1

H 0 2

H1

1

He 0 1

He1

1

Li 0 2

Li1

1

Be 0 1

Be1

1

B 0 2

B1

1

C 0 3

C1

1

N 0 4

N1

1

O 0 3

O1

1

F 0 2

F1

1

Ne 0 1

Ne1

1

Na 0 2

Na1

1

Mg 0 1

Mg1

1

Al 0 2

Al1

1

Si 0 3

Si1

1

P 0 4

P1

1

S 0 3

S1

1

Cl 0 2

Cl1

1

Ar 0 1

Ar1

4

CH3 0 2 Methyl radical

C1 0.0000 0.0000 0.0000

H2 1.0790 0.0000 0.0000

H3 -0.5395 -0.9344 0.0000

H4 -0.5395 0.9344 0.0000

5

CH4 0 1 Methane

C1 0.0000 0.0000 0.0000

H2 0.6276 0.6276 0.6276

H3 0.6276 -0.6276 -0.6276

H4 -0.6276 0.6276 -0.6276

H5 -0.6276 -0.6276 0.6276

2

NH 0 3 NH triplet

N1 0.0000 0.0000 0.0000

H2 0.0000 0.0000 1.0362

3

NH2 0 2 radical

N1 0.0000 0.0000 0.0000

H2 0.0000 0.8036 0.6347

H3 0.0000 -0.8036 0.6347

4

NH3 0 1 Ammonia

N1 0.0000 0.0000 0.0000

H2 0.0000 -0.9377 -0.3816

H3 0.8121 0.4689 -0.3816

H4 -0.8121 0.4689 -0.3816

2

OH 0 2 radical

O1 0.0000 0.0000 0.0000

H2 0.0000 0.0000 0.9697

3

H2O 0 1 Water

O1 0.0000 0.0000 0.1173

H2 0.0000 0.7572 -0.4692

H3 0.0000 -0.7572 -0.4692

2

HF 0 1 Hydrogen fluoride

F1 0.0000 0.0000 0.0000

H2 0.0000 0.0000 0.9168

4

SiH3 0 2 Silyl radical

Si1 0.0000 0.0000 0.0819

H2 0.0000 1.3928 -0.3820

H3 1.2062 -0.6964 -0.3820

H4 -1.2062 -0.6964 -0.3820

5

SiH4 0 1 Silane

Si1 0.0000 0.0000 0.0000

H2 0.8544 0.8544 0.8544

H3 -0.8544 -0.8544 0.8544

H4 -0.8544 0.8544 -0.8544

H5 0.8544 -0.8544 -0.8544

4

PH3 0 1 Phosphine

P1 0.0000 0.0000 0.0000

H2 0.0000 -1.1932 -0.7717

H3 1.0333 0.5966 -0.7717

H4 -1.0333 0.5966 -0.7717

3

SH2 0 1 Hydrogen sulfide

S1 0.0000 0.0000 0.0000

H2 0.0000 0.9569 0.9208

H3 0.0000 -0.9569 0.9208

2

HCl 0 1 Hydrogen chloride

Cl1 0.0000 0.0000 0.0000

H2 0.0000 0.0000 1.2746

4

HCCH 0 1 Acetylene

C1 0.0000 0.0000 0.6013

C2 0.0000 0.0000 -0.6013

H3 0.0000 0.0000 1.6644

H4 0.0000 0.0000 -1.6644

6

CH2CH2 0 1 Ethylene CH2=CH2

C1 0.0000 0.0000 0.6695

C2 0.0000 0.0000 -0.6695

H3 0.0000 0.9289 1.2321

H4 0.0000 -0.9289 1.2321

H5 0.0000 0.9289 -1.2321

H6 0.0000 -0.9289 -1.2321

8

CH3CH3 0 1 Ethane CH3-CH3

C1 0.0000 0.0000 0.7680

C2 0.0000 0.0000 -0.7680

H3 -1.0192 0.0000 1.1573

H4 0.5096 0.8826 1.1573

H5 0.5096 -0.8826 1.1573

H6 1.0192 0.0000 -1.1573

H7 -0.5096 -0.8826 -1.1573

H8 -0.5096 0.8826 -1.1573

3

HCN 0 1 Hydrogen cyanide

C1 0.0000 0.0000 0.0000

H2 0.0000 0.0000 1.0640

