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% Most data on the polarizability and Ionization energy are collected
from CCCBDB  (D. J. I. Russell, Nist computational chemistry
comparison and bench- mark database, 2013).
%
% Data of enthalpy of formation are from Burcat's work (A. Burcat,
Ideal gas thermodynamic data in polynomial form for combustion and air
pollution use, 2006).
%
% Ip or dH(A+) = 0 means that the data is not available in the
literature.
%
% Polarizability (A3) / Element number (CHON) / Ionization energy
(eV) / Enthalpy of formation of an ion and its parent neutral (kJ/
mole) / Species / Data source
%
% polar   C  H  O  N   Ip     dH(A+)    dH(A)    species         %
 0.281    0  1  0  0   13.60  1536.244  217.998  % H             %
BLYP,cc-pVTZ
 0.455    0  2  0  0   15.43  1494.677  0.       % H2            %
BLYP,cc-pVDZ
 0.678    0  0  1  0   13.62  1568.787  249.175  % O             %
B3LYP,aug-ccpVDZ, oxygen atom
 0.743    0  1  1  0   13.02  1299.213  37.3     % OH            % BcT
 0.743    0  1  1  0    0.00  0.        0.       % OH*           %
same value as OH
 1.053    0  2  1  0   12.62  981.806  -241.826  % H2O           %
 1.131    0  0  2  0   12.07  1171.828  0.       % O2            % BcT
 1.489    0  1  2  0   11.35  1113.774  12.296   % HO2           % BcT
 1.773    0  2  2  0   10.58  895.122  -135.88   % H2O2          % BcT
 1.081    0  0  0  1   14.53  1872.924  470.818  % N             %
B3LYP aug-cc-pVDZ, nitrogen atom
 1.760    0  0  0  2   15.58  1509.509  0.       % N2            %
1.435 BcT; 1.760 Arm1.3; 1.740 Prager
 1.285    0  0  1  1    9.26  990.807   91.137   % NO            %
BcT, nitric oxide
 2.378    0  0  1  2   12.89  1329.146  81.6     % N2O           %
BcT, nitrous oxide
 2.210    0  0  2  1    9.59  964.409   34.193   % NO2           %
BcT, nitrogen dioxide
 1.286    1  0  0  0   11.26  1809.444  716.67   % C             %
B3LYP,cc-pV(T+d)Z
 1.745    1  1  0  0   10.64  1630.571  592.5    % CH            %
ground,2\Pi_{1/2} C*V;
 1.654    1  2  0  0   10.40  1399.825  391.2    % CH2           %
ground,^3B_1 C2V
 2.009    1  2  0  0    0.00  1399.825  428.8    % CH2(S)        %
^1A_1 C2V
 1.897    1  3  0  0    9.84  1101.792  146.7    % CH3           %
methyl radical
 2.600    1  4  0  0   12.61  1150.0   -74.6     % CH4           %
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2.262 BcT; 2.60 Arm1.3; 2.448 Prager
 1.390    1  1  0  0   10.64  1630.571  667.919  % CH*          %
4\Sigma- C*V; system error, -1.474
 1.950    1  0  1  0   14.01  1238.337 -110.53   % CO           %
1.685 BcT; Arm1.3
 2.138    1  1  1  0    8.12  833.940   42.3     % HCO          %
Formyl radical
 2.292    1  2  1  0   10.89  948.386  -109.164  % CH2O          %
Formaldehyde
 2.524    1  2  1  0    0.00  0.        0.       % HCOH          %
Hydroxycarbene
 2.551    1  3  1  0    7.56  716.400  -17.0     % CH2OH         %
hydroxymethyl radical
 2.669    1  3  1  0   10.72  1061.172  21.0     % CH3O          %
methoxy radical
 2.786    1  4  1  0   10.84  852.493  -200.94   % CH3OH         %
 2.650    1  0  2  0   13.78  943.137  -393.51   % CO2           %
