Test Set

Database was originally assembled with ^{1}H data by Rablen, et al, *J. Phys. Chem. A* **1999**, 103, 7357-7363.

NMR data was aquired from the following sources:

S: Sadtler Index, Sadtler Research Laboratories, Division of Bio-Rad Laboratories, Researchers, Editors, and Publishers: 3316 Spring Garden St., Philadelphia, PA 19104; 1966-present. Numbers are index entries.

M: Silverstein, R. M.; Bassler, G. C.: Morrill, T. C. Spectrometric Identification of Organic Compounds, 5th ed; John Wiley and Sons: New York, 1991. Numbers are page numbers.

P: Properties of Organic Compounds database, Version 5.0, CRC Press: 1996. Numbers are CAS numbers.

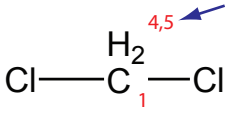
SDBS: Spectral Database for Organic Compounds, National Institute of Advanced Science and Technology (AIST), Japan. Numbers are SDBS entry numbers.

dichloromethane

^{1}H: S-6401 ← Exptl. Data Source

^{13}C: S-163

atom #'s in calc. files



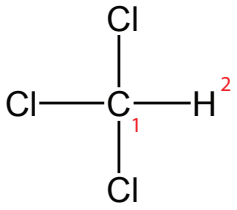
C(1): 53.70 H(4,5): 5.28

Exptl. NMR Shifts

chloroform

^{1}H: S-10513

^{13}C: S-270

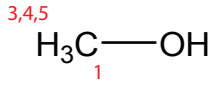


C(1): 77.20 H(2): 7.21

methanol

^{1}H: S-261

^{13}C: P-67-56-1



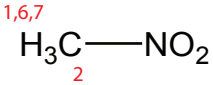
C(1): 49.80 H(3-5): 3.50

acidic H not included

nitromethane

^{1}H: S-9146

^{13}C: S-4002

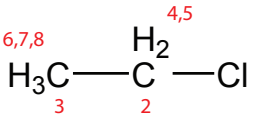


C(2): 63.00 H(1,6,7): 4.22

chloroethane

^{1}H: P-75-00-3

^{13}C: POC-75-00-3



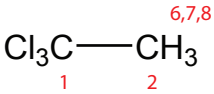
C(2): 39.90 H(4,5): 3.60

C(3): 18.70 H(6-8): 1.50

1,1,1-trichloroethane

^{1}H: S-9171

^{13}C: S-2322



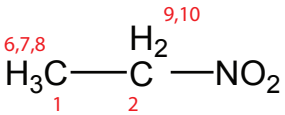
C(1): 95.20 H(6-8): 2.70

C(2): 45.40

nitroethane

^{1}H: S-2

^{13}C: S-402



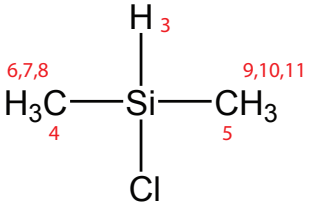
C(1): 12.40 H(6-8): 1.55

C(2): 70.90 H(9,10): 4.40

chlorodimethylsilane

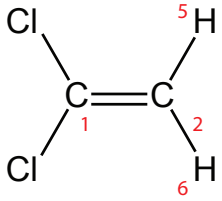
^{1}H: S-53563

^{13}C: SDBS-3863



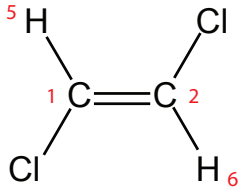
C(4,5): 1.27 H(3-11): 0.54

1,1-dichloroethylene
^{1}H: S-6385
^{13}C: S-1090



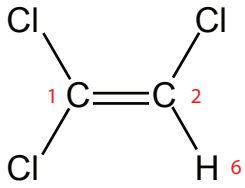
C(1): 128.90 H(5,6): 5.50
C(2): 115.50

trans-1,2-dichloroethylene
^{1}H: S-6742
^{13}C: S-6222



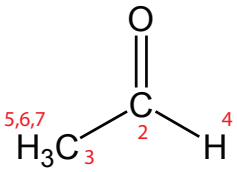
C(1,2): 120.3 H(5,6): 6.36

trichloroethylene
^{1}H: S-9266
^{13}C: S-410



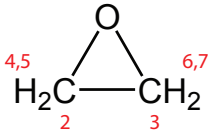
C(1): 124.10 H(6): 6.49
C(2): 116.70

acetaldehyde
^{1}H: S-10493
^{13}C: POC-75-07-0



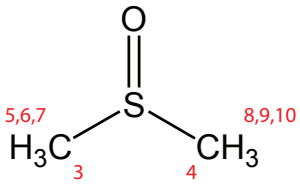
C(2): 199.70 H(4): 9.69
C(3): 30.70 H(5-7): 2.12

