092

H 0.659476 1.335444 -1.361442

H 1.495279 2.166302 -0.046724

H -0.148667 -1.279777 1.594945

N -1.119513 -0.000341 0.260049

O -1.992179 -0.000215 -0.682501

**98** = -365.011260

C -0.065772 -0.145725 1.103360

C -0.066115 -0.143284 -1.103680

C -1.544180 -0.431004 0.783747

C 0.261198 1.334987 0.781550

C -1.544518 -0.429021 -0.784370

C 0.261115 1.336664 -0.778757

H 0.270825 -0.492172 2.080420

H 0.270148 -0.487591 -2.081618

H -2.201745 0.329427 1.210800

H -1.848691 -1.403688 1.175064

H 1.242020 1.607926 1.173836

H -0.479805 2.013471 1.211745

H -1.849371 -1.400629 -1.178096

H -2.202099 0.332615 -1.209277

H -0.479685 2.016315 -1.207426

H 1.241966 1.610146 -1.170593

N 0.565903 -0.917953 -0.001094

O 1.989208 -0.660508 -0.000993

H 2.351082 -1.551780 -0.000362

**98•** = -364.399286

C -0.012422 -0.119010 1.125138

C -0.012734 -0.119252 -1.125109

C -1.455880 -0.525134 0.785286

C 0.205462 1.375521 0.784290

C -1.456005 -0.525711 -0.784849

C 0.205069 1.375338 -0.784752

H 0.366942 -0.445860 2.091065

H 0.366376 -0.446397 -2.091055

H -2.179657 0.176909 1.204921

H -1.682191 -1.519312 1.176276

H 1.167014 1.716976 1.172683

H -0.579672 2.005562 1.208998

H -1.681907 -1.520275 -1.175114

H -2.180141 0.175666 -1.204974

H -0.580242 2.005244 -1.209303

H 1.166405 1.716687 -1.173791

N 0.722695 -0.773277 0.000067

O 1.989659 -0.902846 -0.000024

**99** = -695.692070

O -1.548288 -0.981531 -0.242435

C -2.473740 1.215596 -0.659104

C -1.175355 1.899426 -0.223800

C -2.776190 0.044732 1.588052

C -0.026231 0.916911 -0.128995

C -0.275919 -0.462301 -0.139081

C 1.295606 1.384384 -0.024803

C 0.772435 -1.399416 -0.082774

C 2.092637 -0.930562 -0.006448

C 2.334180 0.452339 0.030488

C 1.595390 2.864887 0.014649

C 0.463059 -2.881004 -0.112647

C 3.275831 -1.873903 0.042300

H -3.334044 1.866702 -0.474547

H -2.442649 1.012212 -1.735297

H -1.317619 2.398567 0.744328

H -0.926010 2.695496 -0.932981

H -3.615878 0.698761 1.842480

H -2.938801 -0.928117 2.059421

H -1.864277 0.475753 2.007518

H 0.963271 3.379587 0.745199

H 2.637457 3.042158 0.277137

H 1.412376 3.335406 -0.959125

H 0.882940 -3.359122 -1.004723

H -0.612376 -3.047130 -0.121988

H 0.878105 -3.394473 0.761051

H 3.978275 -1.680912 -0.779285

H 3.832035 -1.781624 0.985266

H 2.970301 -2.915268 -0.043100

C -2.669721 -0.123846 0.064781

C -3.887702 -0.868296 -0.480849

H -3.970827 -1.853638 -0.014539

H -4.802365 -0.306571 -0.271133

H -3.799213 -1.004082 -1.561792

O 3.619268 0.946474 0.115964

H 4.235777 0.213073 0.197270

**99•** = -695.080185

O -1.463936 -0.982312 -0.152682

C -2.438347 1.181556 -0.683625

C -1.176137 1.903156 -0.207622

C -2.831195 0.040232 1.567058

C 0.001754 0.955868 -0.105647

C -0.223157 -0.444758 -0.105015

C 1.297905 1.434012 -0.018977

C 0.846340 -1.388877 -0.082566

C 2.144973 -0.930196 -0.001438

C 2.427699 0.506793 0.041380

C 1.598533 2.907289 0.002047

C 0.541554 -2.869142 -0.117257

C 3.316164 -1.873017 0.049972

H -3.322056 1.811708 -0.545169

H -2.358335 0.963847 -1.754584

H -1.354185 2.383623 0.763088

H -0.933995 2.714413 -0.900740

H -3.714067 0.656351 1.761169

H -2.973643 -0.930841 2.047644

H -1.966188 0.523084 2.027283

H 1.014749 3.426465 0.769836

H 2.659777 3.061127 0.195561

H 1.355849 3.377121 -0.959443

H 1.225270 -3.388968 -0.793321

H -0.480612 -3.059184 -0.440539

H 0.667602 -3.317197 0.875717

H 3.411581 -2.436826 -0.885869

H 4.235460 -1.309321 0.205907

H 3.203972 -2.606483 0.855638

C -2.638876 -0.145051 0.056158

C -3.790849 -0.948148 -0.544417

H -3.865518 -1.926368 -0.062718

H -4.735448 -0.416946 -0.399160

H -3.636017 -1.099386 -1.615648

O 3.602391 0.931748 0.122062

**100** = -205.699521

H -0.940289 1.035180 0.005247

O -1.091376 0.067639 -0.000977

N 0.172428 -0.521303 0.001020

O 1.058038 0.259104 -0.000571

**100•** = -205.083449

O -1.100473 0.141978 0.000000

N 0.000000 -0.323974 0.000000

O 1.100473 0.141499 0.000000

**101** = -965.902508

O 4.925048 -1.993108 0.159051

C -4.222453 2.767955 -0.038219

C -3.527464 -2.374359 0.185154

C -3.310110 1.536214 0.166504

C -2.975559 -0.926950 0.256400

C 3.843400 -0.111440 1.112952

C 2.620790 -1.739915 -0.327755

C -3.796498 0.209760 0.040453

C -1.093538 0.592702 0.653186

C 3.891664 -1.345963 0.310757

C 1.430705 0.136244 0.705779

C -1.965467 1.683139 0.489086

C -1.633393 -0.698565 0.555101

C 2.695633 0.580476 1.274317

C 1.477402 -1.045543 -0.141172

C -3.447268 4.087416 0.159468

C -5.378924 2.761645 0.992005

C -4.789109 2.785967 -1.479533

C -4.644770 -2.597376 1.239815

C -2.432627 -3.417385 0.497720

C -4.036255 -2.704606 -1.244191

C 0.299699 0.863907 0.972311

H -1.551251 2.677391 0.598977

H -0.990276 -1.538333 0.771348

H 2.682469 1.487058 1.874596

H 0.576620 -1.339137 -0.668172

H -2.628875 4.197458 -0.558552

H -3.039694 4.178209 1.171066

H -4.133093 4.925310 0.006310

H -6.018637 1.886572 0.882238

H -5.995004 3.656566 0.856015

H -4.983974 2.777331 2.012803

H -5.408764 1.914108 -1.685400

H -3.975774 2.815140 -2.211429

H -5.401290 3.682855 -1.620613

H -5.521752 -1.955027 1.120846

H -4.993830 -3.633426 1.193653

H -4.253720 -2.414128 2.244433

H -2.867511 -4.418902 0.437676

H -2.026521 -3.294096 1.505247

H -1.607471 -3.374285 -0.218596

H -3.224553 -2.590878 -1.967861

H -4.384685 -3.741196 -1.281537

H -4.861224 -2.078707 -1.598276

H 0.461641 1.805185 1.497313

H 2.660855 -2.604036 -0.983070

H 4.776461 0.214107 1.560618

O -5.117663 0.081317 -0.277540

H -5.340557 -0.848357 -0.371126

**101•** = -965.289995

O 6.788463 0.131853 0.254918

C -3.406538 -1.964838 0.109965

C -1.279648 2.800005 -0.151073

C -2.165387 -1.065942 0.014117

C -1.113954 1.274279 -0.090515

C 5.204768 -1.495860 -0.413578

C 4.512211 0.646081 0.646376

C -2.322334 0.415068 0.096986

C 0.270764 -0.752099 -0.185024

C 5.605783 -0.206786 0.161184

C 2.831290 -0.966330 -0.093294

C -0.908316 -1.570895 -0.133883

C 0.104185 0.672980 -0.207065

C 3.897943 -1.848567 -0.506343

C 3.210124 0.281373 0.525485

C -3.042442 -3.456007 -0.034134

C -4.403293 -1.612361 -1.023549

C -4.089948 -1.776671 1.488516

C -2.246983 3.184912 -1.299654

C 0.062579 3.511171 -0.414694

C -1.832849 3.321831 1.199990

C 1.511553 -1.416020 -0.270149

H -0.754892 -2.643037 -0.183082

H 0.980641 1.278487 -0.383845

H 3.622661 -2.808598 -0.934520

H 2.440518 0.915389 0.947431

H -2.375977 -3.796772 0.764577

H -2.572512 -3.673321 -0.998771

H -3.957399 -4.051594 0.026881

H -4.754354 -0.584635 -0.939119

H -5.268369 -2.281203 -0.968189

H -3.937341 -1.746740 -2.005224

H -4.436923 -0.752929 1.623095

H -3.398353 -2.024234 2.300356

H -4.950138 -2.450070 1.562481

H -3.243315 2.775642 -1.136980

H -2.324510 4.275343 -1.357781

H -1.869404 2.823663 -2.261835

H -0.110380 4.589921 -0.456909

H 0.507748 3.212019 -1.368948

H 0.790035 3.329237 0.383094

H -1.151184 3.071945 2.019575

H -1.922669 4.412247 1.157905

H -2.813006 2.899328 1.417314

H 1.432438 -2.475066 -0.513143

H 4.799089 1.571944 1.133609

H 6.000356 -2.151212 -0.751262

O -3.429689 0.922186 0.295744

**102** = -498.058177

O 1.743131 1.234963 -0.223927

C 2.619815 -1.034944 0.000186

C 1.389863 -1.535737 -0.160016

C 0.231903 -0.647817 -0.063527

C 0.471324 0.741103 -0.088440

C -1.084842 -1.111468 0.003669

C -0.591783 1.635340 -0.071559

C -1.902740 1.159996 -0.005456

C -2.150967 -0.213731 0.039484

H 3.509065 -1.653011 -0.067427

H 1.225442 -2.586560 -0.377984

C 2.783299 0.424741 0.334025

H 3.712879 0.827890 -0.072275

H 2.804730 0.566873 1.428650

H -1.290094 -2.176780 0.022224

H -2.729447 1.865266 0.016315

H -0.388871 2.699465 -0.112582

O -3.415855 -0.738386 0.112647

H -4.057151 -0.020655 0.123123

**102•** = -497.437022

O 1.631337 1.264819 -0.127037

C 2.586745 -1.008889 -0.019101

C 1.363539 -1.538417 -0.106974

C 0.183054 -0.679561 -0.029523

C 0.396617 0.731509 -0.048715

C -1.107997 -1.156199 0.012570

C -0.688158 1.631192 -0.059335

C -1.974734 1.156542 -0.012209

C -2.259253 -0.270647 0.034928

H 3.482616 -1.618576 -0.074864

H 1.216944 -2.603833 -0.251853

C 2.777229 0.460407 0.211165

H 3.594864 0.858024 -0.394914

H 3.021589 0.657412 1.266209

H -1.305053 -2.223648 0.018454

H -2.824658 1.830020 -0.005536

H -0.472625 2.693801 -0.093883

O -3.428329 -0.708422 0.081980

**103** = -690.790438

C -0.414275 0.267943 0.000002

C 0.977748 -0.047128 -0.000004

C -0.832904 1.633775 0.000003

C 1.948884 1.001858 -0.000005

C -1.376321 -0.786236 -0.000003

C 1.404016 -1.410799 -0.000005

C 0.166600 2.664581 0.000006

C 1.492767 2.365003 0.000000

C -0.923107 -2.147787 0.000000

C 0.404879 -2.442538 -0.000002

C -2.206433 1.913511 0.000017

C 3.311647 0.665453 -0.000009

C -2.743495 -0.445592 0.000007

C 2.779189 -1.694957 -0.000006

C -3.147590 0.890242 0.000006

C 3.717120 -0.666714 -0.000010

H -0.159759 3.700449 0.000008

H 2.233802 3.158528 0.000000

H -1.663148 -2.938794 0.000002

H 0.731909 -3.477962 0.000000

H -2.538847 2.946905 0.000019

H 4.051797 1.459819 -0.000014

H 3.105196 -2.730552 -0.000003

H -4.208050 1.129834 0.000009

H 4.775660 -0.905521 -0.000012

O -3.643032 -1.473912 -0.000016

H -4.536659 -1.115096 0.000127

**103•** = -690.176217

C -0.450944 0.228123 0.000003

C 0.948747 -0.035304 -0.000002

C -0.917336 1.579702 0.000002

C 1.882095 1.044882 0.000001

C -1.368554 -0.850885 -0.000004

C 1.418443 -1.381862 -0.000003

C 0.026904 2.632542 0.000004

C 1.379881 2.381347 0.000003

C -0.887593 -2.176750 -0.000006

C 0.463313 -2.439657 -0.000006

C -2.330441 1.826804 0.000007

C 3.260531 0.756537 0.000001

C -2.827095 -0.591627 -0.000002

C 2.811528 -1.619207 -0.000004

C -3.236532 0.813500 0.000005

C 3.713894 -0.562054 -0.000002

H -0.334798 3.656564 0.000006

H 2.088308 3.204050 0.000004

H -1.617707 -2.978849 -0.000009

H 0.821479 -3.464800 -0.000008

H -2.667212 2.860181 0.000010

H 3.972267 1.576401 0.000003

H 3.171351 -2.643467 -0.000007

H -4.304663 1.003003 0.000010

H 4.779745 -0.763674 -0.000002

O -3.653728 -1.510743 0.000002

**104** = -576.460363

C 0.003446 -1.642118 0.000050

C -1.013302 -0.525191 -0.000022

C 1.315418 -0.883860 0.000026

C -0.379608 0.730395 -0.000012

C 1.074551 0.504840 0.000006

C -2.401692 -0.604811 -0.000012

C 2.615783 -1.372979 0.000026

C -1.121839 1.913497 -0.000042

C 2.138832 1.407610 -0.000009

C -3.153066 0.576952 -0.000030

C 3.680784 -0.466980 0.000017

C -2.512604 1.818833 -0.000048

C 3.442547 0.910716 0.000003

H -0.101038 -2.289198 0.879211