2.139 BcT; Arm1.3
 2.787    1  1  2  0    8.20  604.166  -181.32   % OCHO          %
Hydrocarboxyl
 2.859    1  2  2  0   11.33  0.        0.       % HOCHO         %
formic acid
 2.800    1  2  2  0    0.00  0.        0.       % CH2O2         %
dioxirane
 3.324    1  2  3  0    0.00  0.        0.       % HO2CHO        %
Carbonic acid, H2CO3
 3.511    1  3  2  0    0.00  0.        0.       % HOCH2O        %
CH2OOH
 3.334    1  3  2  0    0.00  0.        0.       % CH3O2         %
methylperoxy radical
 3.647    1  4  2  0    0.00  0.        0.       % CH3O2H        %
methyl peroxide
 3.357    1  4  2  0    0.00  0.        0.       % CH2(OH)2      %
methanediol
 4.159    1  4  3  0    0.00  0.        0.       % HOCH2O2H      %
B3LYP,TZVP; hydroxy methyl peroxide
 2.999    2  0  0  0   11.40  1980.05   826.799  % C2           %
Semi-empirical,PM6, carbon diatomic
 4.120    2  0  0  0    0.00  1980.05   842.402  % C2*          %
BcT, ground 2
 2.974    2  1  0  0   11.61  1697.10   568.056  % C2H          %
ethynyl radical
 2.867    2  2  0  0   11.40  1333.918  228.20   % C2H2         %
acetylene
 3.135    2  2  0  0    0.00  0.        0.       % CCH2         %
vinylidene, ground
 3.395    2  3  0  0    8.25  1122.34   296.580  % C2H3         %
vinyl
 3.584    2  4  0  0   10.51  1074.461  52.500   % C2H4         %
ethylene
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 3.564    2  4  0  0    0.00  1184.77   366.85   % CH3CH          %
methylmethylene
 3.746    2  5  0  0    8.12  909.095   119.7    % C2H5           %
ethyl radical
 4.036    2  6  0  0   11.52  1036.13  -83.852   % C2H6           %
ethane
 3.556    2  0  1  0    0.00  1436.61   385.68   % CCO            %
B3LYP-TZVP
 3.631    2  1  1  0    9.50  1147.93   178.3    % HCCO           %
ketenyl
 3.987    2  3  1  0   10.85  0.        0.       % CH2CHO         %
vinyloxy radical
 3.970    2  3  1  0    7.00  665.789  -10.3     % CH3CO          %
Acetyl
 3.631    2  2  1  0    9.62  885.29   -48.579   % CH2CO          %
ketene
 3.596    2  2  1  0    0.00  1067.     93.3     % HCCOH          %
ethynol
 4.130    2  4  1  0   10.23  828.315  -166.19   % CH3CHO         %
acetaldehyde
 4.218    2  4  1  0    9.33  0.        0.       % C2H3OH         %
CH2CHOH, ethenol
 3.873    2  4  1  0   10.56  828.315  -124.683  % C2H4O          %
ethylene oxide
 4.480    2  5  1  0    9.11  981.63   -11.47    % CH3CH2O        %
CH3CH2O, ethoxy radical
 4.327    2  5  1  0    0.00  0.        0.       % PC2H4OH        %
CH2CH2OH, 2-hydroxy ethyl radical
 4.471    2  5  1  0    0.00  0.        0.       % SC2H4OH        %
CH3OCH2, methoxymethyl radical
 4.591    2  6  1  0   10.48  784.495  -234.95   % C2H5OH         %
Ethanol
 4.658    2  6  1  0   10.03  0.        0.       % CH3OCH3        %
BcT, dimenthyl ether
 4.184    2  2  2  0   10.20  0.        0.       % C2H2O2         %
ethanedial
 4.587    2  4  2  0   10.84  0.        0.       % CH3OCHO        %
BcT, methyl formate
 4.566    2  4  2  0   10.65  888.25   -432.253  % C2H3OOH        %
BcT, CH3COOH, acetic acid
 4.644    2  4  2  0    0.00  0.        0.       % CHOCH2OH       %
hydroxy acetaldehyde, BcT