oxirane
^{1}H: M-214
^{13}C: M-237



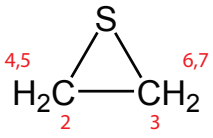
C(2,3): 39.50 H(4-7): 2.54

dimethylsulfoxide
^{1}H: P-67-68-5
^{13}C: S-1043



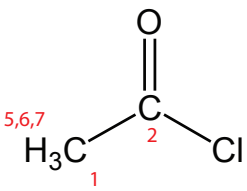
C(3,4): 40.60 H(5-10): 2.50

thiirane
^{1}H: M-214
^{13}C: M-237



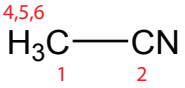
C(2,3): 18.70 H(4-7): 2.27

acetyl chloride
^{1}H: S-8780
^{13}C: S-2939



C(1): 33.70 H(5-7): 2.66
C(2): 170.30

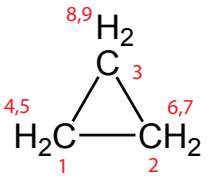
acetonitrile
^{1}H: S-9154
^{13}C: S-65



C(1): 1.70 H(4-6): 1.94
C(2): 117.40

cyclopropane

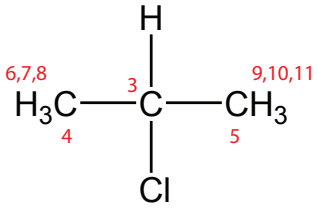
^{1}H: M-214
^{13}C: M-237



C(1-3): -2.90 H(4-9): 0.22

2-chloropropane

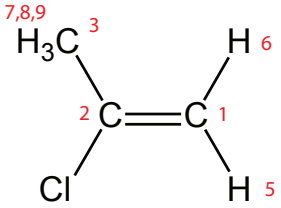
^{1}H: S-6866
^{13}C: S-59



C(2): 53.60 H(3): 4.11
C(4,5): 27.40 H(6-11): 1.51

2-chloropropene

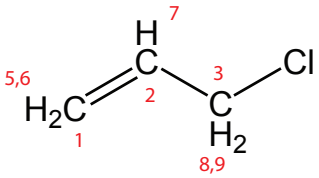
^{1}H: S-61833
^{13}C: SDBS-9806



C(1): 112.63 H(5,6): 5.12
C(2): 138.56 H(7-9): 2.13
C(3): 26.05

3-chloropropene (allylchloride)

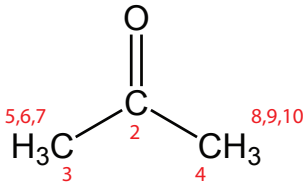
^{1}H: S-7833
^{13}C: S-415



C(1): 118.30 H(5): 5.15
C(2): 134.30 H(6): 5.29
C(3): 45.10 H(7): 5.90
H(8,9): 3.99

acetone

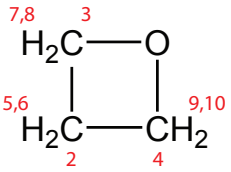
^{1}H: S-9288
^{13}C: S-413



C(3,4): 30.60 H(5-10): 2.11
C(2): 205.80

oxetane

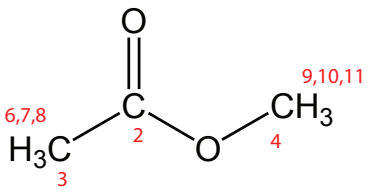
^{1}H: M-214
^{13}C: M-237



C(2): 22.90 H(5,6): 2.72
C(3,4): 72.60 H(7-10): 4.73

methyl acetate

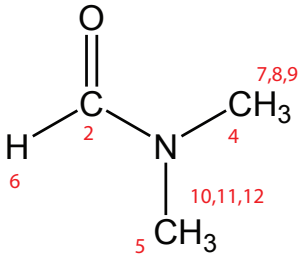
^{1}H: S-10261
^{13}C: S-478



C(2): 171.20 H(6-8): 2.00
C(3): 20.40 H(9-11): 3.65
C(4): 51.40

N,N-dimethylformamide

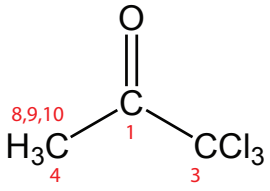
^{1}H: S-9537
^{13}C: S-408



C(2): 162.50 H(6): 7.89
C(4): 31.10 H(7-9): 2.98
C(5): 36.10 H(10-12): 2.81

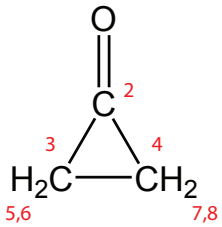
1,1,1-trichloroacetone

^{1}H: S-61585
^{13}C: SDBS-19141



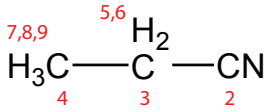
C(1): 187.44 H(8-10): 2.64
C(3): 96.32
C(4): 21.51