H -0.101014 -2.289363 -0.878983

H 2.807880 -2.441882 0.000040

H -0.635847 2.883006 -0.000068

H 1.961033 2.478473 -0.000038

H -4.238938 0.525982 0.000027

H 4.701216 -0.835837 0.000029

H -3.114939 2.721358 -0.000069

H 4.280553 1.600075 -0.000003

O -2.970597 -1.849031 0.000082

H -3.929640 -1.761797 -0.000518

**104•** = -575.831054

C 0.016158 -1.663607 0.000122

C -1.021968 -0.577434 0.000013

C 1.311728 -0.879718 0.000022

C -0.423737 0.679974 -0.000058

C 1.038159 0.503070 -0.000062

C -2.461932 -0.730307 0.000092

C 2.624114 -1.336163 0.000003

C -1.208982 1.846394 -0.000056

C 2.077303 1.433949 -0.000157

C -3.232542 0.508001 0.000083

C 3.664652 -0.402517 -0.000082

C -2.616238 1.739055 0.000009

C 3.392759 0.968990 -0.000158

H -0.084997 -2.315959 0.876342

H -0.085002 -2.316278 -0.875847

H 2.843595 -2.399499 0.000062

H -0.741866 2.826034 -0.000115

H 1.873543 2.500132 -0.000241

H -4.312855 0.410734 0.000124

H 4.694060 -0.745204 -0.000086

H -3.214530 2.644396 0.000007

H 4.213676 1.678396 -0.000225

O -3.017808 -1.852609 0.000169

**105** = -621.631537

C 0.010779 -0.229447 -0.004517

C 1.253527 0.448728 -0.003055

C 1.211856 1.845940 -0.002873

C 0.009639 2.544100 -0.002623

C -1.191826 1.849084 -0.001667

C -1.232197 0.449039 -0.002436

H 2.135737 2.408744 -0.002623

H 0.009871 3.628844 -0.002205

H -2.113614 2.414910 0.000019

C -2.589256 -0.301048 0.000494

C -3.782919 0.679055 0.007056

H -3.789693 1.319561 -0.878995

H -4.714862 0.106206 0.009013

H -3.782381 1.314361 0.896798

C -2.745956 -1.167946 1.279508

H -3.726772 -1.654425 1.280668

H -1.996004 -1.956114 1.394268

H -2.676412 -0.536749 2.169756

C -2.754180 -1.165004 -1.279083

H -3.729751 -1.661483 -1.268436

H -2.703136 -0.530807 -2.168411

H -1.997206 -1.944351 -1.405756

C 2.601719 -0.309204 0.000996

C 3.800907 0.662221 0.004858

H 3.807939 1.303154 0.891662

H 4.726887 0.079801 0.012614

H 3.819133 1.298129 -0.885444

C 2.725969 -1.185446 1.272152

H 1.940357 -1.938294 1.325161

H 3.694484 -1.697294 1.273522

H 2.672161 -0.563813 2.171709

C 2.734675 -1.187504 -1.267969

H 2.674538 -0.568949 -2.169202

H 3.708461 -1.689200 -1.267723

H 1.956815 -1.948431 -1.318982

O 0.072924 -1.602083 -0.007089

H -0.816360 -1.962551 -0.005747

**105•** = -621.013142

C -0.000215 -0.298526 -0.002279

C 1.278549 0.448070 -0.000649

C 1.224148 1.828364 -0.001045

C 0.000292 2.513859 -0.001306

C -1.224032 1.828809 -0.001183

C -1.279010 0.448610 -0.001913

H 2.135805 2.412445 -0.000701

H 0.000502 3.599389 -0.000835

H -2.135002 2.413932 -0.000027

C -2.610124 -0.314936 0.000107

C -3.818387 0.643413 0.002373

H -3.839636 1.281775 -0.886459

H -4.738982 0.053118 0.005008

H -3.834313 1.281930 0.891152

C -2.710725 -1.199971 1.269349

H -3.678999 -1.711493 1.280022

H -1.920308 -1.949040 1.292520

H -2.643626 -0.587748 2.174543

C -2.715279 -1.202320 -1.266966

H -3.682448 -1.715777 -1.270778

H -2.654718 -0.591949 -2.173979

H -1.923010 -1.949488 -1.293667

C 2.609686 -0.315171 0.000712

C 3.817453 0.643826 0.007383

H 3.831187 1.281608 0.896747

H 4.738195 0.053790 0.012573

H 3.841424 1.282771 -0.880979

C 2.710257 -1.205444 1.266162

H 1.915764 -1.950315 1.289926

H 3.675842 -1.722009 1.270905

H 2.650276 -0.596041 2.173801

C 2.716856 -1.196738 -1.270510

H 2.648313 -0.582714 -2.174379

H 3.687962 -1.702659 -1.280086

H 1.930654 -1.950099 -1.297834

O -0.000212 -1.547812 -0.003612

**106** = -460.969504

C 2.739804 0.293883 -0.000003

C 1.776198 1.274605 -0.000004

C 0.394336 0.943937 -0.000002

C 0.027775 -0.439303 0.000002

C 1.041933 -1.431808 0.000007

C 2.369471 -1.071596 0.000004

H -0.331697 2.986513 0.000002

H 3.790594 0.564437 -0.000009

H 2.059282 2.322888 -0.000008

C -0.619433 1.940347 0.000004

C -1.360310 -0.771612 -0.000002

H 0.751023 -2.475329 0.000018

H 3.138928 -1.836343 0.000004

C -2.322498 0.215309 -0.000003

C -1.943880 1.577846 0.000004

H -3.375803 -0.052578 -0.000017

H -2.718334 2.337551 0.000011

O -1.664150 -2.103333 -0.000016

H -2.621169 -2.210132 0.000084

**106•** = -460.349259

C 2.711322 0.395178 -0.000002

C 1.690037 1.328379 0.000003

C 0.337513 0.913273 0.000003

C 0.044766 -0.479047 0.000001

C 1.092321 -1.406758 0.000000

C 2.412930 -0.977312 -0.000003

H -0.496955 2.915367 0.000006

H 3.745906 0.721615 -0.000007

H 1.916433 2.390302 0.000004

C -0.734756 1.855988 0.000004

C -1.367422 -0.939036 0.000001

H 0.842047 -2.461955 0.000002

H 3.219300 -1.703168 -0.000009

C -2.390101 0.093849 -0.000010

C -2.067445 1.439154 -0.000001

H -3.421013 -0.244085 -0.000013

H -2.857787 2.182810 0.000000

O -1.665365 -2.142862 0.000007

**107** = -615.745009

C -0.652422 -1.996881 0.517571

C 0.623774 -1.859739 -0.319686

C -1.608863 -0.863427 0.227599

C 1.229350 -0.487901 -0.126160

C -1.082821 0.425141 -0.004977

C 0.387812 0.628524 0.048400

C -2.990035 -1.061389 0.193039

C 2.617851 -0.300075 -0.119785

C -1.970020 1.473357 -0.293777

C 0.952394 1.895820 0.267480

C -3.861361 -0.007367 -0.075707

C 3.172200 0.964297 0.086836

C -3.345630 1.263597 -0.325521

C 2.332264 2.057658 0.284974

H -0.382999 -1.982990 1.583067

H -1.138452 -2.957660 0.323736

H 0.384101 -2.009890 -1.381774

H 1.348914 -2.629154 -0.048267

H -3.386109 -2.056587 0.375176

H -1.582322 2.460953 -0.517842

H 0.314095 2.752744 0.446160

H -4.932300 -0.179480 -0.103026

H 4.252080 1.089620 0.098728

H -4.011973 2.088588 -0.555031

H 2.761913 3.038201 0.460648

O 3.402219 -1.406886 -0.321390

H 4.328330 -1.148954 -0.272172

**107•** = -615.117518

C -0.667912 -2.013182 0.491799

C 0.620701 -1.890201 -0.329146

C -1.598250 -0.853199 0.215134

C 1.241141 -0.536739 -0.129820

C -1.045480 0.426354 -0.004561

C 0.431506 0.585634 0.041399

C -2.983760 -1.016578 0.186061

C 2.698536 -0.406934 -0.131187

C -1.906331 1.500264 -0.274435

C 1.039140 1.842237 0.260646

C -3.830182 0.061885 -0.065802

C 3.259589 0.917009 0.073432

C -3.286858 1.323424 -0.302627

C 2.438622 1.998923 0.269965

H -0.412302 -2.026956 1.560560

H -1.171542 -2.959194 0.274109

H 0.391293 -2.023023 -1.397019

H 1.345531 -2.663722 -0.068136

H -3.403488 -2.003578 0.358272

H -1.498947 2.482632 -0.487350

H 0.417972 2.711634 0.443808

H -4.904945 -0.084272 -0.089505

H 4.340773 1.000032 0.075435

H -3.934673 2.166437 -0.518308

H 2.859200 2.984676 0.440649

O 3.438545 -1.402257 -0.299706

**108** = -613.563226

C -2.877493 -1.202026 -0.016951

C -1.485716 -1.196246 -0.011671

C -0.746492 0.000191 -0.004167

C -1.485973 1.196518 -0.011691

C -2.877718 1.202000 -0.016937

C -3.581562 -0.000095 -0.011763

H -3.426054 -2.137236 -0.036097

H -0.980809 -2.153728 -0.014546

H -0.981276 2.154093 -0.014559

H -3.426561 2.137040 -0.036016

C 0.746489 0.000212 0.004164

C 1.485943 1.196560 0.011650

C 1.485746 -1.196207 0.011689

C 2.877694 1.202072 0.016853

H 0.981230 2.154127 0.014443

C 2.877521 -1.201950 0.017030

H 0.980864 -2.153703 0.014615

C 3.581560 0.000010 0.011781

H 3.426538 2.137113 0.035807

H 3.426084 -2.137157 0.036291

O -4.966848 -0.000091 -0.075869

H -5.325464 -0.002268 0.817850

O 4.966846 0.000213 0.075882

H 5.325473 -0.005492 -0.817818

**108•** = -612.943101

C -2.806665 -1.205053 -0.012177

C -1.418993 -1.201915 -0.012637

C -0.675364 -0.000097 -0.008586

C -1.418793 1.201818 -0.012951

C -2.806474 1.205199 -0.012438

C -3.511204 0.000143 -0.002953

H -3.357159 -2.139503 -0.028769

H -0.914313 -2.159383 -0.018449

H -0.913933 2.159202 -0.018979

H -3.356855 2.139707 -0.029147

C 0.795990 -0.000120 -0.004616

C 1.542479 1.216548 -0.001308

C 1.542623 -1.216714 -0.001704

C 2.910205 1.231502 0.004187

H 1.021894 2.166214 -0.003627

C 2.910350 -1.231510 0.003787

H 1.022173 -2.166442 -0.004360

C 3.686075 0.000042 0.007639

H 3.463869 2.164620 0.006475

H 3.464124 -2.164563 0.005763

O -4.890368 0.000422 -0.065097

H -5.258486 -0.003226 0.824859

O 4.931281 0.000118 0.013694

**109** = -460.969234

C -2.924672 0.395829 0.000334

C -1.862149 1.268065 0.000154

C -0.525949 0.787478 -0.000490

C -0.290998 -0.626282 -0.000141

C -1.413487 -1.499985 -0.000219

C -2.694605 -1.001781 0.000151

H 0.428521 2.730856 -0.000799

H -3.941722 0.773344 0.000848

H -2.031608 2.341118 0.000328

C 0.594542 1.657656 -0.000050

C 1.039977 -1.111486 -0.000400

H -1.241732 -2.572270 -0.000338

H -3.539629 -1.682762 0.000067

C 2.102425 -0.235397 0.000667

C 1.876939 1.164632 -0.000368

H 2.725003 1.845322 -0.000077

H 1.231341 -2.179109 -0.000319

O 3.368629 -0.751992 0.000064

H 4.008657 -0.032944 0.001949

**109•** = -460.343125

C -2.857930 0.432686 0.000006

C -1.765527 1.287818 0.000003

C -0.455100 0.783430 -0.000002

C -0.258407 -0.640402 -0.000002

C -1.399642 -1.492130 -0.000004

C -2.672591 -0.965287 0.000002

H 0.524141 2.723678 0.000000

H -3.862993 0.840752 0.000011

H -1.916681 2.363095 0.000005

C 0.696673 1.650924 -0.000001

C 1.050119 -1.148524 -0.000005

H -1.247100 -2.566949 -0.000011

H -3.535204 -1.622372 0.000005

C 2.210307 -0.285356 -0.000011

C 1.958868 1.159401 -0.000006

H 2.828702 1.807241 -0.000006

H 1.230828 -2.219105 -0.000007

O 3.367211 -0.752713 0.000017

**110** = -307.368080

C -1.953067 -0.528942 0.006560

C -0.557948 -0.525425 0.004977

C 0.143089 0.680333 -0.009147

C -0.557555 1.886597 -0.023371

C -1.952582 1.890798 -0.010778

C -2.647062 0.681211 0.003140

H -2.495413 -1.467916 0.019609

H -0.011853 -1.462824 0.016740

H 1.227316 0.700011 0.004054

H -2.477341 2.839821 0.001328

H -3.731923 0.686081 0.013441

O 0.136503 3.087791 0.024645

H 0.305812 3.389991 -0.873594

**110•** = -306.742088

C -1.945961 -0.516688 0.006934

C -0.537379 -0.525822 0.007368

C 0.163944 0.658392 0.006911

C -0.530456 1.934515 0.005799

C -1.982886 1.897986 0.005392

C -2.658020 0.698615 0.005977

H -2.488392 -1.456192 0.007357

H -0.009775 -1.474006 0.008184

H 1.248135 0.684656 0.007282

H -2.502162 2.850111 0.004634

H -3.742970 0.681560 0.005671

O 0.096061 3.019586 0.005420

**111** = -520.971162

C 1.152102 0.170362 0.588120

C 0.189265 0.560933 -0.601125

C 0.979099 -1.754966 -0.887727

C 0.604933 -0.474294 -1.696349

C -1.123835 0.018385 -0.055489

C 2.644002 0.383214 0.288608

C 0.830795 0.908238 1.899493

H 0.368487 -2.617398 -1.167938

H 2.023036 -2.037204 -1.043088

H 1.456417 -0.091406 -2.265903

H -0.209737 -0.640602 -2.405288

H 2.872213 1.451637 0.219598

H 3.248692 -0.026456 1.104941

H 2.976887 -0.087581 -0.637443

H 1.389692 0.465594 2.731077

H 1.130745 1.958383 1.826433