N3 0.0000 0.0000 -1.1560

2

CO 0 1 Carbon monoxide

C1 0.0000 0.0000 0.0000

O2 0.0000 0.0000 1.1283

3

HCO 0 2 radical

C1 0.0000 0.0000 0.0000

H2 1.0800 0.0000 0.0000

O3 -0.5899 1.0427 0.0000

4

CH2O 0 1 Formaldehyde CH2=O

O1 0.0000 0.0000 1.2050

C2 0.0000 0.0000 0.0000

H3 0.0000 0.9429 -0.5876

H4 0.0000 -0.9429 -0.5876

6

CH3OH 0 1 Methanol CH3-OH

C1 -0.0503 0.6685 0.0000

O2 -0.0503 -0.7585 0.0000

H3 -1.0807 1.0417 0.0000

H4 0.4650 1.0417 0.8924

H5 0.4650 1.0417 -0.8924

H6 0.8544 -1.0677 0.0000

2

N2 0 1 nitrogen molecule

N1 0.0000 0.0000 0.5488

N2 0.0000 0.0000 -0.5488

6

NH2NH2 0 1 Hydrazine NH2-NH2

N1 0.0000 0.7230 -0.1123

N2 0.0000 -0.7230 -0.1123

H3 -0.4470 1.0031 0.7562

H4 0.4470 -1.0031 0.7562

H5 0.9663 1.0031 0.0301

H6 -0.9663 -1.0031 0.0301

2

NO 0 2 radical

O1 0.0000 0.0000 0.0000

N2 0.0000 0.0000 1.1508

2

O2 0 3 oxygen molecule

O1 0.0000 0.0000 0.0000

O2 0.0000 0.0000 1.2075

4

HOOH 0 1 Hydrogen peroxide

O1 0.0000 0.7375 -0.0528

O2 0.0000 -0.7375 -0.0528

H3 0.8190 0.8170 0.4220

H4 -0.8190 -0.8170 0.4220

2

F2 0 1 fluorine molecule

F1 0.0000 0.0000 0.0000

F2 0.0000 0.0000 1.4119

3

CO2 0 1 Carbon dioxide

C1 0.0000 0.0000 0.0000

O2 0.0000 0.0000 1.1621

O3 0.0000 0.0000 -1.1621

2

P2 0 1

P1 0.0000 0.0000 0.0000

P2 0.0000 0.0000 1.8934

2

S2 0 3

S1 0.0000 0.0000 0.0000

S2 0.0000 0.0000 1.8892

2

Cl2 0 1 chlorine molecule

Cl1 0.0000 0.0000 0.0000

Cl2 0.0000 0.0000 1.9879

2

NaCl 0 1 Sodium Chloride

Na1 0.0000 0.0000 0.0000

Cl2 0.0000 0.0000 2.3608

2

SiO 0 1 Silicon monoxide

Si1 0.0000 0.0000 0.0000

O2 0.0000 0.0000 1.5097

2

CS 0 1 Carbon monosulfide

C1 0.0000 0.0000 0.0000

S2 0.0000 0.0000 1.5349

2

ClO 0 2 radical

O1 0.0000 0.0000 0.0000

Cl2 0.0000 0.0000 1.5696

2

ClF 0 1

F1 0.0000 0.0000 0.0000

Cl2 0.0000 0.0000 1.6283

8

SiH3SiH3 0 1 Disilane SiH3-SiH3

Si1 0.0000 0.0000 1.1600

Si2 0.0000 0.0000 -1.1600

H3 0.0000 1.3865 1.6483

H4 -1.2008 -0.6933 1.6483

H5 1.2008 -0.6933 1.6483

H6 0.0000 -1.3865 -1.6483

H7 -1.2008 0.6933 -1.6483

H8 1.2008 0.6933 -1.6483

5

CH3Cl 0 1 Methyl chloride

C1 0.0000 0.0000 0.0000

Cl2 0.0000 0.0000 1.7810

H3 1.0424 0.0000 -0.3901

H4 -0.5212 0.9027 -0.3901

H5 -0.5212 -0.9027 -0.3901

6

CH3SH 0 1 staggered Methanethiol

C1 -0.8500 -0.0344 -0.2000

S2 0.9000 -0.5125 -0.1219