cyclopropanone
^{1}H: M-214
^{13}C: data not available



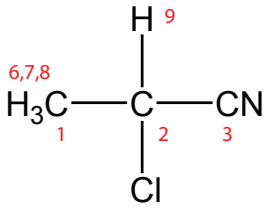
C: N/A H(5-8): 1.65

propionitrile
^{1}H: S-1877
^{13}C: S-1807



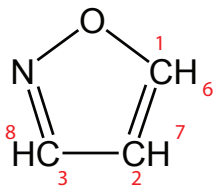
C(2): 121.00 H(5,6): 2.34
C(3): 10.60 H(7-9): 1.25
C(4): 10.90

2-Cl-propionitrile
^{1}H: S-45921
^{13}C: SDBS-15228



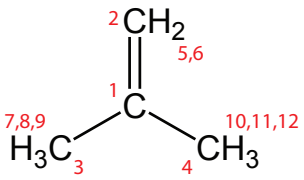
C(1): 23.40 H(6-8): 1.85
C(2): 37.83 H(9): 4.53
C(3): 117.90

isoxazole
^{1}H: S-12784
^{13}C: SDBS-9665



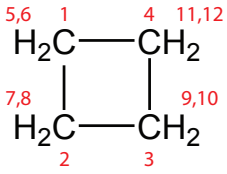
C(1): 157.81 H(6): 8.49
C(2): 103.61 H(7): 6.32
C(3): 149.08 H(8): 8.24

2-methylpropene
(isobutylene)
^{1}H: S-31633
^{13}C: JPC 1975 79 2031-2037



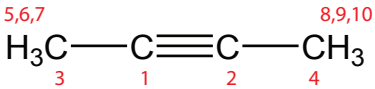
C(1): 141.35 H(5,6): 4.60
C(2): 110.57 H(7-12): 1.72
C(3,4): 23.45

cyclobutane
^{1}H: M-214
^{13}C: M-237



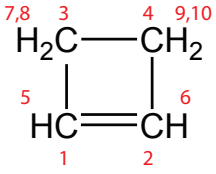
C(1-4): 2240 H(5-12): 1.96

2-butyne
^{1}H: S-8170
^{13}C: SDBS-263



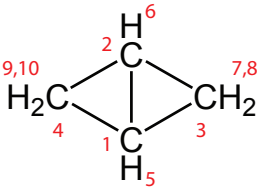
C(1,2): 74.56 H(5-10): 1.70
C(3,4): 3.33

cyclobutene
^{1}H: M-217
^{13}C: M-238



C(1,2): 137.20 H(5,6): 5.95
C(3,4): 30.20 H(7-10): 2.57

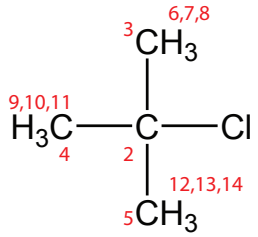
bicyclobutane
^{1}H: J. Am. Chem. Soc.
1966 88 5272-5275
^{13}C: data not available



C: N/A H(5,6): 1.37
H(7,9): 1.47
H(8,10): 0.44

2-chloro-2-methylpropane (t-butylchloride)