H -0.229780 0.891436 2.158600

C 0.162643 2.005915 -1.070532

H 1.149754 2.313997 -1.429082

H -0.551535 2.130658 -1.888957

H -0.143721 2.680536 -0.266350

C 0.713766 -1.330925 0.577575

H 1.201573 -1.963046 1.323622

C -0.820559 -1.237802 0.741488

H -1.354660 -2.106993 0.346173

H -1.140595 -1.115082 1.780361

N -2.242022 0.581386 -0.270046

O -3.302393 -0.145410 0.336305

H -4.067442 0.392755 0.108747

**111•** = -520.346231

C 1.131430 0.246964 0.546869

C 0.100415 0.507696 -0.621282

C 1.006689 -1.770366 -0.809359

C 0.542233 -0.557543 -1.674974

C -1.147959 -0.080408 0.016835

C 2.595471 0.524369 0.172117

C 0.819280 1.042034 1.826144

H 0.427592 -2.674525 -1.015120

H 2.055662 -2.014624 -0.991699

H 1.356245 -0.163926 -2.290460

H -0.281912 -0.806275 -2.347854

H 2.754583 1.596606 0.018841

H 3.253356 0.212190 0.990249

H 2.923460 0.007630 -0.730687

H 1.425797 0.673289 2.660304

H 1.066359 2.099015 1.685755

H -0.230418 0.990857 2.122751

C -0.044305 1.920320 -1.162908

H 0.902120 2.272678 -1.583860

H -0.797157 1.954217 -1.956292

H -0.358385 2.618366 -0.381587

C 0.783469 -1.276051 0.641541

H 1.341643 -1.833835 1.397419

C -0.744494 -1.266150 0.882521

H -1.235572 -2.191879 0.565212

H -1.014650 -1.093842 1.929458

N -2.329612 0.359989 -0.155733

O -3.441851 0.011117 0.264084

**112** = -400.755710

C 2.301704 -0.855823 0.000448

C 0.985575 -1.302981 0.000101

C -0.093011 -0.397894 -0.000208

C 0.191067 0.981298 -0.000452

C 1.512159 1.422767 -0.000308

C 2.569515 0.513345 0.000224

H 3.116509 -1.572047 0.000748

H 0.781496 -2.369735 0.000290

H 1.715967 2.488498 -0.000641

H 3.594754 0.868318 0.000374

C -1.438063 -0.991254 -0.000518

H -1.465763 -2.079822 -0.001216

N -2.622054 -0.502004 -0.000074

H -0.618253 1.695743 -0.000756

O -2.666221 0.899692 0.000491

H -3.614252 1.068795 0.002060

**112•** = -400.137954

C 2.267526 -0.835954 -0.000301

C 0.961676 -1.313313 0.000046

C -0.126432 -0.422576 0.000404

C 0.126328 0.959420 0.000519

C 1.436853 1.429665 0.000149

C 2.510108 0.538425 -0.000279

H 3.096567 -1.535723 -0.000623

H 0.776318 -2.383268 -0.000037

H 1.620009 2.498944 0.000179

H 3.528458 0.912036 -0.000598

C -1.477708 -0.989946 0.000258

H -1.602574 -2.066659 0.000441

N -2.577968 -0.322681 -0.000115

H -0.699399 1.661516 0.000848

O -2.857964 0.872200 -0.000522

**113** = -151.533605

O -1.740674 1.580547 -0.000456

H -1.950426 2.523039 0.000510

O -0.284683 1.674637 -0.000547

H -0.074930 0.732149 0.002247

**113•** = -150.905396

O -1.685448 1.606257 0.000000

H -1.973932 2.539108 0.000000

O -0.359109 1.642348 0.000000

**114** = -339.468321

C 1.760375 -0.000088 0.017660

N 1.163460 -1.194198 0.004326

C -0.171270 -1.187083 -0.012381

C -0.901683 0.000103 -0.007686

C -0.171189 1.187203 -0.012214

N 1.163601 1.194072 0.004403

H -0.681480 -2.147203 -0.035686

H 2.846151 -0.000167 0.029915

H -0.681265 2.147411 -0.035341

O -2.276347 0.000362 -0.090660

H -2.659453 -0.002866 0.793017

**114•** = -338.838243

C 1.692685 0.000007 0.000001

N 1.097129 -1.208415 0.000003

C -0.221248 -1.216360 0.000002

C -1.011888 -0.000006 -0.000001

C -0.221310 1.216377 -0.000001

N 1.097143 1.208415 0.000000

H -0.735060 -2.175141 0.000003

H 2.777776 -0.000053 -0.000002

H -0.735009 2.175240 -0.000002

O -2.262131 -0.000020 -0.000003

**115** = -382.498330

C -2.250480 0.001191 0.200425

C -1.564288 1.211000 0.080333

C -0.191516 1.214442 -0.158537

C 0.480716 -0.001008 -0.283787

C -0.193430 -1.215298 -0.157250

C -1.566243 -1.209768 0.081333

H -3.319638 0.002112 0.384475

H -2.098970 2.150433 0.171877

H 0.366741 2.138729 -0.255344

H 0.363590 -2.140447 -0.253015

H -2.102279 -2.148342 0.173630

O 1.824612 -0.002293 -0.594199

O 2.555960 0.001411 0.701048

H 3.457431 0.001215 0.348488

**115•** = -381.869249

C -2.202096 -0.000620 0.167337

C -1.514009 1.209306 0.065132

C -0.134396 1.217523 -0.138810

C 0.525162 0.000548 -0.233086

C -0.133578 -1.216859 -0.139295

C -1.513307 -1.209941 0.064446

H -3.274546 -0.000969 0.326061

H -2.048949 2.149036 0.143904

H 0.422103 2.143449 -0.223931

H 0.423570 -2.142368 -0.224786

H -2.047406 -2.150189 0.142560

O 1.917759 0.001238 -0.492675

O 2.627063 -0.001076 0.632906

**116** = -383.780434

C 0.180950 1.722058 -0.344555

C -1.148868 1.140737 0.150854

C -1.172526 -0.354243 0.019191

C -0.059456 -1.115871 -0.068269

C 1.286859 -0.541907 0.017746

C 1.372925 0.966153 0.252462

H -1.315740 1.395339 1.206584

H -1.997603 1.551639 -0.404473

H 0.216202 1.645221 -1.437162

H 0.236489 2.785605 -0.095677

H -0.119059 -2.195876 -0.180700

H 1.410455 1.119419 1.340090

H 2.325417 1.314698 -0.152724

O -2.429383 -0.853735 0.007318

O 2.289233 -1.233682 -0.058405

H -2.394268 -1.818264 -0.031819

**116•** = -383.150154

C -0.001245 1.690011 -0.368425

C -1.266931 1.045211 0.213264

C -1.285675 -0.466438 0.026804

C 0.000219 -1.148703 -0.061715

C 1.285914 -0.465763 0.025589

C 1.267314 1.046286 0.208197

H -1.324249 1.239721 1.293358

H -2.179897 1.449348 -0.229960

H -0.003507 1.578041 -1.459090

H -0.001601 2.763816 -0.162742

H 0.001031 -2.227091 -0.187776

H 1.329709 1.243238 1.287584

H 2.178085 1.450007 -0.239910

O -2.331477 -1.106406 -0.036882

O 2.331834 -1.106182 -0.033586

**117** = -304.169354

O -0.529165 -0.799638 -0.001638

O 0.123935 1.342682 -0.000280

C 1.796100 -0.421323 0.000603

C 0.414244 0.168434 -0.000838

H 1.769617 -1.510390 -0.006866

H 2.331810 -0.054495 -0.877608

H 2.323121 -0.068720 0.890138

O -1.851191 -0.239315 0.001318

H -1.635248 0.721102 0.000546

**117•** = -303.525223

O -0.686121 -0.720449 -0.000187

O 0.237380 1.399728 0.000167

C 1.690240 -0.556006 0.000051

C 0.413445 0.230192 -0.000029

H 1.729287 -1.200823 0.881920

H 1.729317 -1.201073 -0.881629

H 2.533003 0.132666 -0.000022

O -1.877974 -0.151265 -0.000030

**118** = -323.420660

C 0.190701 -1.195026 0.000209

C 0.922901 0.000542 -0.000069

C 0.225523 1.206962 -0.000144

C -1.167375 1.165150 0.000112

C -1.805115 -0.072370 -0.000259

N -1.139078 -1.233823 0.000034

H 0.755130 2.156347 0.000022

H 0.721216 -2.143387 -0.000103

H -1.746344 2.082106 0.000444

H -2.888892 -0.139913 0.000312

O 2.282860 -0.092454 -0.000113

H 2.669744 0.789693 0.000893

**118•** = -322.789217

C 0.258190 -1.209301 0.000169

C 1.029148 0.029569 0.000094

C 0.252554 1.251280 -0.000148

C -1.118829 1.168632 -0.000256

C -1.732259 -0.101096 -0.000170

N -1.058989 -1.268838 0.000048

H 0.784317 2.196610 -0.000218

H 0.812555 -2.145081 0.000331

H -1.738923 2.058814 -0.000401

H -2.815470 -0.181937 -0.000232

O 2.279702 0.014869 0.000256

**119** = -209.061690

C -1.742284 2.180282 0.086474

H -1.020715 1.594085 0.674364

N -1.394299 3.253108 -0.501197

C -3.151761 1.686076 -0.007381

H -3.742558 2.360821 -0.628221

H -3.181625 0.681683 -0.442897

H -3.607887 1.625062 0.986585

O -0.067951 3.637912 -0.361021

H 0.391482 2.981895 0.193461

**119•** = -208.445668

C -1.748983 1.940946 0.154938

H -1.123412 1.226991 0.693027

N -1.192697 2.989445 -0.320929

C -3.215371 1.694356 -0.017863

H -3.676699 2.505863 -0.583207

H -3.391375 0.753554 -0.550184

H -3.714554 1.617814 0.954011

O -0.048344 3.435576 -0.329794

**120** = -346.646055

C -1.857377 1.019335 -0.092059

C -0.491900 1.292422 -0.023819

C 0.438370 0.254507 0.087814

C -0.019328 -1.065881 0.121463

C -1.384212 -1.340200 0.043955

C -2.307925 -0.299987 -0.057449

H -2.567310 1.835221 -0.181021

H -0.146615 2.322058 -0.065777

H 0.701203 -1.872817 0.188304

H -1.727422 -2.369621 0.063528

H -3.369583 -0.515657 -0.117287

C 1.910236 0.571358 0.225570

H 2.149090 0.694895 1.293400

H 2.121709 1.528136 -0.272658

O 2.688863 -0.481317 -0.335695

H 3.600839 -0.361009 -0.055780

**120•** = -345.992618

C -1.799148 1.036888 -0.022087

C -0.428399 1.288391 -0.006043

C 0.486502 0.230585 0.019301

C 0.014492 -1.082697 0.028143

C -1.357096 -1.334859 0.010480

C -2.266822 -0.277581 -0.013590

H -2.500982 1.864179 -0.043184

H -0.069422 2.314826 -0.016630

H 0.728492 -1.898972 0.042380

H -1.715925 -2.359002 0.014704

H -3.333348 -0.475996 -0.027579

C 1.976456 0.527049 0.048351

H 2.243664 1.024483 1.009033

H 2.238037 1.310022 -0.693917

O 2.831697 -0.513275 -0.084017

**121** = -280.886305

N 0.151534 0.031394 -0.000443

O 0.212837 1.241024 -0.000094

O 1.023259 -0.786538 0.000458

O -1.153368 -0.515927 -0.000613

H -1.722559 0.271781 0.005095

**121•** = -280.233793

N -0.000040 -0.000405 0.000166

O -1.129705 0.499028 -0.000048

O 0.997088 0.728688 -0.000048

O 0.132652 -1.227362 -0.000048

**122** = -115.673209

C -2.413315 1.400106 -0.084382

H -2.006576 0.380190 -0.052592

H -1.879138 1.969898 -0.856836

H -3.464683 1.339563 -0.370621

O -2.369802 2.038881 1.185029

H -1.450029 2.103520 1.457634

**122•** = -115.017896

C -2.449338 1.443566 -0.082037

H -2.010826 0.427838 0.001577

H -1.857707 1.972640 -0.845480

H -3.491884 1.302764 -0.407685

O -2.338807 1.988127 1.163860

**123** = -194.250685

C 1.268738 -0.682049 -0.083300

H 1.303552 -1.692602 0.335907

H 2.159355 -0.138936 0.243808

H 1.299253 -0.758483 -1.174597

C 0.000002 0.049238 0.351752

H 0.000021 0.135689 1.447657

C -1.268747 -0.682034 -0.083294

H -1.303634 -1.692556 0.335977

H -2.159355 -0.138861 0.243735

H -1.299213 -0.758537 -1.174588

O 0.000001 1.364587 -0.230313

H 0.000051 2.016656 0.473666

**123•** = -193.594728

C 1.288039 -0.628385 -0.077644

H 1.313998 -1.613156 0.397731

H 2.165202 -0.058891 0.236594

H 1.337071 -0.770315 -1.161424

C 0.000023 0.127433 0.292100

H -0.000077 0.266944 1.399095

C -1.287848 -0.628705 -0.077641

H -1.313434 -1.613561 0.397572

H -2.165149 -0.059527 0.236773

H -1.336910 -0.770465 -1.161438

O -0.000248 1.424614 -0.145725

**124** = -229.039750

C -1.394990 -0.121131 -0.000108

H -1.921169 0.831146 -0.008501

H -1.674673 -0.697653 0.885417

H -1.672481 -0.712351 -0.876562

C 0.091477 0.127251 0.000031

O 0.631058 1.204678 0.000028

O 0.789029 -1.036875 0.000058

H 1.728698 -0.800279 -0.000581

**124•** = -228.376581

C -1.389486 0.002570 0.002691

H -1.765721 0.906855 0.485000

H -1.764055 -0.887836 0.511805

H -1.740340 -0.013943 -1.033434

C 0.104970 0.001204 0.007903

O 0.814318 1.038035 -0.001682

O 0.807833 -1.041500 -0.001685

**125** = -76.408434

O -1.685208 1.627906 0.000000

H -0.724718 1.667425 0.000000

H -1.968564 2.546485 0.000000

**125•** = -75.727869

O -1.679890 1.645627 0.000000

H -0.705466 1.645627 0.000000

(4) O-O BDE (**126**-**135**)