H3 1.4219 0.5781 0.4250

H4 -0.9406 0.8688 -0.8219

H5 -1.4219 -0.8688 -0.6469

H6 -1.2031 0.1656 0.8219

3

SO2 0 1 Sulfur dioxide

S1 0.0000 0.0000 0.0000

O2 0.0000 1.2371 0.7215

O3 0.0000 -1.2371 0.7215

4

BF3 0 1

B1 0.0000 0.0000 0.0000

F2 0.0000 1.3070 0.0000

F3 1.1319 -0.6535 0.0000

F4 -1.1319 -0.6535 0.0000

4

BCl3 0 1

B1 0.0000 0.0000 0.0000

Cl2 0.0000 1.7421 0.0000

Cl3 1.5087 -0.8711 0.0000

Cl4 -1.5087 -0.8711 0.0000

4

AlCl3 0 1

Al1 0.0000 0.0000 0.0000

Cl2 0.0000 2.0600 0.0000

Cl3 1.7840 -1.0300 0.0000

Cl4 -1.7840 -1.0300 0.0000

5

CF4 0 1

C1 0.0000 0.0000 0.0000

F2 0.7593 0.7593 0.7593

F3 -0.7593 -0.7593 0.7593

F4 -0.7593 0.7593 -0.7593

F5 0.7593 -0.7593 -0.7593

5

CCl4 0 1

C1 0.0000 0.0000 0.0000

Cl2 1.0202 1.0202 1.0202

Cl3 -1.0202 -1.0202 1.0202

Cl4 -1.0202 1.0202 -1.0202

Cl5 1.0202 -1.0202 -1.0202

3

OCS 0 1 O=C=S Linear

C1 0.0000 0.0000 0.0000

O2 0.0000 0.0000 1.1600

S3 0.0000 0.0000 -1.5600

3

CS2 0 1 Linear

C1 0.0000 0.0000 0.0000

S2 0.0000 0.0000 1.5540

S3 0.0000 0.0000 -1.5540

4

CF2O 0 1

O1 0.0000 0.0000 1.3143

C2 0.0000 0.0000 0.1403

F3 0.0000 1.0614 -0.6309

F4 0.0000 -1.0614 -0.6309

5

SiF4 0 1

Si1 0.0000 0.0000 0.0000

F2 0.8972 0.8972 0.8972

F3 -0.8972 -0.8972 0.8972

F4 -0.8972 0.8972 -0.8972

F5 0.8972 -0.8972 -0.8972

3

N2O 0 1

N1 0.0000 0.0000 -1.1998

N2 0.0000 0.0000 -0.0716

O3 0.0000 0.0000 1.1126

4

NF3 0 1

N1 0.0000 0.0000 0.4731

F2 0.0000 1.2279 -0.1226

F3 1.0634 -0.6140 -0.1226

F4 -1.0634 -0.6140 -0.1226

4

PF3 0 1

P1 0.0000 0.0000 0.4602

F2 0.0000 1.3578 -0.2557

F3 1.1759 -0.6789 -0.2557

F4 -1.1759 -0.6789 -0.2557

3

O3 0 1 Ozone

O1 0.0000 0.0000 0.0000

O2 0.0000 1.0885 0.6697

O3 0.0000 -1.0885 0.6697

3

F2O 0 1

O1 0.0000 0.0000 0.6074

F2 0.0000 1.1063 -0.2700

F3 0.0000 -1.1063 -0.2700

4

ClF3 0 1

Cl1 0.0000 0.0000 0.3572

F2 0.0000 0.0000 -1.2408

F3 0.0000 1.6964 0.2831

F4 0.0000 -1.6964 0.2831

6

CF2CF2 0 1 C2F4 CF2=CF2

C1 0.0000 0.0000 0.6555

C2 0.0000 0.0000 -0.6555

F3 0.0000 1.0961 1.3893

F4 0.0000 -1.0961 1.3893

F5 0.0000 -1.0961 -1.3893

F6 0.0000 1.0961 -1.3893

6

CF3CN 0 1

C1 0.0000 0.0000 -0.3406

C2 0.0000 0.0000 1.1518

N3 0.0000 0.0000 2.3054

F4 0.0000 1.2540 -0.7780

F5 1.0860 -0.6270 -0.7780

F6 -1.0860 -0.6270 -0.7780

7

CH3CCH 0 1 Propyne