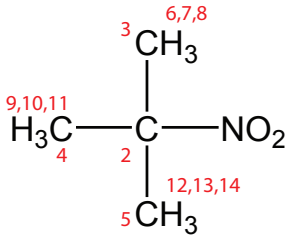
^{1}H: S-6768
^{13}C: S-328



C(2): 66.50 H(6-14): 1.61
C(3-5): 34.50

2-methyl-2-nitropropane

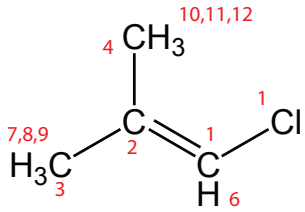
^{1}H: S-19967
^{13}C: S-5376



C(2): 85.20 H(8-16): 1.61
C(3-5): 27.80

1-chloro-2-methylpropene

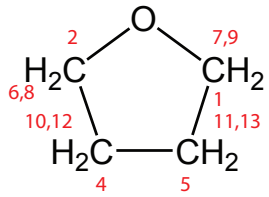
^{1}H: S-53505
^{13}C: SDBS-3999



C(1): 111.64 H(6): 5.79
C(2): 134.91 H(7-9): 1.80
C(3): 22.85 H(10-12): 1.80
C(4): 18.16

tetrahydrofuran

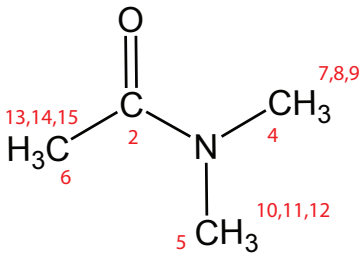
^{1}H: S-14667
^{13}C: S-22



C(2,3): 68.00 H(6-9): 3.71
C(4,5): 26.00 H(10-13): 1.81

N,N-dimethylacetamide

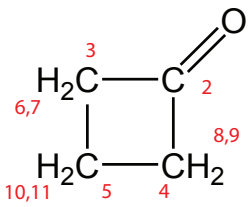
^{1}H: S-8875
^{13}C: S-95



C(2): 170.00 H(7-9): 2.83
C(4): 34.80 H(10-12): 3.01
C(5): 37.90 H(13-15): 1.98
C(6): 21.40
C4 & C5 assignment switched

cyclobutanone

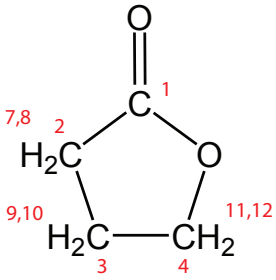
^{1}H: S-5006
^{13}C: Analytica Chimica Acta 2004 502 141-147



C(2): 208.90 H(6-9): 3.08
C(3,4): 47.80 H(10,11): 2.03
C(5): 9.90

butyrolactone

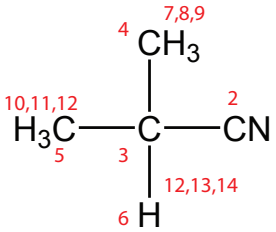
^{1}H: M-214
^{13}C: M-246



C(1): 177.90 H(7,8): 2.31
C(2): 27.70 H(9,10): 2.08
C(3): 22.20 H(11,12): 4.38
C(4): 68.60

2-methylpropanenitrile

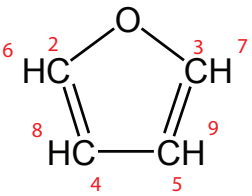
^{1}H: P-78-82-0
^{13}C: S-1873



C(2): 123.83 H(6): 2.70
C(3): 19.87 H(7-12): 1.30
C(4,5): 19.98

furan

^{1}H: S-16937
^{13}C: S-570

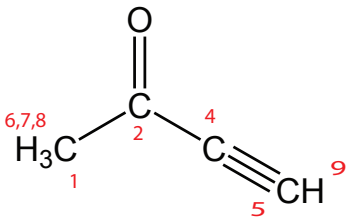


C(2,3): 142.80 H(6,7): 7.40
C(4,5): 109.70 H(8,9): 6.30

3-butyne-2-one

^{1}H: S-13388

^{13}C: ?