**126(A-B)** = -1070.547065

CL 2.017296 0.062508 -0.000213

O 0.447097 -0.599327 0.000452

O -0.447097 0.599327 0.000452

CL -2.017296 -0.062508 -0.000213

**126(A•)** = -535.263041

CL 0.000000 0.000000 0.517997

O 0.000000 0.000000 -1.100743

**126(B•)** = -535.263041

CL 0.000000 0.000000 0.517997

O 0.000000 0.000000 -1.100743

**127(A-B)** = -465.812208

C -1.803390 -0.001272 -0.029450

C -2.027937 -1.299626 -0.816298

H -1.841360 -2.166917 -0.176887

H -3.059866 -1.348243 -1.176442

H -1.357950 -1.352191 -1.676084

C -2.028818 1.236795 -0.907994

H -3.060098 1.257124 -1.272559

H -1.845403 2.148180 -0.332161

H -1.357042 1.228806 -1.767950

C -2.697574 0.043879 1.216287

H -2.511754 -0.822028 1.856798

H -2.510569 0.953221 1.793156

H -3.748185 0.034035 0.914329

O -0.484645 0.019962 0.549709

O 0.484779 -0.020942 -0.549709

C 1.803410 0.001356 0.029420

C 2.027376 -1.232526 0.914136

H 3.060414 -1.255360 1.273504

H 1.360026 -1.216562 1.777423

H 1.836893 -2.146370 0.344536

C 2.697686 -0.051088 -1.215989

H 2.509616 0.809450 -1.863056

H 3.748267 -0.036062 -0.914120

H 2.513043 -0.965291 -1.785870

C 2.029159 1.303327 0.809854

H 3.059811 1.350809 1.173760

H 1.847608 2.167709 0.165068

H 1.355997 1.362463 1.666758

**127(A•)** = -232.881815

C -0.000497 0.026778 0.086384

C 0.020880 -1.387740 -0.580310

H -0.860464 -1.961173 -0.288325

H 0.018441 -1.247210 -1.664686

H 0.919691 -1.933760 -0.288922

C 1.265635 0.811090 -0.315185

H 1.289464 0.990064 -1.394285

H 1.282302 1.778743 0.193693

H 2.160613 0.254809 -0.026849

C -1.289242 0.773217 -0.315435

H -2.167642 0.190033 -0.029318

H -1.335578 1.739118 0.194926

H -1.317185 0.953412 -1.394274

O 0.003713 -0.263014 1.430665

**127(B•)** = -232.881815

C -0.000497 0.026778 0.086384

C 0.020880 -1.387740 -0.580310

H -0.860464 -1.961173 -0.288325

H 0.018441 -1.247210 -1.664686

H 0.919691 -1.933760 -0.288922

C 1.265635 0.811090 -0.315185

H 1.289464 0.990064 -1.394285

H 1.282302 1.778743 0.193693

H 2.160613 0.254809 -0.026849

C -1.289242 0.773217 -0.315435

H -2.167642 0.190033 -0.029318

H -1.335578 1.739118 0.194926

H -1.317185 0.953412 -1.394274

O 0.003713 -0.263014 1.430665

**128(A-B)** = -356.019889

O -1.750748 0.031336 -0.138169

H -1.969073 0.322282 0.762286

O -0.626489 -0.776058 0.052790

N 0.630779 0.076961 0.000705

O 1.596957 -0.620748 -0.014787

O 0.474483 1.257843 0.004263

**128(A•)** = -75.727868

O 0.000000 0.000000 0.108268

H 0.000000 0.000000 -0.866144

**128(B•)** = -280.233529

O -0.633707 -1.055698 0.000035

N 0.025148 -0.000015 -0.000125

O 1.244530 -0.000490 0.000038

O -0.632828 1.056201 0.000035

**129(A-B)** = -304.162032

O 1.732297 0.122007 -0.000240

H 2.443154 -0.533993 -0.000159

O 0.605928 -0.803384 -0.000196

C -0.595932 -0.135070 0.000030

O -1.574560 -0.827675 0.000094

C -0.557211 1.368776 0.000283

H -0.024627 1.737617 0.879784

H -0.024866 1.737897 -0.879246

H -1.584126 1.728649 0.000478

**129(A•)** = -75.727868

O 0.000000 0.000000 0.108268

H 0.000000 0.000000 -0.866141

**129(B•)** = -228.377513

O -0.803790 1.044039 0.000025

C -0.105060 -0.001990 -0.000131

O -0.818640 -1.036449 0.000029

C 1.389822 -0.008901 0.000030

H 1.754058 0.518512 -0.885492

H 1.753739 0.520455 0.884517

H 1.763072 -1.034335 0.001144

**130(A-B)** = -308.673733

C 0.385301 0.000322 0.028111

C 0.385004 1.276936 0.878667

H -0.488233 1.307640 1.532759

H 1.284411 1.314339 1.500038

H 0.368768 2.161311 0.235956

C 0.384132 -1.261562 0.900364

H -0.492319 -1.282740 1.550403

H 0.373240 -2.156782 0.272729

H 1.280733 -1.285958 1.526463

C 1.565499 -0.008650 -0.951220

H 1.537593 -0.901009 -1.581542

H 1.542129 0.875557 -1.593102

H 2.504530 -0.007605 -0.391725

O -0.742277 -0.007113 -0.869723

O -1.960920 -0.000447 -0.056718

H -2.604895 -0.006551 -0.775983

**130(A•)** = -232.881803

C 0.013812 -0.023693 -0.086939

C -0.441156 1.314789 0.581514

H -1.473295 1.544553 0.311897

H -0.367294 1.194293 1.666282

H 0.204576 2.137699 0.268883

C -0.949695 -1.157793 0.328111

H -1.974975 -0.902600 0.051181

H -0.673726 -2.086079 -0.179769

H -0.901941 -1.330744 1.407636

C 1.470028 -0.340304 0.299899

H 1.804643 -1.247685 -0.211179

H 2.127201 0.481119 0.002655

H 1.570430 -0.499131 1.378117

O -0.109194 0.243823 -1.428901

**130(B•)** = -75.727868

O 0.000000 0.000000 0.108268

H 0.000000 0.000000 -0.866140

**131(A-B)** = -250.677265

O -1.074551 -0.348098 -0.000002

H -1.808367 0.288982 0.000002

O 0.021461 0.594725 -0.000002

F 1.137010 -0.251333 0.000003

**131(A•)** = -75.727868

O 0.000000 0.000000 0.108268

H 0.000000 0.000000 -0.866141

**131(B•)** = -174.893036

O 0.000000 0.000000 -0.714688

F 0.000000 0.000000 0.635278

**132(A-B)** = -190.810075

O 1.136720 -0.337004 0.000002

H 1.865663 0.297644 -0.000013

O 0.020356 0.603256 0.000002

C -1.133025 -0.208517 -0.000001

H -1.178715 -0.837765 0.898176

H -1.966724 0.499016 -0.000030

H -1.178682 -0.837804 -0.898153

**132(A•)** = -75.727868

O 0.000000 0.000000 -0.108268

H 0.000000 0.000000 0.866141

**132(B•)** = -115.017874

O -0.790767 -0.000353 0.007677

C 0.573145 -0.000988 0.014223

H 1.010657 -0.922991 0.427837

H 0.869055 0.034572 -1.055537

H 1.007554 0.897170 0.480944

**133(A-B)** = -825.693824

C 1.731773 0.003336 -0.000044

F 1.955484 -0.745770 -1.075295

F 2.546884 1.047291 -0.001521

F 1.951407 -0.739420 1.080514

O 0.462081 0.560134 -0.004356

O -0.462092 -0.560142 -0.005891

C -1.731774 -0.003339 -0.000012

F -1.957139 0.745653 -1.075065

F -1.949730 0.739542 1.080736

F -2.546896 -1.047285 -0.000224

**133(A•)** = -412.816727

C -0.011065 0.010150 0.034774

F -0.878437 -0.640805 -0.744722

F 0.565133 1.008691 -0.638878

F 0.946595 -0.846095 0.402882

O -0.704152 0.530373 1.077227

**133(B•)** = -412.816727

C -0.011065 0.010150 0.034774

F -0.878437 -0.640805 -0.744722

F 0.565133 1.008691 -0.638878

F 0.946595 -0.846095 0.402882

O -0.704152 0.530373 1.077227

**134(A-B)** = -349.816204

F 0.729963 1.520355 0.000000

O 0.729963 0.125113 0.000000

O -0.729963 -0.125113 0.000000

F -0.729963 -1.520355 0.000000

**134(A•)** = -174.893036

F 0.000000 0.000000 0.635281

O 0.000000 0.000000 -0.714692

**134(B•)** = -174.893036

F 0.000000 0.000000 0.635281

O 0.000000 0.000000 -0.714692

**135(A-B)** = -151.533596

O 0.000000 0.729480 0.000000

H 0.954028 0.878080 0.000000

O 0.000000 -0.729480 0.000000

H -0.954028 -0.878080 0.000000

**135(A•)** = -75.727868

O 0.000000 0.000000 -0.108268

H 0.000000 0.000000 0.866141

**135(B•)** = -75.727868

O 0.000000 0.000000 -0.108268

H 0.000000 0.000000 0.866141

(5) O-C BDE (**136**-**160**)