C1 0.0000 0.0000 -1.2455

C2 0.0000 0.0000 0.2135

C3 0.0000 0.0000 1.4195

H4 0.0000 0.0000 2.4755

H5 0.0000 1.0465 -1.6003

H6 0.9063 -0.5232 -1.6003

H7 -0.9063 -0.5232 -1.6003

7

CH2CCH2 0 1 Allene

C1 0.0000 0.0000 0.0000

C2 0.0000 0.0000 1.3080

C3 0.0000 0.0000 -1.3080

H4 0.0000 0.9327 1.8662

H5 0.0000 -0.9327 1.8662

H6 0.9327 0.0000 -1.8662

H7 -0.9327 0.0000 -1.8662

7

cylC3H4 0 1 Cyclopropene

C1 0.0000 0.0000 0.8628

C2 0.0000 0.6476 -0.5001

C3 0.0000 -0.6476 -0.5001

H4 0.0000 1.5745 -1.0386

H5 0.0000 -1.5745 -1.0386

H6 0.9154 0.0000 1.4509

H7 -0.9154 0.0000 1.4509

9

cylC3H6 0 1 Cyclopropane

C1 0.0000 0.8666 0.0000

C2 0.7505 -0.4333 0.0000

C3 -0.7505 -0.4333 0.0000

H4 0.0000 1.4525 0.9108

H5 1.2579 -0.7262 0.9108

H6 -1.2579 -0.7262 0.9108

H7 0.0000 1.4525 -0.9108

H8 1.2579 -0.7262 -0.9108

H9 -1.2579 -0.7262 -0.9108

11

CH3CH2CH3 0 1 Propane

C1 0.0000 0.5863 -0.0000

C2 -1.2681 -0.2626 0.0000

C3 1.2681 -0.2626 -0.0000

H4 0.0000 1.2449 0.8760

H5 -0.0003 1.2453 -0.8758

H6 -2.1576 0.3742 0.0000

H7 2.1576 0.3743 -0.0000

H8 -1.3271 -0.9014 0.8800

H9 -1.3271 -0.9014 -0.8800

H10 1.3271 -0.9014 -0.8800

H11 1.3272 -0.9014 0.8800

10

CH3CCCH3 0 1 Dimethylacetylene 2-butyne

C1 0.0000 0.0000 0.6070

C2 0.0000 0.0000 -0.6070

C3 0.0000 0.0000 2.0750

C4 0.0000 0.0000 -2.0750

H5 0.0000 1.0440 2.4695

H6 -0.9041 -0.5220 2.4695

H7 0.9041 -0.5220 2.4695

H8 0.0000 1.0440 -2.4695

H9 0.9041 -0.5220 -2.4695

H10 -0.9041 -0.5220 -2.4695

10

cylC4H6 0 1 Cyclobutene

C1 0.0000 0.6710 0.8107

C2 0.0000 -0.6710 0.8107

C3 0.0000 0.7821 -0.7023

C4 0.0000 -0.7821 -0.7023

H5 0.0000 1.4165 1.5962

H6 0.0000 -1.4165 1.5962

H7 0.8986 1.2425 -1.1233

H8 -0.8986 -1.2425 -1.1233

H9 -0.8986 1.2425 -1.1233

H10 0.8986 -1.2425 -1.1233

14

isobutane 0 1 isobutane

C1 0.0000 0.0000 0.3650

H2 0.0000 0.0000 1.4730

C3 0.0000 1.4528 -0.0987

C4 1.2582 -0.7264 -0.0987

C5 -1.2582 -0.7264 -0.0987

H6 0.0000 1.4867 -1.1931

H7 1.2875 -0.7433 -1.1931

H8 -1.2875 -0.7433 -1.1931

H9 0.8941 1.9575 0.2821

H10 -0.8941 1.9575 0.2821

H11 1.2482 -1.7530 0.2821

H12 2.1422 -0.2045 0.2821

H13 -2.1422 -0.2045 0.2821

H14 -1.2482 -1.7530 0.2821

12

benzene 0 1 Benzene

C1 0.0000 1.3970 0.0000

C2 1.2098 0.6985 0.0000

C3 1.2098 -0.6985 0.0000

C4 0.0000 -1.3970 0.0000

C5 -1.2098 -0.6985 0.0000