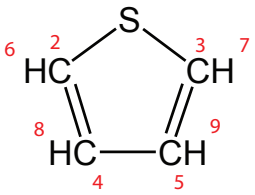


C(1): 32.20 H(6-8): 2.38
C(2): 183.80 H(9): 3.40
C(4): 81.90
C(5): 78.80

thiophene

^{1}H: S-10285

^{13}C: S-1202

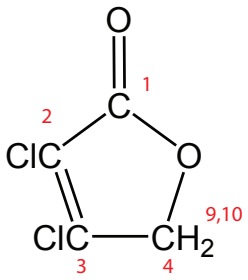


C(2,3): 125.00 H(6,7): 7.10
C(4,5): 126.70 H(8,9): 6.90

3,4-dichloro-2(5H)-furanone

^{1}H: S-53884

^{13}C: Synthesis 2007 12 1887-1889

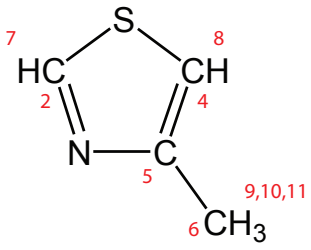


C(1): 165.70 H(9,10): 4.90
C(2): 121.20
C(3): 148.90
C(4): 70.90

methylthiazole

^{1}H: S-49793

^{13}C: SDBS-3323

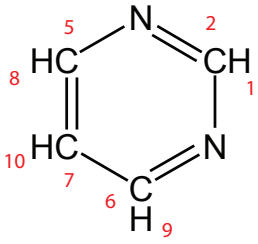


C(2): 152.14 H(7): 8.72
C(4): 113.11 H(8): 6.92
C(5): 153.49 H(9-11): 2.50
C(6): 16.77

pyrimidine

^{1}H: S-33550

^{13}C: POC-289-95-2

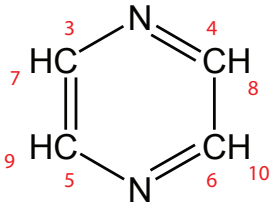


C(2): 159.20 H(1): 9.21
C(5,6): 157.60 H(8,9): 8.74
C(7): 122.60 H(10): 7.32

1,4-pyrizine

^{1}H: S-553

^{13}C: POC-290-37-9

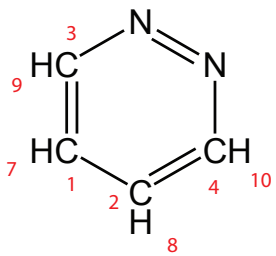


C(3-6): 146.10 H(7-10): 8.48

1,2-pyrazine

^{1}H: M-219

^{13}C: POC-289-80-5

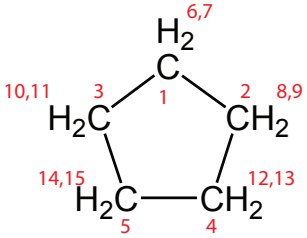


C(1,2): 127.70 H(7,8): 7.50
C(3,4): 152.60 H(9,10): 9.24

cyclopentane

^{1}H: S-3435

^{13}C: POC-287-92-3

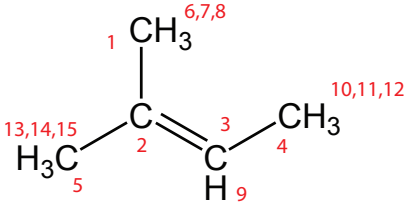


C(1-5): 26.50 H(6-15): 1.50

2-methyl-2-butene

^{1}H: S-3411

^{13}C: S-428

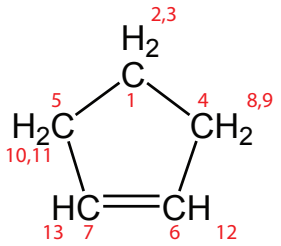


C(1): 17.30 H(6-8): 1.58
C(2): 132.00 H(9): 5.12
C(3): 118.80 H(10-12): 1.48
C(4): 13.40 H(13-15): 1.58
C(5): 25.60

cyclopentene

^{1}H: S-5162

^{13}C: S-5162

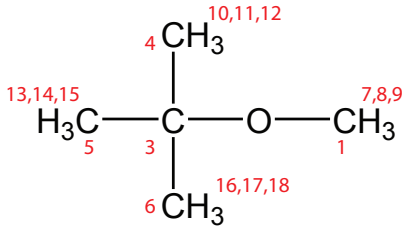


C(1): 22.98 H(2,3): 1.85
C(4,5): 32.59 H(8-11): 2.29
C(6,7): 130.77 H(12,13): 5.66

methyl tert-butyl ether

^{1}H: S19010

^{13}C: ?