 4.401    2  4  2  0    0.00  0.        0.       % C2H4O2         %
1,3-dioxetane
 5.137    2  5  2  0    0.00  0.        0.       % C2H5O2         %
BcT, ethylperoxy radical
 5.090    2  6  2  0   10.16  0.        0.       % C2H6O2         %
1,2-ethanediol
 5.629    2  6  2  0    9.10  0.        0.       % CH3OOCH3       %
dimethylperoxide
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 4.618    2  2  3  0    0.00  0.        0.       % CHOCOOH       % oxo
acetic acid
 5.174    2  3  3  0    0.00  0.        0.       % CH3CO3        %
CH3C(O)OO, acetyl peroxy radical
 5.109    2  4  3  0    0.00  0.        0.       % HOCH2COOH     %
BcT, hydroxyacetic acid
 4.441    3  0  0  0   13.00  1988.93   822.025  % C3            %
BcT, carbon trimer
 5.845    3  0  2  0   10.61  935.95   -95.59    % C3O2          %
carbon suboxide
 4.943    3  3  0  0    8.67  1201.645  348.427  % C3H3          %
propargyl radical
 4.829    3  4  0  0   10.36  0.        0.       % C3H4-P        %
CH3CCH, propyne
 5.368    3  4  0  0    9.69  0.        0.       % C3H4-A        %
CH2CCH2, allene
 4.729    3  4  0  0    8.16  0.        0.       % CC3H4         %
cyclopropene
 5.499    3  5  0  0    8.18  0.        0.       % C3H5-A        %
C3H5, allyl
 5.323    3  5  0  0    0.00  0.        0.       % C3H5-S        %
CH3CHCH, 1-propenyl
 5.499    3  5  0  0    0.00  0.        0.       % C3H5-T        % the
same as C3H5-A
 5.494    3  6  0  0    9.73  0.        0.       % C3H6          %
CH2CHCH3, propene
 5.642    3  7  0  0    7.37  0.        0.       % IC3H7         %
Isopropyl raidcal
 5.619    3  7  0  0    8.09  0.        0.       % NC3H7         % n-
propyl raidcal
 5.819    3  8  0  0   10.94  0.        0.       % C3H8          %
Propane
 5.769    3  4  1  0    0.00  0.        0.       % C2H3CHO       %
BcT, CH2CHCHO, acrolein
 5.496    3  4  1  0    8.95  0.        0.       % CH3CHCO       %
B3LYP,TZVP; methylketene
 6.272    3  4  1  0   10.51  0.        0.       % C3H4O         % 2-
propyn-1-ol, B3LYP, aug-cc-pVTZ
 5.842    3  6  1  0    9.70  0.        0.       % CH3COCH3      %
BcT, acetone
 5.832    3  6  1  0    9.96  0.        0.       % CH3CH2CHO     %
propanal
 5.921    3  6  1  0    9.67  0.        0.       % C3H6O1-2      %
B2PLYP, cc-pVTZ, 2-propylene-1-ol
 5.599    3  6  1  0    0.00  0.        0.       % C3H6O1-3      %
BcT, 1,3-propylene oxide, oxetane
 5.702    3  6  1  0   10.22  0.        0.       % C3H6O         %
propylene oxide
 6.393    3  8  1  0   10.17  0.        0.       % CH3CHOHCH3    %
isopropyl alcohol
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 6.353    3  8  1  0   10.22  0.        0.       % C3H7OH        % 1-
propanol
 6.507    3  8  1  0    9.72  0.        0.       % CH3OC2H5      %
ethane,methoxy-
 6.304    3  6  2  0    0.00  0.        0.       % AC3H5OOH      %
Propanoic acid
 6.915    3  8  2  0    0.00  0.        0.       % NC3H7O2H      %
Propylene glycol, HOCH2CH(OH)CH3
 6.854    3  8  2  0    0.00  0.        0.       % IC3H7O2H      %
1,3-Propanediol, HO(CH2)3OH
 5.638    3  2  2  0    0.00  0.        0.       % C3H2O2        %
propiolic acid