C6 -1.2098 0.6985 0.0000

H7 0.0000 2.4810 0.0000

H8 2.1486 1.2405 0.0000

H9 2.1486 -1.2405 0.0000

H10 0.0000 -2.4810 0.0000

H11 -2.1486 -1.2405 0.0000

H12 -2.1486 1.2405 0.0000

5

CH2F2 0 1 Difluoromethane

C1 0.0000 0.0000 0.5003

H2 -0.9029 0.0000 1.1002

H3 0.9029 0.0000 1.1002

F4 0.0000 1.0962 -0.2890

F5 0.0000 -1.0962 -0.2890

5

CF3H 0 1 Trifluoromethane

C1 0.0000 0.0000 0.3086

H2 0.0000 0.0000 1.4066

F3 0.0000 1.2609 -0.1207

F4 1.0920 -0.6305 -0.1207

F5 -1.0920 -0.6305 -0.1207

5

CH2Cl2 0 1 Dichloromethane

C1 0.0000 0.0000 0.7761

H2 -0.8854 0.0000 1.3734

H3 0.8854 0.0000 1.3734

Cl4 0.0000 1.4675 -0.2178

Cl5 0.0000 -1.4675 -0.2178

5

CCl3H 0 1 Chloroform

C1 0.0000 0.0000 0.5231

H2 0.0000 0.0000 1.5961

Cl3 0.0000 1.6562 -0.0928

Cl4 1.4343 -0.8281 -0.0928

Cl5 -1.4343 -0.8281 -0.0928

7

CH3NO2 0 1 Nitromethane CH3-NO2

C1 1.4008 0.0000 0.0000

N2 -0.0878 0.0000 0.0000

H3 1.7215 -1.0392 0.0000

H4 1.7215 0.5196 0.9000

H5 1.7215 0.5196 -0.9000

O6 -0.6498 1.0874 0.0000

O7 -0.6498 -1.0874 0.0000

8

CH3SiH3 0 1 Methylsilane CH3-SiH3

C1 0.0000 0.0000 -1.2367

Si2 0.0000 0.0000 0.6319

H3 0.0000 -1.0237 -1.6272

H4 -0.8866 0.5119 -1.6272

H5 0.8866 0.5119 -1.6272

H6 0.0000 1.3893 1.1514

H7 -1.2031 -0.6946 1.1514

H8 1.2031 -0.6946 1.1514

5

HCOOH 0 1 Formic Acid HOCOcis

C1 0.0000 0.4199 0.0000

O2 -1.0543 -0.4121 0.0000

O3 1.1506 0.0721 0.0000

H4 -0.0799 1.5140 0.0000

H5 -0.6905 -1.3134 0.0000

9

CH3CONH2 0 1 Acetamide

C1 -1.3674 -0.3302 0.0013

C2 0.0720 0.1552 -0.0019

N3 1.0259 -0.8416 -0.0326

O4 0.3726 1.3376 0.0057

H5 -2.0656 0.5484 -0.0612

H6 -1.5426 -1.0080 -0.8780

H7 -1.5719 -0.9088 0.9430

H8 2.0050 -0.5675 0.0710

H9 0.7853 -1.8244 0.1113

8

cylNHC2H4 0 1 Aziridine cyclic CH2-NH-CH2-ring

N1 -0.0037 0.8559 -0.1934

H2 -0.0140 1.4040 0.6620

C3 -0.7380 -0.4043 0.0261

C4 0.7425 -0.3952 0.0380

H5 -1.2757 -0.4486 0.9652

H6 -1.2332 -0.8641 -0.8216

H7 1.2820 -0.7584 -0.8280

H8 1.2404 -0.5270 0.9918

4

NCCN 0 1 Cyanogen

C1 0.0000 0.0000 0.6950

C2 0.0000 0.0000 -0.6950

N3 0.0000 0.0000 1.8450

N4 0.0000 0.0000 -1.8450

10

CH3NHCH3 0 1 Dimethylamine

N1 0.0934 -0.5520 0.0000

H2 -0.6454 -1.2544 0.0000

C3 -0.0220 0.2554 1.2139

C4 -0.0220 0.2554 -1.2139

H5 -0.9221 0.8833 1.2437

H6 -0.9221 0.8833 -1.2437

H7 0.8440 0.9287 1.2609