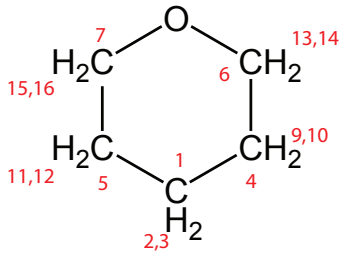


C(1): 49.41 H(7-9): 3.11
C(3): 72.80 H(10-18): 1.12
C(4-6): 27.06

tetrahydropyran

^{1}H: S-7566

^{13}C: S-2848

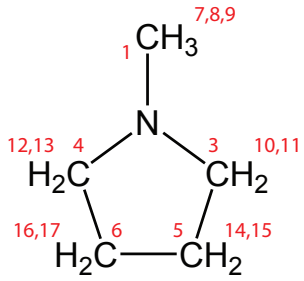


C(1): 24.00 H(2,3): 1.59
C(4,5): 27.10 H(9-12): 1.59
C(6,7): 68.80 H(13-16): 3.56

N-methylpyrrolidine

^{1}H: S-5091

^{13}C: POC-120-94-5

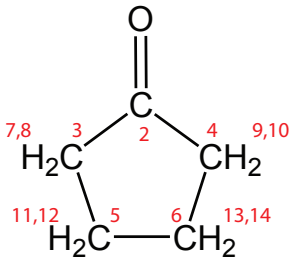


C(1): 42.90 H(7-9): 2.34
C(3,4): 56.90 H(10-13): 2.48
C(5,6): 24.60 H(14-17): 1.78

cyclopentanone

^{1}H: S-1195

^{13}C: S-42

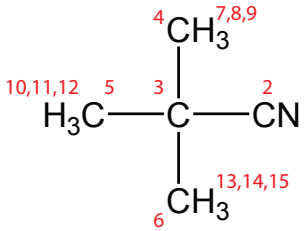


C(2): 219.60 H(11-14): 2.02
C(3,4): 38.20
C(5,6): 23.40

t-butylcyanide (pivalonitrile)