 5.647    3  4  2  0    9.70  0.        0.       % C3H4O2        %
beta-propiolactone
 6.950    3  4  2  0    0.00  0.        0.       % HOCHCCHOH     %
allenediol
 6.347    3  6  2  0   10.25  0.        0.       % CH3COOCH3     %
methyl acetate
 6.549    3  6  2  0   10.61  0.        0.       % HCOOC2H5      %
ethyl formate
 6.126    3  6  2  0    9.90  0.        0.       % C3H6O2        %
1,3-dioxolane, B3LYP,TZVP
 6.171    3  4  3  0   10.40  0.        0.       % C2H4CO3       %
ethylene carbonate
 6.648    3  6  3  0   10.30  0.        0.       % C3H6O3        %
1,3,5-trioxane
 7.044    4  0  0  0   12.54  0.        0.       % C4            %
carbon tetramer
 6.517    4  2  0  0   10.17  1447.72   458.299  % C4H2          %
BcT, diacetylene
 8.008    4  4  0  0    9.15  0.        0.       % C4H4          %
BcT, H2CCCCH2
 6.790    4  4  0  0    9.58  0.        0.       % C2H3CCH       %
BcT, 1-Buten-3-yne
 7.420    4  6  0  0    9.03  0.        0.       % C4H612        %
BcT, 1,2-Butadiene
 6.907    4  6  0  0    9.58  0.        0.       % C4H6-2        % 2-
Butyne
 6.686    4  6  0  0   10.18  0.        0.       % CHCCH2CH3     % 1-
Butyne
 7.624    4  6  0  0    9.07  0.        0.       % CH2CHCHCH2    %
1,3-Butadiene
 7.575    4  9  0  0    6.70  0.        0.       % C(CH3)3       %
tert-butyl radical
 7.617    4  7  0  0    0.00  0.        0.       % C4H71-1       %
BcT, CH3CHCHCH2, methylallyl radical
 7.617    4  7  0  0    0.00  0.        0.       % C4H71-2       % the
same as C4H71-1
 7.617    4  7  0  0    0.00  0.        0.       % C4H71-3       %
 7.617    4  7  0  0    0.00  0.        0.       % C4H71-4       %
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 7.617    4  7  0  0    0.00  0.        0.       % C4H72-2       %
 7.351    4  8  0  0    9.55  0.        0.       % C4H8-1        %
BcT, 1-Butene
 7.367    4  8  0  0    9.10  0.        0.       % C4H8-2        %
BcT, 2-Butene,(Z)-; 7.501,0.00 (E)-
 7.347    4  8  0  0    9.22  0.        0.       % IC4H8         %
CH2C(CH3)CH3, 1-Propene,2-methyl-
 7.485    4  9  0  0    7.25  0.        0.       % IC4H9         %
CH3CHCH2CH3, 2-Butyl
 7.369    4  9  0  0    7.93  0.        0.       % TC4H9         %
CH2CH(CH3)2, Isobutyl
 6.437    4  4  1  0    8.88  0.        0.       % C4H4O         %
BcT, Furan
 7.907    4  6  1  0    9.75  0.        0.       % C2H5CHCO      % 2-
Butenal, CHOCHCHCH3
 7.762    4  6  1  0    9.75  0.        0.       % SC3H5CHO      %
cis-2-Butenal
 7.841    4  6  1  0    8.68  0.        0.       % CH2CHOCHCH2   %
vinyl ether
 6.951    4  6  1  0    9.16  0.        0.       % C4H6O         %
furan,2,3-dihydro-
 7.625    4  8  1  0    9.71  0.        0.       % C4H8O1-2      %
CHOCH(CH3)CH3, Propanal, 2-methyl-
 7.567    4  8  1  0    9.52  0.        0.       % C4H8O1-3      %
B3LYPultrafine, ccpVTZ
 8.215    4  8  1  0    8.98  0.        0.       % C4H8O1-4      %
C2H3OC2H5, ethene, ethoxy-
 7.343    4  8  1  0    8.64  0.        0.       % C4H8O2-3      %
CH2C(CH3)OCH3, 1-Propene, 2-methoxy-
 7.389    4  4  2  0    9.60  0.        0.       % C4H4O2        % 2-
oxetanone,4-methylene-
 8.080    4  6  2  0    0.00  0.        0.       % C4H6O2        % 2-