H8 0.8440 0.9287 -1.2609

H9 -0.0138 -0.3909 2.0843

H10 -0.0138 -0.3909 -2.0843

5

CH2CO 0 1 Ketene H2C=C=O

C1 0.0000 0.0000 0.0000

C2 0.0000 0.0000 1.3150

O3 0.0000 0.0000 2.4750

H4 0.0000 0.9451 -0.5206

H5 0.0000 -0.9451 -0.5206

7

cylOC2H4 0 1 Oxirane cyclic CH2-O-CH2-ring

O1 0.0000 0.0000 0.8517

C2 0.0000 0.7297 -0.3725

C3 0.0000 -0.7297 -0.3725

H4 -0.9230 1.2565 -0.5859

H5 0.9230 1.2565 -0.5859

H6 0.9230 -1.2565 -0.5859

H7 -0.9230 -1.2565 -0.5859

6

OCHCHO 0 1 Glyoxal O=CH-CH=O Trans

C1 0.0000 0.7630 0.0000

C2 0.0000 -0.7630 0.0000

H3 1.0481 1.1907 0.0000

H4 -1.0481 -1.1907 0.0000

O5 -1.0367 1.3908 0.0000

O6 1.0367 -1.3908 0.0000

9

CH3CH2OH 0 1 Ethanol trans

C1 1.1879 -0.3829 0.0000

C2 0.0000 0.5526 0.0000

O3 -1.1867 -0.2472 0.0000

H4 -1.9237 0.3850 0.0000

H5 2.0985 0.2306 0.0000

H6 1.1184 -1.0093 0.8869

H7 1.1184 -1.0093 -0.8869

H8 -0.0227 1.1812 0.8852

H9 -0.0227 1.1812 -0.8852

9

CH3OCH3 0 1 DimethylEther CH3-O-CH3

O1 0.0000 0.0000 0.5952

C2 0.0000 1.1669 -0.1963

C3 0.0000 -1.1669 -0.1963

H4 0.0000 2.0489 0.4542

H5 0.0000 -2.0489 0.4542

H6 0.8950 1.1787 -0.8287

H7 -0.8950 1.1787 -0.8287

H8 -0.8950 -1.1787 -0.8287

H9 0.8950 -1.1787 -0.8287

7

cylSC2H4 0 1 Thiooxirane cyclic CH2-S-CH2-ring

S1 0.0000 0.0000 0.8622

C2 0.0000 0.7421 -0.7942

C3 0.0000 -0.7421 -0.7942

H4 -0.9174 1.2493 -1.0661

H5 0.9174 1.2493 -1.0661

H6 0.9174 -1.2493 -1.0661

H7 -0.9174 -1.2493 -1.0661

10

CH3SOCH3 0 1 Dimethylsulfoxide

S1 0.0000 0.1432 0.4202

O2 0.0000 1.4024 -0.3667

C3 1.3425 -0.8664 -0.2227

C4 -1.3425 -0.8664 -0.2227

H5 2.2553 -0.4311 0.0751

H6 -2.2553 -0.4311 0.0751

H7 1.3057 -1.8579 0.2349

H8 1.2255 -0.9383 -1.3113

H9 -1.3057 -1.8579 0.2349

H10 -1.2255 -0.9383 -1.3113

6

CH2CHF 0 1 Vinyl fluoride CH2=CHF

C1 0.0000 0.4476 0.0000

C2 1.1877 -0.1487 0.0000

F3 -1.1356 -0.2769 0.0000

H4 -0.2349 1.5038 0.0000

H5 1.2321 -1.2348 0.0000

H6 2.0966 0.4290 0.0000

8

CH3CH2Cl 0 1 Ethyl chloride CH3-CH2-Cl

C1 1.5949 -0.3563 -0.0000

C2 0.4757 0.6568 -0.0004

H3 2.5527 0.1648 0.0000

H4 1.5351 -0.9919 -0.8828

H5 1.5347 -0.9917 0.8828

Cl6 -1.1206 -0.1505 -0.0005

H7 0.5089 1.2945 -0.8790

H8 0.4949 1.2796 0.8893

6

CH2CHCl 0 1 Vinyl chloride CH2=CHCl

C1 0.0000 0.0000 1.3320

C2 0.0000 0.0000 0.0000

Cl3 0.0000 1.4589 2.2543