^{1}H: S-21352

^{13}C: S-2537

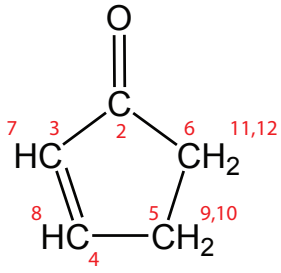


C(2): 125.90 H(7-15): 1.39
C(3): 28.12
C(4-6): 28.41

2-cyclopentenone

^{1}H: S-14728

^{13}C: SDBS-382

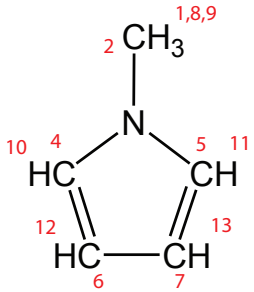


C(2): 210.45 H(7): 6.09
C(3): 134.37 H(8): 7.72
C(4): 165.25 H(9,10): 2.69
C(5): 29.03 H(11,12): 2.22
C(6): 34.02

N-methylpyrrole

^{1}H: S-21175

^{13}C: S-2958

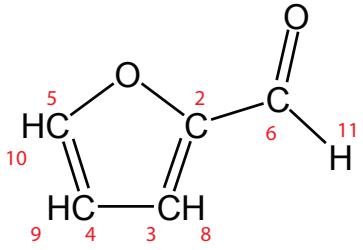


C(2): 35.60 H(1,8,9): 3.62
C(4,5): 121.60 H(10,11): 6.57
C(6,7): 108.30 H(12,13): 6.11

furfural

^{1}H: S-10203

^{13}C: S-1618

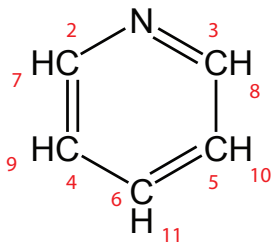


C(2): 153.30 H(8): 7.11
C(3): 121.90 H(9): 6.52
C(4): 112.90 H(10): 7.61
C(5): 148.60 H(11): 9.63
C(6): 178.10

pyridine

^{1}H: S-10200

^{13}C: S-1201

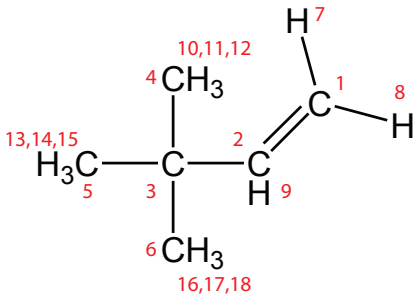


C(2,3):	149.90	H(7,8):	8.51
C(4,5):	123.70	H(9,10):	7.14
C(6):	135.70	H(11):	7.55

3,3-dimethyl-1-butene

^{1}H: S-5318

^{13}C: S-232

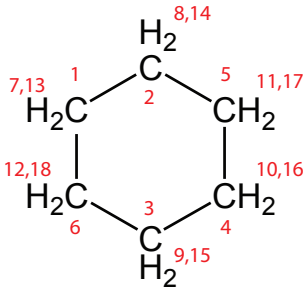


C(1):	109.00	H(7):	4.78
C(2):	149.80	H(8):	4.82
C(3):	33.70	H(9):	5.80
C(4-6):	29.40	H(10-18):	1.00

cyclohexane

^{1}H: S-1196

^{13}C: S-1403

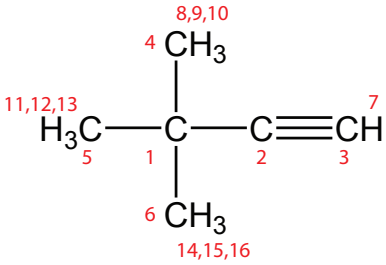


C(1-6):	27.30	H(7-18):	1.42

t-butylacetylene

^{1}H: S-13789

^{13}C: SDBS-22638

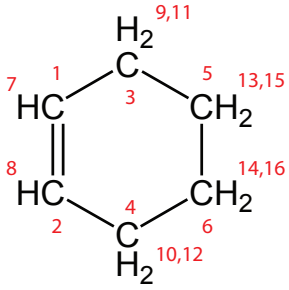


C(1):	27.25	H(7):	1.89
C(2):	92.97	H(8-16):	1.21
C(3):	66.52		
C(4-6):	30.92		

cyclohexene

^{1}H: S-3409

^{13}C: S-1808

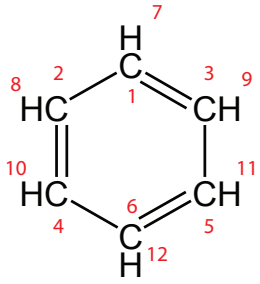


C(1,2):	127.30	H(7,8):	5.58
C(3,4):	25.40	H(9-12):	1.97
C(5,6):	22.90	H(13-16):	1.62

benzene

^{1}H: S-3429

^{13}C: S-425

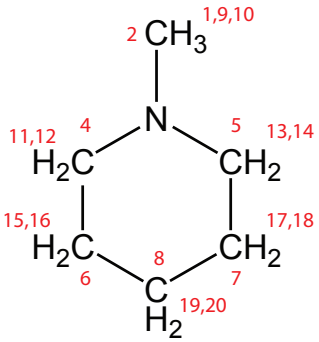


C(1-6):	128.50	H(7-12):	7.23

N-methylpiperidine

^{1}H: S-2849

^{13}C: SDBS-2418

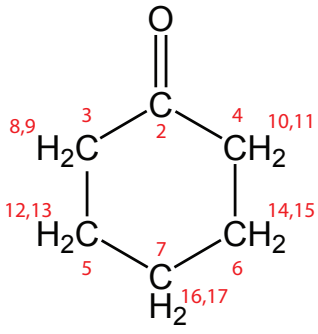


C(2):	46.85	H(1,9,10):	2.10
C(4,5):	56.59	H(11-14):	2.23
C(6,7):	26.01	H(15-18):	1.42
C(8):	23.85	H(19,20):	1.42

cyclohexanone

^{1}H: S-10208

^{13}C: S-409

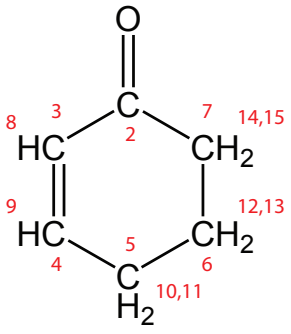


C(1):	211.20	H(8-11):	2.25
C(3,4):	41.90	H(12-15):	1.79
C(5,6):	27.20	H(16,17):	1.79
C(7):	25.10		

2-cyclohexenone

^{1}H: S-9880

^{13}C: S-2313

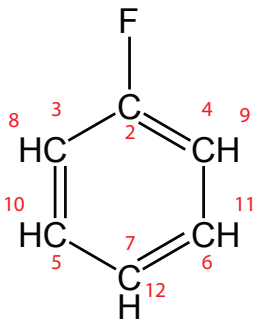


C(2):	198.70	H(8):	5.88
C(3):	129.80	H(9):	6.91
C(4):	150.60	H(10,11):	2.10
C(5):	25.80	H(12,13):	2.10
C(6):	22.90	H(14,15):	2.10
C(7):	38.20		