**136(A-B)** = -523.315338

C -0.012759 -1.949014 -1.212697

C -1.267512 -1.075159 -1.090706

C -1.285364 -0.227507 0.203394

C 1.281678 -0.242656 0.204102

C 1.252721 -1.090802 -1.089450

H -1.310032 -0.392308 -1.946616

H -2.172930 -1.692312 -1.126649

H -0.018423 -2.736593 -0.449948

H -0.015600 -2.464436 -2.179168

H 1.302812 -0.408238 -1.945155

H 2.150552 -1.718840 -1.125989

N 0.002848 0.539498 0.385105

C 2.447231 0.762045 0.132279

H 2.467886 1.394175 1.025500

H 3.391657 0.212458 0.083605

H 2.377173 1.398829 -0.749484

C 1.542751 -1.119398 1.447931

H 2.594862 -1.417961 1.449423

H 1.347982 -0.552519 2.361782

H 0.951700 -2.032773 1.474923

C -2.437731 0.792282 0.135583

H -3.389355 0.255480 0.085476

H -2.448677 1.421849 1.030856

H -2.359728 1.431667 -0.743559

C -1.555383 -1.103907 1.446133

H -1.338134 -0.546334 2.360677

H -2.614209 -1.377295 1.456992

H -0.986162 -2.031610 1.462206

O 0.009084 1.534290 -0.672820

C 0.019348 2.854908 -0.143197

H 0.914605 3.380991 -0.496244

H -0.871176 3.392959 -0.490199

H 0.022701 2.827248 0.948166

**136(A•)** = -483.453382

C -0.001007 -2.126329 0.011913

C -1.244222 -1.394725 -0.494627

C -1.328460 0.071935 -0.027697

C 1.328947 0.071841 -0.027228

C 1.243792 -1.395836 -0.491988

H -1.239386 -1.414650 -1.591439

H -2.160133 -1.902312 -0.173829

H -0.002078 -2.186828 1.105903

H -0.000937 -3.157870 -0.354818

H 1.240823 -1.417283 -1.588782

H 2.158496 -1.904007 -0.168837

N 0.000413 0.751655 -0.204960

C 2.347522 0.823570 -0.899412

H 2.448795 1.859036 -0.573636

H 3.321199 0.329798 -0.826927

H 2.033077 0.820854 -1.946723

C 1.756118 0.171183 1.452777

H 2.789591 -0.171322 1.561774

H 1.697236 1.210721 1.782915

H 1.128040 -0.437354 2.107611

C -2.346713 0.826433 -0.898168

H -3.318294 0.327468 -0.833331

H -2.454245 1.858902 -0.564888

H -2.028441 0.833677 -1.944255

C -1.756110 0.168360 1.452575

H -1.687631 1.205586 1.788066

H -2.793026 -0.164463 1.558858

H -1.135126 -0.449468 2.105104

O -0.000008 2.024916 -0.059614

**136(B•)** = -39.801328

C 0.000013 -0.000173 0.000274

H 0.950798 -0.515192 -0.000549

H -0.922267 -0.564656 -0.000549

H -0.028607 1.080884 -0.000548

**137(A-B)** = -424.000426

O 0.846923 -0.595669 0.068367

C -0.469029 -0.238467 0.025282

C -0.935674 1.080160 0.054522

H -0.249908 1.915966 0.113263

C -2.311533 1.324462 0.003768

H -2.663931 2.350654 0.027144

C -3.222341 0.276655 -0.076870

H -4.287341 0.476093 -0.115960

C -2.746423 -1.037957 -0.107975

H -3.443824 -1.866977 -0.171246

C -1.383538 -1.298199 -0.057252

H -1.001097 -2.312535 -0.080276

C 1.824960 0.434511 0.203833

C 3.170107 -0.215274 0.324149

C 4.218433 0.101268 -0.430137

H 1.799070 1.109715 -0.661680

H 1.610910 1.024421 1.107728

H 3.256680 -0.970477 1.102108

H 5.184766 -0.369077 -0.284154

H 4.149517 0.844620 -1.219785

**137(A•)** = -306.742092

O 2.300337 -0.000439 -0.001058

C 1.047225 -0.000052 0.001153

C 0.290325 1.240174 0.000854

H 0.857645 2.164509 -0.000214

C -1.085772 1.224807 0.000052

H -1.643183 2.155894 -0.001721

C -1.781982 0.000335 -0.000451

H -2.866851 0.000738 -0.001801

C -1.086380 -1.224663 0.000258

H -1.644209 -2.155459 -0.000079

C 0.289633 -1.240088 0.000270

H 0.855608 -2.165247 -0.000539

**137(B•)** = -117.188167

C -1.228131 0.196352 0.000111

C 0.000218 -0.442859 0.000050

C 1.227853 0.196213 -0.000017

H -1.295426 1.279751 0.000271

H -2.155548 -0.363417 -0.000628

H -0.000072 -1.531810 -0.000233

H 2.156012 -0.362412 0.000340

H 1.295393 1.279649 -0.000615

**138(A-B)** = -500.237322

C 0.849311 2.303853 -0.000018

C -0.513426 2.152418 0.000025

C -1.086036 0.850228 0.000018

C -0.232212 -0.296067 -0.000044

C 1.186946 -0.094564 -0.000106

C 1.713703 1.180959 -0.000089

H -3.141041 1.518578 0.000126

H 1.287399 3.296414 -0.000006

H -1.168248 3.017591 0.000072

C -2.492045 0.648121 0.000073

C -0.809071 -1.592077 -0.000054

H 2.783734 1.343155 -0.000143

C -2.176225 -1.749115 -0.000009

C -3.026218 -0.618973 0.000059

H -0.153382 -2.453914 -0.000086

H -2.607267 -2.744635 -0.000022

H -4.102468 -0.756263 0.000097

O 1.928881 -1.235411 -0.000199

C 3.342436 -1.118888 0.000232

H 3.724707 -2.139591 0.000554

H 3.701571 -0.596895 -0.894880

H 3.700975 -0.596519 0.895360

**138(A•)** = -460.349271

C 2.067648 1.438144 -0.000015

C 0.734961 1.856680 0.000009

C -0.337104 0.914197 0.000007

C -0.044730 -0.478197 0.000025

C 1.366987 -0.939055 0.000061

C 2.390910 0.092778 -0.000006

H -1.917611 2.390375 -0.000007

H 2.858064 2.182108 -0.000034

H 0.498972 2.916309 -0.000001

C -1.690046 1.328664 -0.000002

C -1.091481 -1.406659 0.000006

H 3.421517 -0.244922 -0.000048

C -2.412425 -0.977350 -0.000008

C -2.710943 0.395262 -0.000013

H -0.841939 -2.461983 0.000012

H -3.218035 -1.703902 -0.000015

H -3.745050 0.723147 -0.000024

O 1.662677 -2.143489 -0.000033

**138(B•)** = -39.801328

C -0.000011 -0.000176 -0.000484

H -0.949919 -0.516833 0.000968

H 0.923262 -0.563039 0.000968

H 0.026721 1.080929 0.000966

**139(A-B)** = -244.973343

C -1.303655 0.417740 -0.000810

H -2.318963 0.027698 -0.003981

H -1.121662 1.025466 -0.890464

H -1.127349 1.024851 0.890597

O -0.467244 -0.751417 0.001915

N 0.913141 -0.513481 -0.002280

O 1.216983 0.627655 0.001169

-39.801326

C 0.000005 -0.000177 0.000345

H -0.931923 -0.548582 -0.000690

H 0.941736 -0.531564 -0.000690

H -0.009844 1.081206 -0.000689

**139(B•)** = -205.083460

O -1.100928 -0.141046 0.000000

N 0.000000 0.323900 0.000000

O 1.100928 -0.142367 0.000000

**140(A-B)** = -500.236044

C -3.145748 -0.986216 0.000706

C -1.869833 -1.494982 -0.000043

C -0.739138 -0.629340 -0.000521

C -0.962151 0.786545 -0.000405

C -2.295610 1.278171 0.000192

C -3.364253 0.414792 0.000915

H 0.770361 -2.190774 -0.000631

H -3.996863 -1.659448 0.000988

H -1.706462 -2.568487 -0.000296

C 0.585710 -1.121590 -0.000755

C 0.165467 1.642942 -0.000648

H -2.456538 2.352442 0.000375

H -4.378372 0.799994 0.001377

C 1.449363 1.145286 -0.000836

C 1.664103 -0.257728 -0.000911

H 0.008580 2.717603 -0.000367

H 2.286535 1.831837 -0.001123

O 2.902328 -0.830851 -0.000923

C 4.043448 0.010962 0.002026

H 4.077487 0.644897 0.896329

H 4.904482 -0.656973 0.005927

H 4.084008 0.642670 -0.893517

**140(A•)** = -460.343137

C -2.672691 -0.965149 -0.000003

C -1.399524 -1.492073 0.000003

C -0.257952 -0.640273 0.000002

C -0.455816 0.783422 0.000004

C -1.765934 1.287788 -0.000002

C -2.858616 0.432346 -0.000005

H 1.231519 -2.219443 0.000011

H -3.535126 -1.622854 -0.000004

H -1.247229 -2.566965 0.000004

C 1.050460 -1.148770 0.000009

C 0.696648 1.650588 0.000002

H -1.917859 2.363024 -0.000003

H -3.863741 0.840569 -0.000011

C 1.959184 1.159471 0.000005

C 2.211242 -0.285344 0.000002

H 0.523553 2.723488 0.000004

H 2.828914 1.807616 0.000000

O 3.367246 -0.752184 -0.000013

**140(B•)** = -39.801327

C 0.000007 0.000173 0.000185

H -0.929274 0.553055 -0.000370

H 0.944266 0.527058 -0.000370

H -0.015036 -1.081149 -0.000370

**141(A-B)** = -346.636578

C -1.583241 1.206800 0.083635

C -0.211198 1.210902 -0.166904

C 0.471743 -0.000268 -0.291480

C -0.211678 -1.211160 -0.166590

C -1.583695 -1.206483 0.083923

C -2.271848 0.000321 0.213013

H -2.115289 2.148339 0.172968

H 0.335004 2.140737 -0.284777

H 0.334240 -2.141195 -0.284201

H -2.116135 -2.147776 0.173506

H -3.339239 0.000534 0.405358

O 1.820003 -0.000657 -0.583242

C 2.664966 0.000356 0.565167

H 2.499538 -0.892111 1.182107

H 3.691459 -0.000357 0.196229

H 2.500098 0.894268 1.180162

**141(A•)** = -306.742089

C -1.086245 1.224291 0.000004

C 0.289995 1.239482 0.000068

C 1.048089 0.000004 -0.000086

C 0.290001 -1.239479 0.000037

C -1.086236 -1.224298 0.000027

C -1.782732 -0.000002 -0.000050

H -1.643525 2.155356 0.000010

H 0.854804 2.165339 0.000057

H 0.854828 -2.165326 0.000045

H -1.643520 -2.155359 0.000054

H -2.867571 -0.000010 -0.000081

O 2.300969 0.000001 -0.000011

**141(B•)** = -39.801327

C 0.000014 -0.000181 -0.000403

H -0.924655 -0.560754 0.000806

H 0.948639 -0.519150 0.000807

H -0.024069 1.080991 0.000805

**142(A-B)** = -232.316758

C -2.447094 -0.287302 0.039066

H -3.368800 0.274414 -0.033222

H -2.499545 -1.358966 0.190019

C -1.279764 0.343642 -0.073285

H -1.220052 1.422044 -0.222574

O -0.087256 -0.306102 -0.039967

C 1.065745 0.526607 0.106697

H 1.050138 1.314317 -0.659572

H 1.046535 1.010697 1.092548

C 2.302042 -0.340601 -0.041442

H 3.202171 0.269823 0.073809

H 2.315949 -1.124919 0.719075

H 2.326073 -0.812668 -1.026559

**142(A•)** = -153.133357

C -1.166412 -0.171035 0.000022

H -2.061447 0.441115 0.000022

H -1.264555 -1.251634 -0.000072

C 0.131673 0.407633 -0.000037

H 0.189283 1.512962 0.000028

O 1.168144 -0.265254 0.000014

**142(B•)** = -79.089757

C -0.794077 0.000010 -0.020564

H -1.350603 0.927410 0.045692

H -1.350374 -0.927523 0.045716

C 0.693212 0.000023 -0.001747

H 1.092805 -0.001193 1.026837

H 1.106631 -0.886780 -0.493204

H 1.106731 0.887888 -0.491177

**143(A-B)** = -384.721501

C -1.724722 1.367348 -0.064983

C -0.363138 1.062585 -0.113505

C 0.038686 -0.273854 -0.058846

C -0.908657 -1.297090 0.023725

C -2.261957 -0.977857 0.062060

C -2.677602 0.355277 0.023663

H -2.036454 2.405682 -0.109458

H 0.371851 1.852502 -0.217806

H -0.567616 -2.325546 0.058082

H -2.995745 -1.774341 0.127480

H -3.733405 0.599948 0.056611

O 1.356168 -0.664376 -0.127294

C 2.320728 0.187287 0.341037

H 2.002268 0.844370 1.147244

C 3.566088 0.150347 -0.120458

H 3.851708 -0.514828 -0.926514

H 4.321497 0.782962 0.326561

**143(A•)** = -231.470881

C 1.211981 0.632351 -0.000015

C 1.224465 -0.770904 0.000005

C 0.000555 -1.397536 0.000001

C -1.223778 -0.771749 0.000001

C -1.212573 0.631549 -0.000008

C -0.000521 1.324165 -0.000002

H 2.152044 1.176673 -0.000007

H 2.159262 -1.323311 0.000024

H -2.158052 -1.325024 0.000014

H -2.153125 1.175037 -0.000006

H -0.000902 2.409367 0.000086

**143(B•)** = -153.133378

O -1.168927 -0.265095 0.000016

C -0.132911 0.406654 -0.000079

H -0.189720 1.511707 0.000208

C 1.168246 -0.171218 0.000022

H 1.270265 -1.251162 0.000039

H 2.058860 0.447594 -0.000034

**144(A-B)** = -384.721502

C -1.724709 1.367321 -0.064990

C -0.363064 1.062544 -0.113488

C 0.038666 -0.273844 -0.058730

C -0.908703 -1.297076 0.023756

C -2.261974 -0.977855 0.062070

C -2.677601 0.355331 0.023672

H -2.036349 2.405693 -0.109635

H 0.371828 1.852561 -0.217888

H -0.567626 -2.325538 0.058021

H -2.995774 -1.774349 0.127389

H -3.733403 0.600054 0.056587

O 1.356175 -0.664456 -0.127367

C 2.320704 0.187357 0.340938

H 2.002054 0.844475 1.147058

C 3.566123 0.150333 -0.120374

H 3.851757 -0.515041 -0.926274

H 4.321457 0.783120 0.326552

**144(A•)** = -306.742088

C -1.086087 1.224273 -0.000019

C 0.290149 1.239365 0.000001

C 1.048057 -0.000041 -0.000015

C 0.289948 -1.239355 -0.000002

C -1.086271 -1.224230 -0.000013

C -1.782744 0.000079 0.000000

H -1.643329 2.155478 -0.000003

H 0.854885 2.165336 0.000048

H 0.854788 -2.165258 0.000032

H -1.643461 -2.155474 0.000006

H -2.867692 0.000113 0.000124

O 2.300813 -0.000093 0.000010

**144(B•)** = -77.860816

C -0.707039 0.143734 -0.000001

H -1.601604 -0.463081 0.000003

C 0.587186 -0.029248 0.000001

H 1.286248 0.804968 0.000000

H 1.034474 -1.028799 -0.000002

**145(A-B)** = -538.331177

O 0.000246 -1.190846 0.000341

C -1.197408 -0.504759 0.036888

C -1.380660 0.645854 0.807554

H -0.549058 1.064912 1.362468

C -2.640747 1.239238 0.855082

H -2.784355 2.131621 1.455516

C -3.713167 0.691310 0.150386

H -4.690940 1.157974 0.194818

C -3.518243 -0.463335 -0.607312

H -4.345162 -0.899539 -1.157965

C -2.262018 -1.063584 -0.669718

H -2.091448 -1.961128 -1.253284

C 1.197196 -0.504982 -0.036622

C 1.380494 0.645861 -0.807246

C 2.262296 -1.063429 0.669714

C 2.640439 1.239298 -0.855179

C 3.518419 -0.463166 0.606932

C 3.713133 0.691431 -0.150851

H 0.548544 1.064946 -1.361681

H 2.091890 -1.960962 1.253406

H 2.783767 2.131711 -1.455622

H 4.345494 -0.899337 1.157371

H 4.690889 1.158148 -0.195529

**145(A•)** = -306.742094

O 2.300432 -0.000127 -0.000894

C 1.047340 -0.000043 0.000919

C 0.290128 1.240051 0.000765

H 0.856886 2.164725 -0.000095

C -1.085955 1.224758 0.000075

H -1.643589 2.155684 -0.001647

C -1.782091 0.000185 -0.000414

H -2.866958 0.000375 -0.001446

C -1.086235 -1.224673 0.000242

H -1.643884 -2.155594 -0.000063

C 0.289831 -1.240118 0.000193

H 0.855984 -2.165134 -0.000274

**145(B•)** = -231.470874

C -0.000822 -1.397049 -0.000397

C -1.224900 -0.771261 0.000715

C 1.224025 -0.772131 -0.000051

C -1.212010 0.632690 0.000215

C 1.212951 0.631457 0.000541

C 0.000672 1.323934 -0.000243

H -2.160006 -1.321635 -0.001467

H 2.157887 -1.324736 -0.000916

H -2.151528 1.177102 -0.000966

H 2.153079 1.174768 -0.000009