H4 0.0000 -0.9058 1.9384

H5 0.0000 0.9249 -0.5557

H6 0.0000 -0.9391 -0.5313

7

CH3CClO 0 1 Acetyl Chloride HCCOcis

C1 0.0000 0.5272 0.0000

C2 1.4961 0.6994 0.0000

O3 -0.8349 1.3710 0.0000

Cl4 -0.4665 -1.2092 0.0000

H5 1.7591 1.7726 0.0000

H6 1.9367 0.2285 0.8973

H7 1.9367 0.2285 -0.8973

11

prplCl 0 1 Propyl Chloride CH3-CH2-CH2-Cl

Cl1 1.7375 0.1388 0.0000

C2 0.0000 0.5937 0.0000

H3 -0.1639 1.2199 0.9054

H4 -0.1639 1.2199 -0.9054

C5 -0.8957 -0.6405 0.0000

H6 -0.6638 -1.2607 0.8947

H7 -0.6638 -1.2607 -0.8947

C8 -2.3710 -0.2543 0.0000

H9 -2.6338 0.3458 0.8998

H10 -2.6338 0.3458 -0.8998

H11 -3.0133 -1.1633 0.0000

13

NC3H9 0 1 Trimethyl Amine NCH33

N1 0.0000 -0.0000 -0.3852

C2 -0.9758 -0.9757 0.0634

C3 1.3330 -0.3571 0.0634

C4 -0.3572 1.3328 0.0634

H5 -1.0253 -1.0252 1.1492

H6 1.4006 -0.3752 1.1492

H7 -0.3753 1.4004 1.1492

H8 -1.9833 -0.7091 -0.3156

H9 -0.7093 -1.9833 -0.3156

H10 1.6060 -1.3629 -0.3156

H11 2.0722 0.3776 -0.3156

H12 0.3774 2.0722 -0.3156

H13 -1.3631 1.6057 -0.3156

9

cylOC4H4 0 1 Furan

O1 0.0000 0.0000 1.1626

C2 0.0000 1.0920 0.3487

C3 0.0000 -1.0920 0.3487

C4 0.0000 0.7169 -0.9596

C5 0.0000 -0.7169 -0.9596

H6 0.0000 2.0473 0.8439

H7 0.0000 -2.0473 0.8439

H8 0.0000 1.3509 -1.8290

H9 0.0000 -1.3509 -1.8290

10

cylNHC4H4 0 1 Pyrrole Planar

N1 0.0000 0.0000 1.1218

H2 0.0000 0.0000 2.1178

C3 0.0000 1.1209 0.3341

C4 0.0000 -1.1209 0.3341

C5 0.0000 0.7076 -0.9847

C6 0.0000 -0.7076 -0.9847

H7 0.0000 2.1084 0.7614

H8 0.0000 -2.1084 0.7614

H9 0.0000 1.3566 -1.8429

H10 0.0000 -1.3566 -1.8429

3

NO2 0 2 radical

N1 0.0000 0.0000 0.0000

O2 0.0000 1.0989 0.4653

O3 0.0000 -1.0989 0.4653

7

SF6 0 1

S1 0.0000 0.0000 0.0000

F2 0.0000 0.0000 1.5607

F3 0.0000 1.5607 0.0000

F4 1.5607 0.0000 0.0000

F5 0.0000 -1.5607 0.0000

F6 -1.5607 0.0000 0.0000

F7 0.0000 0.0000 -1.5607

5

CFCl3 0 1

C1 0.0000 0.0000 0.2472

F2 0.0000 0.0000 1.5922

Cl3 0.0000 1.6732 -0.3101

Cl4 1.4491 -0.8366 -0.3101

Cl5 -1.4491 -0.8366 -0.3101

5

CClF3 0 1

C1 0.0000 0.0000 -0.3471

Cl2 0.0000 0.0000 1.4049

F3 0.0000 1.2425 -0.8074

F4 1.0760 -0.6212 -0.8074

F5 -1.0760 -0.6212 -0.8074

5

CBrF3 0 1

C1 0.0000 0.0000 -0.8088

Br2 0.0000 0.0000 1.1146

F3 0.0000 1.2455 -1.2651

F4 1.0787 -0.6228 -1.2651

F5 -1.0787 -0.6228 -1.2651

4

HCCF 0 1

