C1

Atoms # full

1 1 12 -0.132000 -18.804256151 0.4267336236 -5.6537640425

2 1 12 -0.191000 -18.463364812 -0.1034249514 -4.4790551831

56 1 20 0.125000 -19.256812331 -0.1767726401 -6.4526988488

57 1 20 0.137000 -18.650439977 1.491355303 -5.8864704647

58 1 20 0.154000 -18.609754632 -1.1671207751 -4.2318550584

Bonds

113 39 2 58

114 10 2 1

115 39 1 57

116 3 1 56

Angles

201 36 58 2 1

202 25 2 1 57

203 25 2 1 56

204 20 57 1 56

Dihedrals

251 47 58 2 1 57

252 47 58 2 1 56

1 1 1 2 57 56

C2

Atoms # full

3 1 64 0.329000 -17.85311522 0.7072082234 -3.4181088269

4 1 61 -0.356000 -17.579841045 1.9113379122 -3.4183516495

5 1 3 -0.277000 -17.572172904 -0.0183992929 -2.2906506157

Bonds

110 13 5 3

111 5 3 4

Angles

196 81 5 3 4

C3

Atoms # full

6 1 64 -0.013000 -16.934135764 0.6927181995 -1.2170674706

7 1 12 -0.025000 -16.606269079 -0.34882025 -0.1556026214

8 1 4 -0.281000 -15.248491551 -0.7283760099 -0.3636816703

59 1 20 0.107000 -16.009489029 1.1970479356 -1.6014702501

60 1 20 0.107000 -17.65073761 1.457592116 -0.8215746606

61 1 20 0.083000 -16.716238235 0.1024716916 0.8662377774

62 1 20 0.083000 -17.275154073 -1.2450830648 -0.2484545036

Bonds

103 18 8 7

104 4 7 62

105 4 7 61

106 26 7 6

107 4 6 60

108 4 6 59

Angles

183 8 8 7 62

184 8 8 7 61

185 13 8 7 6

186 14 62 7 61

187 15 62 7 6

188 15 61 7 6

189 15 7 6 60

190 15 7 6 59

192 102 60 6 59

Dihedrals

231 47 8 7 6 60

232 47 8 7 6 59

235 47 62 7 6 60

236 47 62 7 6 59

238 47 61 7 6 60

239 47 61 7 6 59

C8

21 1 63 0.080000 -2.6152283304 0.349161419 2.8356396144

22 1 63 -0.180000 -1.8194444932 1.0873701054 3.7288521013

23 1 63 -0.092000 -0.8988937923 2.0023513434 3.2292818217

24 1 63 -0.099000 -0.75498857 2.2002075512 1.8506604987

54 1 63 -0.092000 -1.5555719863 1.4534135548 0.9761645337

55 1 63 -0.180000 -2.4808338958 0.5291150407 1.4536003336

80 1 20 0.137000 -0.2866216106 2.5722371975 3.944797364

79 1 20 0.142000 -1.9349045925 0.9331878663 4.8106662999

114 1 20 0.137000 -1.4455583251 1.595691464 -0.1107292832

115 1 20 0.142000 -3.0900845958 -0.0453998798 0.7428081322

Bonds

68 3 55 115

69 17 55 21

70 17 21 22

64 17 24 54

65 17 24 23

67 15 54 55

66 39 54 114

72 3 22 79

73 15 22 23

74 39 23 80

Angles

114 27 54 24 23

115 25 24 54 114

116 27 24 54 55

117 25 114 54 55

118 25 54 55 115

119 27 54 55 21

120 25 115 55 21

121 27 55 21 22

124 25 21 22 79

125 27 21 22 23

126 25 79 22 23

127 27 24 23 22

128 25 24 23 80

129 25 22 23 80

Dihedrals

146 47 24 54 55 115

147 15 24 54 55 21

148 15 54 24 23 22

149 47 54 24 23 80

150 15 54 55 21 22

151 47 54 55 21 20

152 47 114 54 55 115

153 47 114 54 55 21

154 47 55 21 22 79

155 15 55 21 22 23

157 47 115 55 21 22

159 15 21 22 23 24

160 47 21 22 23 80

165 47 79 22 23 24

166 47 79 22 23 80

167 47 23 24 54 114

Impropers

5 1 22 21 79 23

6 1 23 24 22 80

17 1 54 24 114 55

18 1 55 54 115 21

C9

Atoms # full

25 1 63 0.036000 0.2044925953 3.2120184173 1.2711887559

26 1 12 -0.204000 -0.6251365917 4.3653994692 0.7069965196

27 1 12 -0.204000 1.1434737014 3.7923291157 2.3284979703

81 1 20 0.079000 -1.2645228709 4.7965751499 1.5147838431

82 1 20 0.079000 0.0418976256 5.170672733 0.3167432334

83 1 20 0.079000 -1.2892177249 4.0065384388 -0.1151280698

84 1 20 0.079000 1.7010303694 2.9786155138 2.8503288063

85 1 20 0.079000 1.8826834377 4.4720870462 1.8399348735

86 1 20 0.079000 0.5668318641 4.3816862241 3.0810233667

Bonds

55 27 25 27

56 27 25 26

58 4 27 86

59 4 27 85

60 4 27 84

61 4 26 83

62 4 26 82

63 4 26 81

Angles

97 13 27 25 26

100 14 25 27 86

101 14 25 27 85

102 14 25 27 84

103 47 86 27 85

104 47 86 27 84

105 47 85 27 84

106 14 25 26 83

107 14 25 26 82

108 14 25 26 81

109 47 83 26 82

110 47 83 26 81

111 47 82 26 81

Dihedrals

130 47 27 25 26 83

131 47 27 25 26 82

132 47 27 25 26 81

135 47 26 25 27 86

136 47 26 25 27 85

137 47 26 25 27 84