fluorobenzene

^{1}H: S-8774

^{13}C: S-1419

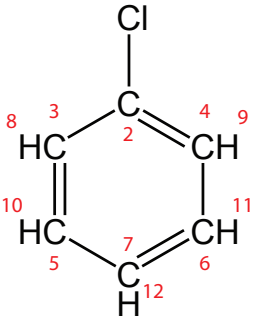


C(2):	163.30	H(8,9):	7.00
C(3,4):	115.50	H(10,11):	7.00
C(5,6):	130.20	H(12):	7.00
C(7):	124.20		

chlorobenzene

^{1}H: S-714

^{13}C: S-1402

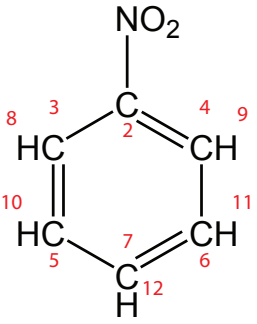


C(2):	134.40	H(8,9):	7.22
C(3,4):	128.60	H(10,11):	7.22
C(5,6):	129.70	H(12):	7.22
C(7):	126.40		

nitrobenzene

^{1}H: S-4

^{13}C: S-1401

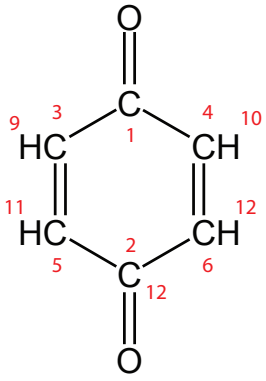


C(2):	148.30	H(8,9):	8.20
C(3,4):	123.50	H(10,11):	7.57
C(5,6):	129.50	H(12):	7.57
C(7):	134.80		

p-benzoquinone

^{1}H: S-10391

^{13}C: S-2810

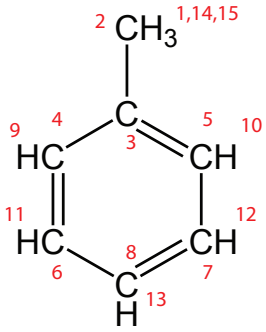


C(1,2):	187.20	H(9-12):	6.79
C(3-6):	136.60		

toluene

^{1}H: S-10216

^{13}C: S-91

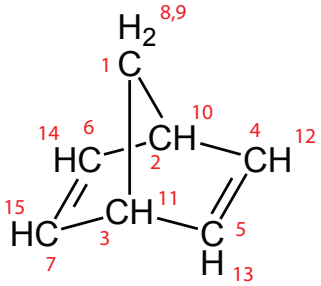


C(2):	21.40	H(9,10):	7.04
C(3):	137.70	H(11,12):	7.04
C(4,5):	130.00	H(13):	7.04
C(6,7):	129.20	H(1,14,15):	2.29
C(8):	126.60		

2,5-norbornadiene

^{1}H: S-16943

^{13}C: S-2992

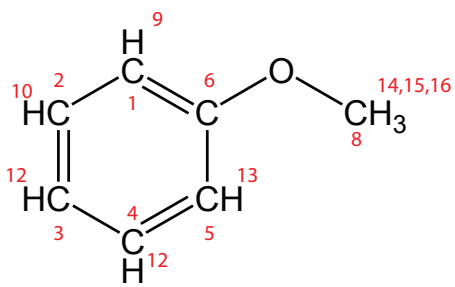


C(1):	75.20	H(8,9):	1.96
C(2,3):	50.30	H(10,11):	3.52
C(4-7):	143.20	H(12-15):	6.69

anisole

^{1}H: S-9115

^{13}C: S-526

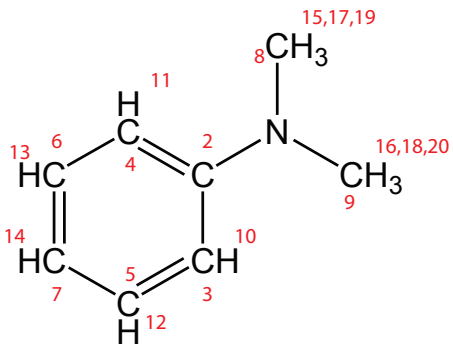


C(1):	159.90	H(9,13):	6.80
C(2,6):	114.10	H(10,12):	7.19
C(3,5):	129.50	H(11):	6.80
C(4):	120.70	H(14-16):	3.70
C(8):	54.80		

N,N-dimethylaniline

^{1}H: S-1

^{13}C: S-2

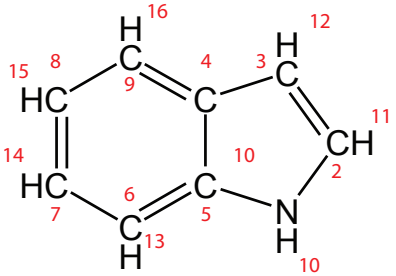


C(2):	150.70	H(10,11):	6.56
C(3,4):	112.70	H(12,13):	7.10
C(5,6):	129.00	H(14):	6.50
C(7):	116.60	H(15-20):	2.85
C(8,9):	40.20		

indole

^{1}H: S-473

^{13}C: S-451



C(2):	121.70	H(11):	6.76
C(3):	101.90	H(12):	6.38
C(4):	127.60	H(13):	7.03
C(5):	135.60	H(14):	7.03
C(6):	111.10	H(15):	7.03
C(7):	124.30	H(16):	7.50
C(8):	119.70		
C(9):	120.60		

H10 not included

C3 & C6 assignment swapped