H 0.001080 2.408657 -0.001327

**146(A-B)** = -320.159160

C -1.765596 0.004930 0.000249

H -2.538792 -0.762979 -0.006249

H -1.840918 0.629914 -0.891262

H -1.846001 0.619908 0.898369

O -0.547977 -0.755934 -0.000409

N 0.623041 0.048718 0.000057

O 1.632079 -0.600000 0.000230

O 0.473149 1.248754 -0.000165

**146(A•)** = -39.801326

C -0.000005 -0.000176 0.000364

H -0.942362 -0.530444 -0.000728

H 0.931254 -0.549702 -0.000728

H 0.011137 1.081201 -0.000727

**146(B•)** = -280.233717

O -0.625938 1.062509 0.000013

N 0.013254 0.000042 -0.000044

O -0.624472 -1.063369 0.000013

O 1.238812 0.000823 0.000013

**147(A-B)** = -154.944828

C 1.170503 0.195657 0.000025

H 2.021680 -0.487617 0.001496

H 1.227614 0.838801 0.892267

H 1.229104 0.836577 -0.893759

O -0.000002 -0.590429 0.000004

C -1.170505 0.195660 -0.000019

H -1.227359 0.839076 -0.892101

H -2.021674 -0.487627 -0.001904

H -1.229338 0.836318 0.893936

**147(A•)** = -39.801326

C -0.000005 -0.000177 -0.000345

H 0.931923 -0.548582 0.000690

H -0.941736 -0.531564 0.000690

H 0.009844 1.081206 0.000689

**147(B•)** = -115.017872

O 0.790764 -0.000152 -0.007690

C -0.573146 -0.000250 -0.014253

H -0.868975 0.007877 1.056096

H -1.008175 0.907877 -0.460405

H -1.010088 -0.913037 -0.448659

**148(A-B)** = -268.309206

C 1.802904 -0.522749 0.000501

H 1.704601 -1.607173 -0.018954

H 2.352257 -0.215354 0.893541

H 2.371707 -0.183508 -0.868292

C 0.458453 0.166835 -0.000996

O 0.297376 1.362827 -0.000191

O -0.559203 -0.720873 -0.001476

C -1.879341 -0.153011 0.000857

H -2.026837 0.479406 -0.876961

H -2.561769 -1.000890 -0.018788

H -2.037441 0.445438 0.900617

**148(A•)** = -228.377498

C 1.389701 -0.006457 -0.000007

H 1.761779 -1.032125 -0.017060

H 1.753715 0.506696 0.893860

H 1.754597 0.536377 -0.875744

C -0.105036 -0.000762 -0.000401

O -0.807027 1.041939 0.000039

O -0.815233 -1.037893 0.000135

**148(B•)** = -39.801330

C -0.000020 -0.000178 -0.000387

H -0.957555 -0.502531 0.000773

H 0.914717 -0.576807 0.000773

H 0.042959 1.080407 0.000772

**149(A-B)** = -576.751420

C -2.120446 -0.120785 0.690846

C -0.813890 0.311561 0.458409

C -0.632475 1.488711 -0.254188

C -1.688254 2.257879 -0.724574

C -2.987240 1.808939 -0.482882

C -3.202424 0.623211 0.219842

H -2.287973 -1.034456 1.249586

H 0.038718 -0.240961 0.837066

H -1.501554 3.189351 -1.247388

H -3.828128 2.394934 -0.835784

H -4.214261 0.284192 0.409754

O 0.689493 1.974665 -0.430235

C 1.406702 1.688680 -1.508463

C 0.890946 0.862800 -2.535331

C 2.690265 2.293647 -1.471606

C 1.500600 0.476748 -3.712167

H -0.114527 0.489751 -2.367713

C 3.705018 2.238448 -2.400269

H 2.869702 2.879694 -0.574605

C 2.777979 0.786516 -4.221223

H 0.897143 -0.166907 -4.346616

C 3.755538 1.568714 -3.640951

H 4.599331 2.796678 -2.137714

H 3.015570 0.352564 -5.187872

H 4.678595 1.685285 -4.200856

**149(A•)** = -306.742089

C 1.086252 -1.224289 0.000003

C -0.289988 -1.239482 0.000068

C -1.048089 -0.000008 -0.000086

C -0.290008 1.239479 0.000037

C 1.086229 1.224300 0.000027

C 1.782732 0.000008 -0.000050

H 1.643529 -2.155357 0.000011

H -0.854802 -2.165336 0.000058

H -0.854830 2.165329 0.000043

H 1.643517 2.155359 0.000054

H 2.867571 0.000017 -0.000081

O -2.300969 -0.000007 -0.000011

**149(B•)** = -269.875399

C -0.001119 1.556895 0.001869

C 1.281081 1.072578 -0.005742

C -1.282577 1.071084 0.005499

C 1.594802 -0.292548 0.001749

H 2.104550 1.784833 -0.013560

C -1.594353 -0.294422 -0.004885

H -2.106493 1.782870 0.014062

C 0.700309 -1.370532 0.004598

H 2.652378 -0.543759 0.002407

C -0.698409 -1.370837 -0.002539

H -2.651365 -0.547865 -0.010322

H 1.161427 -2.354378 0.009579

H -1.158907 -2.355003 -0.005459

**150(A-B)** = -115.673209

C 0.665036 -0.019860 0.000001

H 1.082667 0.988377 -0.000818

H 1.031867 -0.544508 -0.892664

H 1.032007 -0.543108 0.893436

O -0.749634 0.121914 0.000001

H -1.139687 -0.756910 0.000030

**150(A•)** = -39.801326

C -0.000005 0.000177 0.000345

H 0.931923 0.548582 -0.000690

H -0.941736 0.531564 -0.000690

H 0.009844 -1.081206 -0.000689

**150(B•)** = -75.727868

O 0.000000 0.000000 -0.108268

H 0.000000 0.000000 0.866141

**151(A-B)** = -154.962431

C 1.225846 -0.223185 -0.000012

H 2.074814 0.467838 -0.001737

H 1.292840 -0.859918 -0.886184

H 1.294504 -0.857421 0.887829

C -0.084637 0.548332 0.000016

H -0.137462 1.193955 -0.888977

H -0.137419 1.193970 0.888992

O -1.155808 -0.396895 0.000025

H -1.988064 0.085852 -0.000145

**151(A•)** = -79.089756

C 0.693220 -0.000014 -0.001762

H 1.092614 0.002069 1.026891

H 1.106782 0.886344 -0.493852

H 1.106676 -0.888379 -0.490296

C -0.794054 0.000009 -0.020643

H -1.350539 0.927420 0.045861

H -1.350529 -0.927427 0.045829

**151(B•)** = -75.727868

O 0.000000 0.000000 0.108268

H 0.000000 0.000000 -0.866140

**152(A-B)** = -310.921366

C 1.161107 -1.266867 0.217789

C -0.323204 -1.263554 -0.181322

C -1.039967 -0.000216 0.305250

C -0.323948 1.263376 -0.181373

C 1.160359 1.267194 0.217719

C 1.876853 0.000329 -0.272802

H -0.418006 -1.304121 -1.273698

H -0.835533 -2.146613 0.214777

H 1.244851 -1.327864 1.311457

H 1.651336 -2.161179 -0.180988

H -0.418171 1.303781 -1.273769

H -0.836236 2.146476 0.214726

H 1.650642 2.161577 -0.180817

H 1.244635 1.328009 1.311395

H 1.900159 0.000129 -1.370539

H 2.919218 0.000492 0.063935

H -1.042495 -0.000273 1.405835

O -2.392028 -0.000381 -0.180372

H -2.991379 0.001063 0.569104

**152(A•)** = -235.048435

C 1.268541 0.711449 0.242701

C 1.288012 -0.779450 -0.158542

C -0.001622 -1.463222 0.165356

C -1.289275 -0.776924 -0.159806

C -1.267060 0.713112 0.244223

C 0.001003 1.411227 -0.269066

H 1.474716 -0.835257 -1.248393

H 2.130401 -1.294037 0.315625

H 1.303914 0.788263 1.336629

H 2.164183 1.211624 -0.141751

H -1.474231 -0.829507 -1.250184

H -2.133837 -1.290259 0.311869

H -2.162344 1.216060 -0.137430

H -1.299618 0.787940 1.338401

H -0.000039 1.404735 -1.368051

H 0.002301 2.462896 0.038184

H -0.003040 -2.519609 0.415908

**152(B•)** = -75.727868

O 0.000000 0.000000 -0.108267

H 0.000000 0.000000 0.866138

**153(A-B)** = -323.436767

C -0.999861 -1.228105 -0.000342

C -1.815387 -0.104427 -0.000386

C -1.199244 1.152177 0.000083

C 0.183731 1.236216 0.000113

C 0.903153 0.032413 -0.000254

N 0.339797 -1.169325 0.000378

H -1.796735 2.057777 0.000859

H -1.426579 -2.227119 0.001633

H -2.893749 -0.206180 -0.000114

H 0.709639 2.182748 0.000921

O 2.254186 0.085135 -0.000303

H 2.561000 -0.832671 0.001193

**153(A•)** = -247.529611

C -1.313482 0.294126 -0.000195

C -0.320148 1.267404 -0.000106

C 1.020761 0.867383 0.000117

C 1.333813 -0.493268 0.000209

C 0.240770 -1.353967 0.000083

N -0.997520 -1.016617 -0.000084

H 1.814432 1.608669 0.000255

H -2.367983 0.550427 -0.000366

H -0.590193 2.317202 -0.000247

H 2.356100 -0.850041 0.000302

**153(B•)** = -75.727868

O 0.000000 0.000000 -0.108268

H 0.000000 0.000000 0.866141

**154(A-B)** = -268.309206

C 1.802904 -0.522749 0.000501

H 1.704601 -1.607173 -0.018954

H 2.352257 -0.215354 0.893541

H 2.371707 -0.183508 -0.868292

C 0.458453 0.166835 -0.000996

O 0.297376 1.362827 -0.000191

O -0.559203 -0.720873 -0.001476

C -1.879341 -0.153011 0.000857

H -2.026837 0.479406 -0.876961

H -2.561769 -1.000890 -0.018788

H -2.037441 0.445438 0.900617

**154(A•)** = -153.142541

C 1.171565 0.089558 -0.000005

H 1.899528 -0.719104 0.000035

H 1.304076 0.713815 0.889902

H 1.304088 0.713867 -0.889877

C -0.252315 -0.447474 -0.000016

O -1.252899 0.179865 0.000008

**154(B•)** = -115.017956

O 0.790952 -0.002492 0.006927

C -0.573632 -0.006685 0.012263

H -0.873904 0.233411 -1.028780

H -1.018470 -0.979159 0.271312

H -0.993447 0.805788 0.628473

**155(A-B)** = -232.316758

C -2.447094 -0.287302 0.039066

H -3.368800 0.274414 -0.033222

H -2.499545 -1.358966 0.190019

C -1.279764 0.343642 -0.073285

H -1.220052 1.422044 -0.222574

O -0.087256 -0.306102 -0.039967

C 1.065745 0.526607 0.106697

H 1.050138 1.314317 -0.659572

H 1.046535 1.010697 1.092548

C 2.302042 -0.340601 -0.041442

H 3.202171 0.269823 0.073809

H 2.315949 -1.124919 0.719075

H 2.326073 -0.812668 -1.026559

**155(A•)** = -77.860817

C -0.587190 0.029244 0.000022

H -1.034615 1.028742 -0.000052

H -1.286201 -0.805029 -0.000023

C 0.707040 -0.143687 -0.000016

H 1.601713 0.462945 0.000037

**155(B•)** = -154.307523

O -1.257442 -0.363866 0.000015

C -0.181373 0.475257 -0.000003

H -0.302051 1.159674 -0.865629

H -0.301852 1.159738 0.865577

C 1.190779 -0.194352 -0.000012

H 1.989373 0.554739 -0.000377

H 1.308967 -0.823995 0.885935

H 1.308664 -0.824654 -0.885535

**156(A-B)** = -189.736553

C -0.132757 0.361163 -0.000024

H -0.041982 1.463462 0.000037

O -1.174103 -0.219829 0.000009

O 1.057047 -0.279750 0.000000

H 1.774976 0.366187 0.000034

**156(A•)** = -113.844513

C 0.061696 0.584375 0.000000

H -0.863747 1.222373 0.000000

O 0.061696 -0.591078 0.000000

**156(B•)** = -75.727869

O 0.000000 0.000000 -0.108269

H 0.000000 0.000000 0.866150

**157(A-B)** = -460.969232

C -2.924539 0.395986 0.000044

C -1.862037 1.268161 0.000086

C -0.525788 0.787360 -0.000003

C -0.291092 -0.626191 0.000086

C -1.413476 -1.499998 0.000078

C -2.694578 -1.001762 -0.000055

H 0.428415 2.730792 -0.000140

H -3.941532 0.773361 0.000117

H -2.031341 2.341112 0.000101

C 0.594736 1.657772 -0.000044

C 1.040077 -1.111797 -0.000102

H -1.241491 -2.572115 -0.000093

H -3.539709 -1.682412 -0.000342

C 2.102163 -0.235701 -0.000055

C 1.876917 1.164746 -0.000159

H 1.231298 -2.179623 -0.000045

H 2.725379 1.844759 0.000040

O 3.368352 -0.751875 0.000026

H 4.007866 -0.032337 0.000888

**157(A•)** = -75.727869

O 0.000000 0.000000 0.108267

H 0.000000 0.000000 -0.866137

**157(B•)** = -385.067419

C -2.343825 0.790445 0.000001

C -1.126515 1.428585 -0.000003

C 0.086510 0.687582 -0.000004

C 0.017765 -0.744315 -0.000002

C -1.256073 -1.373597 0.000001

C -2.408624 -0.624063 0.000003

H 1.397907 2.414236 -0.000008

H -3.261945 1.367894 0.000005

H -1.075318 2.513062 -0.000001

C 1.357144 1.328520 -0.000001

C 1.236669 -1.494233 -0.000003

H -1.303565 -2.457994 0.000001

H -3.376182 -1.114687 0.000010

C 2.397158 -0.796196 0.000000

C 2.526314 0.593808 0.000007

H 1.203228 -2.579740 -0.000008

H 3.496735 1.078010 0.000010

**158(A-B)** = -460.969504

C 2.739805 0.293875 -0.000003

C 1.776198 1.274602 -0.000004

C 0.394340 0.943939 -0.000002

C 0.027777 -0.439303 0.000002

C 1.041927 -1.431805 0.000007

C 2.369471 -1.071596 0.000004

H -0.331695 2.986518 0.000002

H 3.790597 0.564428 -0.000009

H 2.059286 2.322885 -0.000008

C -0.619430 1.940351 0.000004

C -1.360314 -0.771613 -0.000003

H 0.751014 -2.475327 0.000019

H 3.138925 -1.836348 0.000004

C -2.322498 0.215310 -0.000002

C -1.943875 1.577848 0.000004

H -3.375805 -0.052575 -0.000016

H -2.718329 2.337554 0.000011

O -1.664153 -2.103329 -0.000016

H -2.621170 -2.210145 0.000083

**158(A•)** = -75.727868

O 0.000000 0.000000 0.108269

H 0.000000 0.000000 -0.866148

**158(B•)** = -385.067172

C 2.395184 0.730207 -0.000022

C 1.191634 1.393472 -0.000194

C -0.036157 0.677461 -0.000115

C 0.014738 -0.760701 0.000138

C 1.274575 -1.418620 0.000312

C 2.437453 -0.686603 0.000233

H -1.331935 2.409800 -0.000491

H 3.323059 1.291659 -0.000086

H 1.161187 2.478851 -0.000394

C -1.303401 1.324953 -0.000294

C -1.226637 -1.410583 0.000199

H 1.296880 -2.502364 0.000508

H 3.396822 -1.191981 0.000360

C -2.446788 -0.821911 0.000033

C -2.474490 0.604389 -0.000224

H -3.369858 -1.391931 0.000078

H -3.432813 1.113584 -0.000367

**159(A-B)** = -307.368080

C -1.855740 -0.000157 0.016582

C -1.155058 1.206189 0.004404

C 0.239667 1.210212 -0.010772

C 0.933952 0.000192 -0.012102

C 0.239765 -1.209927 -0.011057

C -1.154993 -1.206355 0.004332

H -2.940121 -0.000186 0.026313

H -1.693796 2.147908 0.004698

H 0.798575 2.139265 -0.035003

H 0.798736 -2.138961 -0.035665

H -1.693455 -2.148218 0.004593

O 2.319920 0.000502 -0.089332

H 2.685149 -0.004745 0.801400

**159(A•)** = -231.470868

C -0.000428 1.324119 -0.000002

C 1.212377 0.632236 0.000033

C 1.224782 -0.771169 -0.000034

C 0.000417 -1.397007 -0.000001

C -1.224249 -0.771862 0.000038

C -1.212795 0.631664 -0.000027

H -0.000666 2.408663 0.000004

H 2.151824 1.176392 0.000032

H 2.158576 -1.323426 -0.000037

H -2.157739 -1.324641 0.000015

H -2.152624 1.175127 -0.000060

**159(B•)** = -75.727869

O 0.000000 0.000000 -0.108267

H 0.000000 0.000000 0.866139

**160(A-B)** = -188.589950

C 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.161356

O 0.000000 0.000000 -1.161356

**160(A•)** = -113.315016

C 0.000000 0.000000 -0.645063

O 0.000000 0.000000 0.483798

**160(B•)** = -75.068852

O -4.163086 2.637511 0.000000

(6) N-C BDE (**161**-**180**)