C1 0.0000 0.0000 -0.0942

C2 0.0000 0.0000 -1.2922

F3 0.0000 0.0000 1.1848

H4 0.0000 0.0000 -2.3452

5

HCCCN 0 1

N1 0.0000 0.0000 1.9018

C2 0.0000 0.0000 0.7413

C3 0.0000 0.0000 -0.6351

C4 0.0000 0.0000 -1.8409

H5 0.0000 0.0000 -2.9033

6

NCCCCN 0 1

C1 0.0000 0.0000 2.5100

C2 0.0000 0.0000 3.7000

C3 0.0000 0.0000 1.1400

C4 0.0000 0.0000 5.0700

N5 0.0000 0.0000 0.0000

N6 0.0000 0.0000 6.2100

4

C2N2 0 1

C1 0.0000 0.0000 0.6950

C2 0.0000 0.0000 -0.6950

N3 0.0000 0.0000 1.8450

N4 0.0000 0.0000 -1.8450

5

C3O2 0 1

C1 0.0000 0.0000 0.0308

C2 0.0000 1.2509 0.0123

C3 0.0000 -1.2509 0.0123

O4 0.0000 2.3964 -0.0207

O5 0.0000 -2.3964 -0.0207

3

FCN 0 1

C1 0.0000 0.0000 0.0000

F2 0.0000 0.0000 -1.2620

N3 0.0000 0.0000 1.1590

6

HCCCCH 0 1

C1 0.0000 0.0000 0.6890

C2 0.0000 0.0000 -0.6890

C3 0.0000 0.0000 1.8940

C4 0.0000 0.0000 -1.8940

H5 0.0000 0.0000 2.9520

H6 0.0000 0.0000 -2.9520

4

H2CS 0 1

S1 0.0000 0.0000 0.5846

C2 0.0000 0.0000 -1.0262

H3 0.0000 0.9244 -1.5980

H4 0.0000 -0.9244 -1.5980

6

HCONH2 0 1

C1 0.0000 0.4165 0.0000

O2 1.1942 0.2217 0.0000

N3 -0.9373 -0.5551 0.0000

H4 -0.4299 1.4182 0.0000

H5 -0.6608 -1.5171 0.0000

H6 -1.9020 -0.2881 0.0000

8

CH2CHCHO 0 1

C1 -0.1496 -0.7423 0.0000

C2 0.0000 0.7200 0.0000

C3 1.2291 1.2662 0.0000

O4 -1.2313 -1.3044 0.0000

H5 0.8007 -1.3120 0.0000

H6 -0.9066 1.3142 0.0000

H7 1.3716 2.3428 0.0000

H8 2.1072 0.6273 0.0000

6

CH2CCl2 0 1

C1 0.0000 0.0000 1.7363

C2 0.0000 0.0000 0.4123

H3 0.0000 0.9266 2.2713

H4 0.0000 -0.9266 2.2713

Cl5 0.0000 1.4382 -0.5128

Cl6 0.0000 -1.4382 -0.5128

6

CHFCF2 0 1

C1 0.0000 0.4436 0.0000

C2 -0.7139 -0.6916 0.0000

F3 1.3153 0.4857 0.0000

F4 -0.5506 1.6388 0.0000

F5 -0.0873 -1.8784 0.0000

H6 -1.8133 -0.7269 0.0000

6

CH2CF2 0 1

C1 0.0000 0.0000 1.3851

C2 0.0000 0.0000 0.0701

H3 0.0000 0.9419 1.9094

H4 0.0000 -0.9419 1.9094

F5 0.0000 1.0777 -0.6972

F6 0.0000 -1.0777 -0.6972

5

CH3F 0 1

C1 0.0000 0.0000 -0.6289

F2 0.0000 0.0000 0.7541

H3 0.0000 1.0201 -1.0043

H4 0.8835 -0.5101 -1.0043

H5 -0.8835 -0.5101 -1.0043

5

CF2Cl2 0 1

C1 0.0000 0.0000 0.3171

F2 0.0000 1.0758 1.1243

F3 0.0000 -1.0758 1.1243

Cl4 1.4505 0.0000 -0.6512

Cl5 -1.4505 0.0000 -0.6512

3

SiF2 0 1

Si1 0.0000 0.0000 0.5703

F2 0.0000 1.2249 -0.4436

F3 0.0000 -1.2249 -0.4436