**161(A-B)** = -1548.449100

C -0.075985 -0.000707 -0.010200

CL 1.034360 -0.006627 1.371446

CL -1.068467 1.482298 -0.067987

CL -1.081603 -1.473345 -0.072618

N 0.669570 -0.001809 -1.430403

O 1.841998 -0.002829 -1.356285

**161(A•)** = -1418.512635

C -0.000798 -0.000085 -0.298108

CL 0.895756 -1.453145 0.035056

CL 0.811149 1.501996 0.035051

CL -1.706624 -0.048821 0.035108

**161(B•)** = -129.893904

N 0.000000 0.000000 0.612560

O 0.000000 0.000000 -0.535990

**162(A-B)** = -287.618636

C -0.319689 0.042239 -0.002481

C -1.069653 -0.343000 1.284377

H -2.066920 0.106194 1.277332

H -1.177641 -1.428230 1.359687

H -0.537332 0.014618 2.170491

C -0.040286 1.538512 -0.087403

H 0.531480 1.884429 0.777383

H 0.532460 1.784219 -0.985238

H -0.985509 2.087707 -0.118994

C -1.067206 -0.487028 -1.238508

H -0.531021 -0.236516 -2.158416

H -1.178922 -1.573371 -1.188121

H -2.062865 -0.036891 -1.287054

N 0.947523 -0.801915 0.046896

O 1.978077 -0.186636 0.011094

**162(A•)** = -157.668786

C -0.000096 0.000000 -0.153613

C 0.743761 -1.287036 0.015368

H 0.889979 -1.540672 1.081557

H 0.204599 -2.128357 -0.433390

H 1.741836 -1.239385 -0.433386

C 0.742871 1.287514 0.015417

H 1.739226 1.242646 -0.437596

H 0.200796 2.129167 -0.428996

H 0.893613 1.538188 1.081648

C -1.486597 -0.000478 0.015388

H -1.945816 0.885032 -0.437205

H -1.944514 -0.890529 -0.429548

H -1.779353 0.003908 1.081556

**162(B•)** = -129.893908

N 0.000000 0.000000 0.612664

O 0.000000 0.000000 -0.536081

**163(A-B)** = -169.757963

C -1.099301 0.144092 -0.000305

H -1.010629 1.232995 -0.003072

H -1.631696 -0.222041 0.883736

H -1.636746 -0.228097 -0.878230

N 0.231424 -0.519705 -0.000020

O 1.156863 0.248816 -0.000058

**163(A•)** = -39.801327

C -0.000005 0.000168 0.000265

H 0.931898 0.548641 -0.000529

H -0.941738 0.531577 -0.000529

H 0.009870 -1.081224 -0.000529

**163(B•)** = -129.893908

N 0.000000 0.000000 -0.612706

O 0.000000 0.000000 0.536118

**164(A-B)** = -475.949263

O -2.524799 -1.082858 -0.579599

O -2.506368 1.090276 -0.584362

N -2.169375 0.001750 -0.145852

C 0.225100 -0.002139 0.525003

C -1.195905 -0.003606 1.029700

C 0.886833 -1.210058 0.280250

C 0.886779 1.206931 0.285976

C 2.195322 -1.208063 -0.198389

C 2.195246 1.207218 -0.192665

C 2.851015 0.000156 -0.434666

H -1.427572 -0.904242 1.595713

H -1.426625 0.892998 1.602628

H 0.373608 -2.149728 0.458861

H 0.373295 2.145642 0.468683

H 2.702563 -2.148533 -0.385125

H 2.702465 2.148578 -0.374924

H 3.870882 0.001059 -0.804433

**164(A•)** = -205.083448

O -1.100468 0.141714 0.000000

O 1.100468 0.141724 0.000000

N 0.000000 -0.323930 0.000000

**164(B•)** = -270.795572

C -0.994725 0.000000 -0.000147

C -2.400272 -0.000005 0.001232

C -0.251317 -1.218280 -0.000100

C -0.251324 1.218285 -0.000102

C 1.132662 -1.211166 -0.000158

C 1.132660 1.211167 -0.000169

C 1.837713 0.000000 0.000269

H -2.961366 -0.927323 -0.002395

H -2.961362 0.927316 -0.002300

H -0.791635 -2.160149 -0.000141

H -0.791647 2.160149 -0.000127

H 1.675664 -2.150915 -0.000674

H 1.675657 2.150921 -0.000682

H 2.922306 -0.000002 0.001363

**165(A-B)** = -189.183724

C -1.802682 -0.058591 0.000038

H -1.977130 -0.673113 0.888219

H -1.977154 -0.673444 -0.887908

H -2.485750 0.790704 -0.000106

H 1.977092 0.673511 -0.887892

N -0.418731 0.453964 -0.000077

N 0.418739 -0.453979 -0.000029

C 1.802677 0.058601 0.000026

H 2.485754 -0.790685 -0.000197

H 1.977163 0.673072 0.888236

**165(A•)** = -39.801306

C -0.000355 0.000000 -0.000705

H 0.542068 0.935142 0.001408

H 0.540907 -0.935812 0.001408

H -1.080848 0.000669 0.001413

**165(B•)** = -149.303336

N -1.254238 0.246187 0.000000

N -0.308773 -0.441345 -0.000001

C 1.109944 0.110337 0.000000

H 1.792875 -0.735265 -0.000052

H 1.244284 0.719632 0.895089

H 1.244254 0.719723 -0.895033

**166(A-B)** = -361.450913

C -2.174009 0.257604 0.000119

C -1.277816 1.334927 -0.000140

C 0.090152 1.102264 -0.000081

C 0.552765 -0.219413 -0.000168

C -0.334060 -1.297704 -0.000144

C -1.706035 -1.056528 0.000105

H -3.242315 0.448757 0.000404

H -1.656762 2.351670 -0.000038

H 0.810793 1.912734 0.000271

H 0.071315 -2.304338 -0.000383

H -2.406514 -1.884594 0.000115

N 1.954014 -0.580947 0.000153

O 2.729925 0.351938 0.000051

**166(A•)** = -231.470881

C 0.000235 1.324158 0.000013

C 1.212396 0.631762 -0.000117

C 1.224009 -0.771519 0.000059

C -0.000245 -1.397492 -0.000015

C -1.224282 -0.771152 -0.000022

C -1.212170 0.632126 0.000044

H 0.000388 2.409356 0.000221

H 2.152791 1.175531 -0.000099

H 2.158487 -1.324462 0.000236

H -2.158900 -1.323862 -0.000107

H -2.152420 1.176143 -0.000021

**166(B•)** = -129.893908

N 0.000000 0.000000 -0.612683

O 0.000000 0.000000 0.536098

**167(A-B)** = -308.233309

C 2.321675 0.648156 -0.624164

H 2.063260 1.595180 -1.106271

H 2.649926 -0.060770 -1.408833

H 3.171161 0.826886 0.040737

N 1.192260 0.159961 0.151916

C 1.523541 -1.059479 0.879342

H 2.338068 -0.858978 1.580826

H 0.648938 -1.392445 1.439591

H 1.840667 -1.879536 0.206006

C 0.000518 0.001888 -0.667612

H -0.069980 0.891042 -1.323238

H 0.071453 -0.885944 -1.325167

N -1.191514 -0.158079 0.150909

C -1.527431 1.061639 0.875623

H -1.846063 1.879649 0.200619

H -2.342202 0.860167 1.576551

H -0.654654 1.397947 1.436789

C -2.318665 -0.653033 -0.624034

H -3.167543 -0.832263 0.041492

H -2.649361 0.051778 -1.411354

H -2.056733 -1.600914 -1.102454

**167(A•)** = -134.424248

C 1.191038 -0.171273 0.000076

H 2.080840 0.461170 0.003684

H 1.229727 -0.829193 -0.884892

H 1.226261 -0.835255 0.880622

N -0.000198 0.637561 0.000010

C -1.190919 -0.171432 -0.000049

H -1.228732 -0.830338 0.884152

H -2.080725 0.461062 -0.002310

H -1.226698 -0.834148 -0.881491

**167(B•)** = -173.703602

C 0.005630 -1.430842 -0.099315

H 0.941135 -1.957535 0.047996

H -0.924437 -1.966088 0.051879

N 0.000069 -0.081390 0.211786

C 1.220306 0.666005 -0.035745

H 1.363000 0.891009 -1.105362

H 1.193977 1.609171 0.517173

H 2.078594 0.086130 0.311006

C -1.225444 0.657173 -0.036022

H -1.206798 1.600501 0.517121

H -1.369267 0.881712 -1.105630

H -2.079641 0.070814 0.309803

**168(A-B)** = -434.470076

C 2.006654 -0.718713 -0.000557

C 2.146326 0.639971 0.000949

C 0.825003 1.175545 -0.000247

C 0.004136 0.085843 0.000141

O 0.698480 -1.070906 -0.000624

H 2.709062 -1.536218 -0.000405

H 3.074704 1.189304 0.001725

H 0.511894 2.206740 -0.000593

N -1.429195 -0.002691 -0.000033

O -2.032137 1.069208 -0.000457

O -1.939344 -1.115410 0.000804

**168(A•)** = -229.270243

C 0.827556 0.735579 -0.000439

C -0.500459 1.022462 0.000538

C -1.209503 -0.238816 -0.000787

C -0.212920 -1.158360 0.001106

O 1.007289 -0.635809 -0.000564

H 1.729214 1.324079 0.002252

H -0.943106 2.007279 -0.000311

H -2.272462 -0.410078 0.000066

**168(B•)** = -205.083430

N 0.000000 0.322789 0.000000

O -1.100501 -0.141219 0.000000

O 1.100501 -0.141221 0.000000

**169(A-B)** = -436.664940

C 2.517150 -0.000231 0.000229

C 1.822220 -1.210817 0.000260

C 0.430073 -1.219100 0.000102

C -0.241259 0.000321 -0.000424

C 0.430374 1.219567 -0.000552

C 1.822574 1.210587 -0.000198

H 3.601830 -0.000230 0.000696

H 2.363457 -2.150278 0.000719

H -0.135509 -2.141856 0.000654

H -0.134692 2.142606 -0.001042

H 2.364151 2.149878 -0.000373

N -1.723769 -0.000023 -0.000113

O -2.292159 -1.085134 -0.000584

O -2.292797 1.084895 0.001039

**169(A•)** = -231.470881

C 0.000235 1.324158 0.000013

C 1.212396 0.631762 -0.000117

C 1.224009 -0.771519 0.000059

C -0.000245 -1.397492 -0.000015

C -1.224282 -0.771152 -0.000022

C -1.212170 0.632126 0.000044

H 0.000388 2.409356 0.000221

H 2.152791 1.175531 -0.000099

H 2.158487 -1.324462 0.000236

H -2.158900 -1.323862 -0.000107

H -2.152420 1.176143 -0.000021

**169(B•)** = -205.083449

N 0.000000 0.323976 0.000000

O 1.100479 -0.141523 0.000000

O -1.100479 -0.141956 0.000000

**170(A-B)** = -151.095240

C -1.176487 -0.240678 -0.001572

H -2.054529 0.411266 -0.034266

H -1.218395 -0.835086 0.929102

H -1.238333 -0.932031 -0.847820

N 0.027384 0.572178 -0.122888

H 0.025085 1.313457 0.567548

N 1.246009 -0.149937 0.054890

H 1.123308 -0.923189 0.712322

H 1.508035 -0.546040 -0.841466

**170(A•)** = -39.801327

C 0.000006 0.000158 -0.000210

H -0.927771 0.555577 0.000421

H 0.945640 0.524607 0.000421

H -0.017906 -1.081131 0.000420

**170(B•)** = -111.193390

N -0.742235 -0.150785 -0.024487

H -1.144920 0.789688 0.033667

N 0.596617 0.024439 0.070766

H 1.131472 -0.802440 -0.150802

H 1.032778 0.897170 -0.206815

**171(A-B)** = -326.763825

C -1.850975 1.029835 -0.135867

C -0.484976 1.286814 -0.015614

C 0.429597 0.241331 0.146305

C -0.049960 -1.073397 0.180103

C -1.413619 -1.332756 0.054636

C -2.319760 -0.282513 -0.099451

H -2.546341 1.853269 -0.263608

H -0.124500 2.311359 -0.054492

H 0.660671 -1.885655 0.288607

H -1.771268 -2.357292 0.080704

H -3.381106 -0.486065 -0.196895

C 1.908361 0.534896 0.322509

H 2.151648 0.490552 1.391644

H 2.097328 1.572019 0.002826

N 2.747390 -0.460878 -0.352812

H 2.643697 -0.387942 -1.360175

H 3.726123 -0.309360 -0.134653

**171(A•)** = -270.795550

C -1.132309 1.210957 -0.000012

C 0.251659 1.218184 0.000266

C 0.995005 0.000257 -0.000041

C 0.252157 -1.218009 -0.000280

C -1.131878 -1.211149 -0.000077

C -1.837386 -0.000232 -0.000036

H -1.675393 2.150829 -0.000199

H 0.791842 2.160246 0.000304

H 0.792502 -2.160007 -0.000262

H -1.674815 -2.151118 0.000306

H -2.922070 -0.000350 0.000681

C 2.398433 0.000174 -0.000197

H 2.956034 -0.928920 0.003192

H 2.957809 0.928222 -0.001759

**171(B•)** = -55.855919

N 0.000000 0.143165 0.000000

H 0.803714 -0.501079 0.000000

H -0.803714 -0.501077 0.000000

**172(A-B)** = -174.344776

C -1.199168 -0.701328 0.061059

H -1.192611 -1.722684 -0.329850

H -1.292144 -0.755936 1.163718

H -2.086351 -0.194926 -0.329568

C 1.207155 -0.687610 0.061104

H 1.214482 -1.707336 -0.333952

H 2.088365 -0.168008 -0.325618

H 1.298367 -0.745212 1.163744

N 0.000031 -0.000065 -0.373125

C -0.007966 1.388959 0.061066

H 0.874149 1.903755 -0.329725

H -0.895801 1.893681 -0.329933

H -0.008800 1.497000 1.163686

**172(A•)** = -134.424263

C -1.191131 -0.171324 -0.000010

H -1.226430 -0.834391 -0.881589

H -1.230426 -0.828934 0.885421

H -2.081095 0.461600 -0.003983

C 1.191148 -0.171347 -0.000006

H 1.227734 -0.832183 -0.883154

H 2.081124 0.461565 -0.001020

H 1.228963 -0.831060 0.883931

N 0.000004 0.637061 0.000070

**172(B•)** = -39.801328

C -0.000014 0.000171 -0.000328

H 0.923695 0.562350 0.000656

H -0.949501 0.517589 0.000656

H 0.025892 -1.080968 0.000655

**173(A-B)** = -204.044987

C -1.542974 0.282438 -0.000048

H -1.558138 0.917482 0.892943

H -2.433682 -0.341222 -0.000118

H -1.558670 0.918450 -0.892378

N -0.390596 -0.631355 -0.000402

N 0.715660 -0.095271 0.000822

N 1.790413 0.271007 -0.000442

**173(A•)** = -39.801333

C -0.000137 -0.000083 -0.001219

H 0.910283 -0.584679 0.002437

H -0.961908 -0.494438 0.002440

H 0.052444 1.079618 0.002437

**173(B•)** = -164.133098

N -0.822711 -0.820478 0.000000

N 0.000000 -0.000307 0.000000

N 0.822711 0.820785 0.000000

**174(A-B)** = -95.791315

C -0.709240 -0.000015 0.017891

H -1.113848 0.880838 -0.488500

H -1.083637 -0.000990 1.053658

H -1.114133 -0.879699 -0.490304

N 0.752063 -0.000013 -0.120694

H 1.151253 0.815219 0.331327

H 1.151359 -0.815188 0.331335

**174(A•)** = -39.801327

C 0.000005 0.000168 -0.000265

H -0.931898 0.548641 0.000529

H 0.941738 0.531577 0.000529

H -0.009870 -1.081224 0.000529

**174(B•)** = -55.855920

N 0.000000 -0.143164 0.000000

H -0.803721 0.501075 0.000000

H 0.803721 0.501070 0.000000

**175(A-B)** = -291.036334

C -1.889106 0.001000 -0.273883

C -1.173030 -1.267284 0.214150

C 0.310587 -1.260427 -0.184754

C 1.029932 -0.000391 0.315689

C 0.311944 1.259891 -0.185532

C -1.170907 1.267889 0.215157

H 0.812213 -2.153726 0.208646

H -1.257323 -1.331510 1.307417

H -1.663231 -2.159932 -0.189095

H -1.912525 0.001118 -1.371746

H -2.931335 0.001561 0.063973

H 0.972488 0.000306 1.420178

H 0.814872 2.153064 0.206368

H 0.407132 1.294967 -1.278146

H -1.253872 1.330531 1.308598

H -1.661010 2.161416 -0.186333

H 0.407617 -1.296764 -1.277162

N 2.417520 -0.000800 -0.168368

H 2.912367 0.816051 0.178764

H 2.913453 -0.815554 0.182143

**175(A•)** = -235.048437

C -0.004859 1.412020 -0.268569

C -1.270142 0.708147 0.243298

C -1.285635 -0.782505 -0.159461

C 0.004904 -1.463623 0.165277

C 1.291113 -0.774335 -0.159238

C 1.265116 0.716184 0.243006

H -2.127648 -1.299174 0.313204

H -1.304592 0.783621 1.337393

H -2.167471 1.206282 -0.139825

H -0.004980 1.408038 -1.367622

H -0.008076 2.463087 0.040764

H 0.008132 -2.519599 0.417559

H 2.136257 -1.284698 0.314660

H 1.478075 -0.828708 -1.249104

H 1.299489 0.792383 1.337065

H 2.158850 1.220654 -0.140374

H -1.471014 -0.837214 -1.249607

**175(B•)** = -55.855920

N 0.000000 0.143164 0.000000

H 0.803721 -0.501067 0.000000

H -0.803721 -0.501079 0.000000

**176(A-B)** = -209.152853

C 1.364330 -0.341977 -0.000114

H 1.459954 -1.427545 -0.071187

H 1.844721 -0.000511 0.919783

H 1.889173 0.121828 -0.837619

C -0.076987 0.147706 -0.002177

O -0.360876 1.331215 -0.000016

N -1.032281 -0.830513 -0.000109

H -2.001862 -0.555453 0.006982

H -0.803070 -1.808825 -0.003322

**176(A•)** = -153.142542

C 1.171633 0.089526 -0.000015

H 1.899421 -0.719291 -0.001455

H 1.304760 0.712513 0.890699

H 1.303902 0.715074 -0.889064

C -0.252283 -0.447292 -0.000024

O -1.253023 0.179788 0.000007

**176(B•)** = -55.855919

N 0.000000 0.143166 0.000000

H 0.803708 -0.501075 0.000000

H -0.803708 -0.501085 0.000000

**177(A-B)** = -169.859817

C 0.162907 0.385908 0.000085

H 0.137972 1.493046 0.000337

O 1.196294 -0.245915 -0.000012

N -1.084283 -0.157284 -0.000414

H -1.187825 -1.160517 0.001317

H -1.907962 0.420332 0.000831

**177(A•)** = -113.844514

C -0.061693 0.584359 0.000000

H 0.863703 1.222519 0.000000

O -0.061693 -0.591084 0.000000

**177(B•)** = -55.855919

N 0.000000 -0.143166 0.000000

H -0.803711 0.501079 0.000000

H 0.803711 0.501083 0.000000

**178(A-B)** = -132.671489

C 1.107598 0.000009 -0.000053

H 1.476905 0.893333 -0.508344

H 1.476966 -0.886941 -0.519320

H 1.477163 -0.006311 1.027625

N -0.312134 -0.000040 0.000085

C -1.481947 0.000024 -0.000041

**178(A•)** = -39.801327

C 0.000005 0.000168 -0.000265

H -0.931898 0.548641 0.000529

H 0.941738 0.531577 0.000529

H -0.009870 -1.081224 0.000529

**178(B•)** = -92.706549

N 0.000000 0.000000 0.538247

C 0.000000 0.000000 -0.627955

**179(A-B)** = -287.482694

C 1.878288 0.028812 0.000044

C 1.200905 -1.189667 0.000018

C -0.194526 -1.217169 -0.000109

C -0.926419 -0.028627 -0.000035

C -0.240506 1.192439 0.000035

C 1.153731 1.221600 0.000013

H 2.962507 0.049891 0.000073

H 1.757711 -2.120665 -0.000039

H -0.735318 -2.156372 -0.000249

H -0.804782 2.120322 0.000084

H 1.673220 2.173880 0.000022

N -2.368196 -0.115824 -0.000160

H -2.752402 0.348158 0.817069

H -2.752402 0.351231 -0.815634

**179(A•)** = -231.470868

C -0.000443 1.324115 -0.000002

C 1.212371 0.632242 0.000025

C 1.224816 -0.771172 -0.000029

C 0.000434 -1.396947 -0.000001

C -1.224263 -0.771888 0.000033

C -1.212807 0.631642 -0.000020

H -0.000693 2.408656 0.000006

H 2.151810 1.176417 0.000025

H 2.158610 -1.323429 -0.000017

H -2.157739 -1.324691 -0.000001

H -2.152640 1.175103 -0.000049

**179(B•)** = -55.855920

N 0.000000 0.143165 0.000000

H 0.803715 -0.501079 0.000000

H -0.803715 -0.501078 0.000000

**180(A-B)** = -441.079750

C 2.942673 0.369019 0.000012

C 1.891104 1.254675 0.000031

C 0.548783 0.788916 0.000011

C 0.303627 -0.620042 0.000000

C 1.412967 -1.508456 -0.000012

C 2.700567 -1.026540 -0.000012

H -0.383611 2.743425 0.000027

H 3.963657 0.734572 0.000018

H 2.072955 2.324912 0.000040

C -0.564375 1.672988 -0.000002

C -1.038890 -1.088290 -0.000039

H 1.225626 -2.577576 -0.000038

H 3.539135 -1.714262 -0.000027

C -2.099651 -0.214339 -0.000020

C -1.848908 1.186642 -0.000007

H -1.237593 -2.154436 -0.000096

H -2.693029 1.869638 0.000012

N -3.439201 -0.751148 -0.000077

H -3.949780 -0.428641 0.816428

H -3.950331 -0.427035 -0.815599

**180(A•)** = -385.067420

C 2.343821 0.790468 0.000000

C 1.126488 1.428586 0.000001

C -0.086515 0.687574 0.000003

C -0.017753 -0.744346 0.000000

C 1.256086 -1.373596 -0.000002

C 2.408630 -0.624028 -0.000001

H -1.397916 2.414231 0.000007

H 3.261929 1.367941 -0.000003

H 1.075285 2.513064 -0.000001

C -1.357160 1.328511 0.000001

C -1.236660 -1.494273 0.000002

H 1.303600 -2.457993 -0.000001

H 3.376193 -1.114645 -0.000006

C -2.397104 -0.796179 0.000000

C -2.526347 0.593813 -0.000005

H -1.203243 -2.579782 0.000009

H -3.496769 1.078014 -0.000008

**180(B•)** = -55.855920

N 0.000000 -0.143165 0.000000

H -0.803717 0.501078 0.000000

H 0.803717 0.501078 0.000000

(7) N-H BDE (**181**-**200**)

H = -0.500215

**181** = -362.655712

O 2.710800 0.415173 -0.249835

N 1.825161 -0.603622 0.210158

C 0.459192 -0.259497 0.064563

C -0.482330 -1.297122 0.004072

C 0.024259 1.068683 0.066990

C -1.841175 -1.003840 -0.045058

C -1.341023 1.348158 0.012988

C -2.281603 0.320966 -0.039459

H -0.148283 -2.331005 0.002463

H 0.752856 1.868495 0.093629

H -2.559082 -1.816206 -0.091978

H -1.668284 2.382875 0.009770

H 3.225710 0.623425 0.537796

H -3.341301 0.546707 -0.081276

H 2.051929 -1.434418 -0.327399

**181•** = -362.044750

O 2.669042 0.405913 -0.000208

N 1.820055 -0.685432 0.000598

C 0.517327 -0.273635 0.000203

C -0.446388 -1.313662 -0.000453

C 0.078313 1.074883 -0.000355

C -1.798267 -1.012801 -0.000067

C -1.279982 1.353990 -0.000042

C -2.224961 0.320901 0.000387

H -0.095625 -2.339756 -0.001066

H 0.810018 1.872015 -0.000931

H -2.527962 -1.815591 -0.000208

H -1.612720 2.386983 0.000072

H 3.541609 -0.004563 0.000679

H -3.284289 0.553569 0.000885

**182** = -254.905765

N 0.945211 -0.255928 0.390527

H 1.454497 0.191944 -0.385052

F 1.545147 -1.521590 0.382422

F 1.544120 0.386022 1.483148

**182•** = -254.295069

N 1.037024 -0.239623 0.363389

F 1.521506 -1.504574 0.424253

F 1.521528 0.340131 1.489293

**183** = -303.545499

N 2.301744 0.000000 -0.000406

N -1.900413 -0.000002 0.000126

C 0.933940 -0.000006 -0.000024

C 0.197161 1.198308 0.000006

C 0.197160 -1.198310 -0.000026

C -1.189928 1.134983 0.000020

C -1.189932 -1.134973 0.000078

H 0.700273 2.160122 -0.000033

H 0.700252 -2.160139 -0.000114

H -1.767046 2.056994 0.000120

H -1.767049 -2.056985 0.000065

H 2.816926 -0.861196 0.000772

H 2.816911 0.861206 0.000824

**183•** = -302.897408

N 2.345504 0.137843 0.000085

N -1.828290 -0.033072 -0.000083

C 1.007383 0.029232 0.000035

C 0.226841 1.222695 0.000025

C 0.278847 -1.199217 0.000005

C -1.154877 1.129453 -0.000046

C -1.104990 -1.165873 -0.000051

H 0.734726 2.180273 0.000061

H 0.809291 -2.146852 0.000037

H -1.765086 2.028334 -0.000059

H -1.675747 -2.090629 -0.000088

H 2.757090 -0.802269 0.000223

**184** = -518.455421

C -2.783165 1.364554 0.560704

C -1.493382 0.839486 0.540236

C -1.263169 -0.446428 0.023753

C -2.360428 -1.186352 -0.451275

C -3.645830 -0.657221 -0.409135

C -3.868351 0.627684 0.087191

H -2.939359 2.359097 0.966349

H -0.671326 1.414014 0.948743

H -2.195491 -2.179824 -0.858927

H -4.476100 -1.249457 -0.780155

H -4.869130 1.043976 0.109848

N 0.000626 -1.043585 0.011052

C 1.263857 -0.445431 -0.014110

C 2.366137 -1.186257 0.447941

C 1.488191 0.842259 -0.528459

C 3.650509 -0.656001 0.394679

H 2.205833 -2.181026 0.854256

C 2.777486 1.368169 -0.560555

H 0.661428 1.418168 -0.925418

C 3.867661 0.630452 -0.100314

H 4.484803 -1.248957 0.755395

H 2.928845 2.364040 -0.964748

H 4.868123 1.046888 -0.131955

H 0.000893 -2.051308 0.005308

**184•** = -517.826889

C -2.699427 1.343016 0.616213

C -1.421979 0.801821 0.581324

C -1.199472 -0.488442 0.025704

C -2.327581 -1.207297 -0.452426

C -3.591570 -0.641095 -0.441236

C -3.787678 0.638489 0.091890

H -2.854008 2.319955 1.063105

H -0.593565 1.339826 1.026826

H -2.158687 -2.204466 -0.843200

H -4.435507 -1.199338 -0.833071

H -4.781092 1.073116 0.116798

N -0.000281 -1.141901 -0.002939

C 1.199578 -0.488727 -0.028743

C 2.325916 -1.207284 0.453556

C 1.423396 0.800945 -0.584281

C 3.590145 -0.641283 0.445257

H 2.155890 -2.203998 0.844981

C 2.701064 1.341975 -0.616305

H 0.596364 1.338967 -1.032314

C 3.787824 0.637586 -0.088763

H 4.432845 -1.199317 0.840012

H 2.856980 2.318502 -1.063610

H 4.781449 1.071847 -0.112095

**185** = -362.655712

O 2.710800 0.415173 -0.249835

N 1.825161 -0.603622 0.210158

C 0.459192 -0.259497 0.064563

C -0.482330 -1.297122 0.004072

C 0.024259 1.068683 0.066990

C -1.841175 -1.003840 -0.045058

C -1.341023 1.348158 0.012988

C -2.281603 0.320966 -0.039459

H -0.148283 -2.331005 0.002463

H 0.752856 1.868495 0.093629

H -2.559082 -1.816206 -0.091978

H -1.668284 2.382875 0.009770

H 3.225710 0.623425 0.537796

H -3.341301 0.546707 -0.081276

H 2.051929 -1.434418 -0.327399

**185•** = -362.044750

O 2.669042 0.405913 -0.000208

N 1.820055 -0.685432 0.000598

C 0.517327 -0.273635 0.000203

C -0.446388 -1.313662 -0.000453

C 0.078313 1.074883 -0.000355

C -1.798267 -1.012801 -0.000067

C -1.279982 1.353990 -0.000042

C -2.224961 0.320901 0.000387

H -0.095625 -2.339756 -0.001066

H 0.810018 1.872015 -0.000931

H -2.527962 -1.815591 -0.000208

H -1.612720 2.386983 0.000072

H 3.541609 -0.004563 0.000679

H -3.284289 0.553569 0.000885

**186** = -326.764058

C -1.360592 1.350690 -0.010188

C 0.003127 1.059417 -0.048368

C 0.443791 -0.275972 -0.051214

C -0.525546 -1.298306 -0.004671

C -1.879087 -0.992965 0.038464

C -2.312959 0.335802 0.034312

H -1.675697 2.389575 -0.010696

H 0.719702 1.871723 -0.077574

H -0.203658 -2.336425 -0.009322

H -2.603393 -1.800686 0.075418

H -3.370779 0.570887 0.066514

N 1.788949 -0.610365 -0.136788

H 2.003973 -1.546634 0.168431

C 2.835527 0.365398 0.094295

H 2.748358 0.874039 1.066436

H 3.800600 -0.142500 0.053441

H 2.832680 1.128196 -0.690913

**186•** = -326.129125

C -1.289830 -1.365133 0.000154

C 0.061569 -1.062691 0.000198

C 0.502907 0.297932 0.000357

C -0.500105 1.315629 0.000016

C -1.845309 0.996554 -0.000338

C -2.251145 -0.345294 -0.000151

H -1.608574 -2.402748 0.000309

H 0.788434 -1.866426 0.000221

H -0.159431 2.345102 -0.000004

H -2.589348 1.786319 -0.000706

H -3.306718 -0.595117 -0.000277

N 1.783628 0.719462 0.000791

C 2.827802 -0.280240 -0.000633

H 2.777343 -0.932389 -0.885645

H 3.797500 0.220154 -0.002145

H 2.780071 -0.931663 0.885095

**187** = -287.482692

C -1.153586 1.221586 0.000004

C 0.240690 1.192290 0.000024

C 0.926523 -0.028757 -0.000012

C 0.194360 -1.217132 -0.000001

C -1.201117 -1.189491 0.000013

C -1.878432 0.028975 -0.000014

H -1.672922 2.173966 0.000010

H 0.805065 2.120129 0.000004

H 0.734936 -2.156485 -0.000025

H -1.757985 -2.120444 0.000019

H -2.962637 0.050213 -0.000045

N 2.368370 -0.116012 -0.000021

H 2.752161 0.350066 -0.816257

H 2.752160 0.349812 0.816360

**187•** = -286.851464

C -1.080017 1.233461 0.000094

C 0.301340 1.212703 -0.000386

C 1.019954 -0.029697 0.000013

C 0.248174 -1.237934 -0.000432

C -1.132212 -1.198531 0.000056

C -1.806986 0.032511 0.000297

H -1.607971 2.181589 -0.000149

H 0.866596 2.140650 -0.001010

H 0.791737 -2.176179 -0.000840

H -1.700405 -2.122904 -0.000129

H -2.891344 0.056871 0.000680

N 2.353251 -0.136553 0.000499

H 2.767111 0.800766 0.000105

**188** = -363.691836

C -0.246373 -0.672051 0.000006

C -0.248784 0.751225 0.000013

C -1.626030 1.166090 0.000036

C 0.935255 -1.418766 0.000026

C 0.982110 1.429516 0.000047

C -2.388871 0.029171 -0.000102

C 2.134051 -0.717892 0.000015

C 2.156727 0.691887 0.000013

H -2.002754 2.177194 0.000087

H 0.921264 -2.503961 0.000017

H 1.012290 2.514090 0.000073

H -3.462475 -0.084771 -0.000142

H 3.070003 -1.266303 0.000012

H 3.111987 1.206062 0.000014

N -1.566050 -1.080090 -0.000045

H -1.876477 -2.036746 -0.000068

**188•** = -363.050370

C -0.294664 -0.684682 0.000010

C -0.262595 0.743098 -0.000012

C -1.634971 1.137726 0.000010

C 0.867597 -1.423177 0.000010

C 0.957169 1.422460 -0.000025

C -2.384273 -0.088707 -0.000016

C 2.097473 -0.724867 0.000033

C 2.141331 0.667614 0.000027

H -2.034770 2.143219 0.000032

H 0.837252 -2.507167 0.000004

H 0.997939 2.507120 0.000005

H -3.465366 -0.168340 -0.000012

H 3.024813 -1.287949 0.000049

H 3.099925 1.174617 0.000062

N -1.626029 -1.165470 -0.000052

**189** = -517.297859

C 0.725259 0.504853 -0.000537

C -0.725264 0.505001 -0.000238

C 1.131967 -0.855936 -0.000341

C -1.132010 -0.855614 0.000065

C 1.698015 1.510248 -0.000168

C -1.698037 1.510412 -0.000220

C 2.479461 -1.220482 0.000051

C -2.479332 -1.220528 0.000155

C 3.042300 1.152797 0.000303

C -3.042278 1.152730 0.000176

C 3.425138 -0.199292 0.000438

C -3.425105 -0.199372 0.000411

H 1.407806 2.556118 -0.000203

H -1.408064 2.556337 -0.000459

H 2.783414 -2.262272 -0.000082

H -2.783345 -2.262313 0.000020

H 3.805904 1.922849 0.000712

H -3.805988 1.922686 0.000414

H 4.479697 -0.454221 0.000723

H -4.479667 -0.454283 0.000500

N 0.000126 -1.653532 -0.000320

H -0.001328 -2.659088 0.000041

**189•** = -516.660165

C 0.732445 0.520595 0.000053

C -0.732440 0.520598 0.000048

C 1.093119 -0.865124 -0.000038

C -1.093115 -0.865132 -0.000051

C 1.711240 1.496821 0.000124

C -1.711231 1.496825 0.000064

C 2.437939 -1.255387 -0.000062

C -2.437950 -1.255383 -0.000097

C 3.060271 1.094753 0.000095

C -3.060263 1.094760 0.000002

C 3.415969 -0.258764 0.000006

C -3.415971 -0.258757 -0.000067

H 1.458137 2.552418 0.000193

H -1.458125 2.552421 0.000115

H 2.697684 -2.308184 -0.000126

H -2.697702 -2.308179 -0.000156

H 3.839880 1.849288 0.000142

H -3.839870 1.849297 0.000008

H 4.465018 -0.533716 -0.000012

H -4.465020 -0.533703 -0.000108

N -0.000011 -1.702068 -0.000075

**190** = -164.769691

N 0.159458 -1.116229 0.000000

N 0.000000 0.112661 0.000000

N -0.324605 1.194460 0.000000

H 1.156032 -1.336250 0.000000

**190•** = -164.134447

N 1.177442 -0.007489 0.000000

N 0.000000 -0.000252 0.000000

N -1.177442 0.007741 0.000000

**191** = -210.089451

C 0.328664 -1.124403 -0.000057

C -0.985073 -0.709712 -0.000016

C -0.981115 0.715080 -0.000044

C 0.334874 1.122540 0.000119

N 1.121908 -0.003040 -0.000012

H 2.127681 -0.005767 0.000122

H 0.758891 -2.113112 -0.000141

H -1.851084 -1.354073 -0.000053

H -1.843474 1.364328 -0.000085

H 0.770531 2.108878 0.000228

**191** = -209.442202

C 0.424907 -1.063570 -0.000046

C -0.984727 -0.680731 -0.000046

C -0.984297 0.681214 0.000005

C 0.425414 1.063302 0.000103

N 1.247422 -0.000275 -0.000011

H 0.821764 -2.072263 -0.000101

H -1.832600 -1.350550 -0.000087

H -1.831674 1.351658 0.000011

H 0.822780 2.071795 0.000164

**192** = -477.044820

O -3.306825 -0.762228 -0.000454

N -1.046906 -1.045866 -0.000183

C 0.256816 -0.593814 -0.000017

C 0.486143 0.803110 0.000118

C -0.662900 1.672911 0.000059

C 1.341978 -1.485271 0.000008

C -2.196415 -0.252353 -0.000132

C 1.812328 1.272591 0.000279

C -1.925320 1.186771 -0.000076

C 2.637290 -0.991676 0.000176

C 2.880075 0.390501 0.000311

H -0.491945 2.746143 0.000120

H 1.159262 -2.555475 -0.000099

H 1.986085 2.344401 0.000374

H -2.795022 1.832015 -0.000146

H 3.470771 -1.685936 0.000199

H 3.897836 0.763432 0.000436

H -1.224021 -2.042306 -0.000310

**192•** = -476.390998

O -3.260250 -0.819234 -0.000636

N -1.017822 -1.161408 -0.000249

C 0.197939 -0.614320 -0.000067

C 0.437919 0.814351 0.000133

C -0.707344 1.676461 0.000055

C 1.329319 -1.496735 -0.000033

C -2.125942 -0.322502 0.000047

C 1.757792 1.286058 0.000352

C -1.948741 1.135623 -0.000041

C 2.608202 -0.997781 0.000174

C 2.826444 0.400035 0.000363

H -0.558336 2.752583 0.000079

H 1.123588 -2.561067 -0.000190

H 1.939034 2.356701 0.000499

H -2.850171 1.737076 -0.000161

H 3.457725 -1.671833 0.000180

H 3.841388 0.783130 0.000523

**193** = -95.791315

C -0.709240 -0.000005 0.017891

H -1.113965 0.880279 -0.489402

H -1.083637 0.000012 1.053659

H -1.114016 -0.880259 -0.489402

N 0.752063 -0.000004 -0.120694

H 1.151281 0.815218 0.331322

H 1.151331 -0.815189 0.331340

**193•** = -95.139491

C -0.627677 0.011494 0.000003

H -0.970104 0.584149 -0.878692

H -0.970130 0.584202 0.878646

H -1.128185 -0.959395 0.000015

N 0.804329 -0.153275 0.000002

H 1.204182 0.795009 -0.000004

**194** = -322.469645

C -1.291904 -0.773921 -0.115813

C -1.345799 0.740966 0.152287

C 0.861975 -0.005311 -0.011788

H -1.907282 -1.361319 0.564982

H -1.563554 -1.003485 -1.150859

H -1.588176 0.960262 1.200263

H -2.065010 1.247189 -0.494856

O 0.084914 -1.128853 0.089531

N 0.027547 1.083483 -0.179400

H 0.417015 1.991474 0.019002

O 2.061155 -0.019760 0.031614

**194•** = -321.808765

C -1.292898 -0.765069 -0.069875

C -1.302124 0.770351 0.086933

C 0.852394 0.036488 -0.012751

H -1.851000 -1.295393 0.702514

H -1.649179 -1.078907 -1.055386

H -1.607636 1.075700 1.101577

H -1.970290 1.294887 -0.603566

O 0.092283 -1.101794 0.051516

N 0.054026 1.198819 -0.107422

O 2.052179 0.021965 0.021106

**195** = -248.428919

O 0.424866 1.387882 -0.000111

N -0.624253 -0.631044 -0.002808

C 0.484188 0.168945 -0.000088

C -1.976873 -0.103680 0.000964

C 1.815863 -0.567849 0.000813

H -0.495452 -1.629450 0.005865

H -2.540101 -0.460748 -0.866654

H -1.906057 0.982951 -0.043777

H -2.511207 -0.386901 0.913534

H 2.379200 -0.268607 -0.886025

H 2.387422 -0.251258 0.876076

H 1.717966 -1.656239 0.011387

**195•** = -247.765924

O 0.404731 1.375707 0.034993

N -0.643328 -0.621533 0.341013

C 0.468412 0.153900 0.043638

C -1.917353 -0.183069 -0.156299

C 1.756211 -0.619428 -0.115585

H -2.241019 -0.903206 -0.923977

H -1.888442 0.820234 -0.594261

H -2.662879 -0.235787 0.643276

H 2.522873 0.029915 -0.538093

H 2.083390 -0.976925 0.865474

H 1.607898 -1.497574 -0.749979

**196** = -400.838614

C -1.852900 1.226012 -0.141373

C -0.459421 1.192224 -0.159278

C 0.219484 -0.024508 -0.017685

C -0.515484 -1.206334 0.128206

C -1.906511 -1.170003 0.156104

C -2.578115 0.046361 0.023214

H -2.371276 2.171166 -0.263278

H 0.089829 2.114028 -0.322082

H 0.023912 -2.142703 0.214637

H -2.468249 -2.090130 0.277310

H -3.662587 0.073997 0.039623

C 1.721977 -0.136686 -0.038578

O 2.289093 -1.179573 -0.317776

N 2.415722 1.008217 0.258318

H 1.974797 1.771650 0.743033

H 3.416591 0.918653 0.341079

**196•** = -400.169897

C -1.826582 1.231393 -0.031227

C -0.434352 1.210003 -0.037447

C 0.244891 -0.015282 -0.005358

C -0.477760 -1.215023 0.034329

C -1.867793 -1.188215 0.039866

C -2.543003 0.034693 0.006972

H -2.352946 2.179357 -0.061497

H 0.133600 2.132601 -0.080314

H 0.064073 -2.154208 0.059809

H -2.427575 -2.116804 0.070956

H -3.627972 0.053771 0.011274

C 1.729553 -0.066593 0.015412

O 2.377433 -1.111369 -0.103462

N 2.416223 1.125962 0.031463

H 3.328077 0.968651 0.471945

**197** = -286.530738

C -1.414221 0.693779 -0.188289

C -0.007997 1.223790 0.138797

C 0.906142 0.001032 -0.006907

C -1.326167 -0.817287 0.132117

H -2.208466 1.184207 0.376925

H -1.625223 0.827308 -1.252570

H 0.073413 1.575712 1.173046

H 0.332662 2.030092 -0.511782

H -1.950643 -1.421008 -0.531493

H -1.628580 -1.024118 1.167866

O 2.120045 -0.010608 -0.041000

N 0.087996 -1.096059 -0.073804

H 0.483961 -2.022805 -0.031674

**197•** = -285.865470

C -1.407538 0.671460 -0.189119

C -0.008671 1.202445 0.144867

C 0.881812 -0.037218 -0.005754

C -1.261844 -0.842957 0.109791

H -2.207527 1.137885 0.388037

H -1.629703 0.816633 -1.250048

H 0.064794 1.545650 1.183364

H 0.346152 2.012143 -0.494095

H -1.897824 -1.495552 -0.497337

H -1.527162 -1.067144 1.158828

O 2.097889 -0.050407 -0.056014

N 0.120801 -1.215534 -0.057050

**198** = -56.521848

N 0.000001 -0.000051 -0.110357

H 0.817753 -0.474331 0.257547

H -0.819859 -0.470688 0.257545

H 0.002102 0.945379 0.257406

**198•** = -55.855919

N 0.000000 0.143163 0.000000

H 0.803720 -0.501069 0.000000

H -0.803720 -0.501069 0.000000

**199** = -169.859816

C 0.162942 0.386009 -0.000004

H 0.138063 1.492856 -0.000030

O 1.196312 -0.245979 0.000049

N -1.084291 -0.157312 -0.000251

H -1.188374 -1.160542 0.000456

H -1.907799 0.420650 0.000959

**199•** = -169.180769

C 0.099263 0.351735 -0.014351

H 0.038027 1.465631 -0.060425

O 1.148297 -0.239223 0.031704

N -1.156414 -0.234925 -0.116853

H -1.725082 -0.017783 0.710870

**200** = -225.222005

C 0.000196 0.142701 -0.000625

O -0.005349 1.360191 0.012606

N 1.164076 -0.594022 -0.038166

H 2.015692 -0.083198 0.120376

H 1.180989 -1.589481 0.102701

N -1.162292 -0.607263 -0.060124

H -1.166337 -1.570912 0.233103

H -2.001221 -0.085139 0.134760

**200•** = -224.556645

C -0.052727 0.079121 0.014959

O -0.489032 1.225687 -0.026414

N 1.267978 -0.242181 0.050853

H 1.946348 0.498695 -0.021966

H 1.553736 -1.189219 -0.136132

N -0.911178 -1.018927 -0.071725

H -1.769065 -0.761943 0.425753