propenoic acid,methyl ester
 7.619    4  8  1  0    9.82  0.        0.       % CHOCH2CH2CH3  %
Butanal
 8.003    4  8  2  0    9.19  0.        0.       % IC4H7OOH      %
1,4-Dioxane; ethyl acetate
 8.003    4  8  2  0   10.01  0.        0.       % TC3H6OHCHO    %
C4H8O2, the same as above
 8.711    4  10 2  0    9.65  0.        0.       % IC4H9O2H      %
1,3-Butanediol
 8.477    4  10 2  0    9.30  0.        0.       % TC4H9O2H      %
1,4-Butanediol
 7.635    5  5  0  0    0.00  0.        0.       % C5H5          %
cyclopentadienyl radical,B3LYP,TZVP
 8.607    5  6  0  0    9.25  0.        0.       % C5H6          % 1-
buten-3-yne,2-methyl-
 9.458    5  7  0  0    7.25  0.        0.       % C5H7          %
1,3-pentadienyl, SVWN,6-31+G**
 9.288    5  8  0  0    8.86  0.        0.       % C5H8          %
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1,3-butadiene,2-methyl-
 8.733    5  6  1  0    8.38  0.        0.       % C5H6O         % 2-
methylfuran, TPSSh,6-31+G*
 9.172    5  4  2  0    9.22  0.        0.       % C5H4O2        %
furfural
 9.561    6  2  0  0    9.50  0.        0.       % C6H2          %
M06-2X, hexatriyne
 8.945    6  4  0  0    0.00  0.        0.       % C6H4          %
Benzyne
 9.083    6  5  0  0    8.32  1143.     337.3    % C6H5          %
phenyl
 9.304    6  6  0  0    9.24  982.3     82.88    % C6H6          %
benzene
 10.142   6  5  1  0    8.56  0.        0.       % C6H5O         %
phenoxy radical
 10.454   6  4  2  0    0.00  0.        0.       % C6H4O2        %
parabenzoquinone
 1.401    0  2  0  1   10.78  1269.973  186.2    % NH2           %
BcT, amino radical
 1.634    0  3  0  1   10.07  943.294  -45.567   % NH3           %
BcT, ammonia
 1.406    0  0  3  1   12.57  1292.57   74.628   % NO3           %
semi-empirical,PM6,nitrogen trioxide
 1.753    0  1  1  1   10.10  1163.44   214.51   % HNO           %
BcT, nitrosyl hydride
 2.260    0  3  1  1   10.00  854.33   -25.23    % NH2OH         %
BcT, hydroxylamine
 2.372    0  3  1  1    0.00  0.        0.       % NH3O          %
BcT, ammonia oxide
 2.488    0  1  2  1   11.30  0.        0.       % HNO2          %
BcT, nitrous acid
 3.196    0  1  3  1   11.95  0.        0.       % HNO3          %
BcT, nitric acid
 4.189    0  1  4  1    0.00  0.        0.       % HOONO2        %
BcT, peroxy nitric acid
 2.026    0  1  0  2    7.80  0.        0.       % NNH           %
BcT, dinitrogen monohydride
 2.303    0  2  0  2    9.65  1156.7    222.465  % N2H2          %
BcT, trans-diazine
 2.793    0  4  0  2    8.10  879.85    95.18    % N2H4          %
BcT, hydrazine
 3.922    0  0  2  2    0.00  0.        0.       % ONNO          %
BcT, NO dimer
 4.627    0  0  3  2    0.00  0.        0.       % N2O3          %
BcT, dinitrogen trioxide
 4.412    0  0  3  2    0.00  0.        0.       % ONONO         %
BcT, nitrosyl nitrite
 5.316    0  0  4  2   10.80  0.        0.       % N2O4          %
BcT, dinitrogen tetroxide
 2.778    0  0  0  3   11.06  1523.1    449.924  % N3            %
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BcT, azide radical
 3.164   0 1 0 3   10.72 1334.177 291.826 % HN3   %
BcT, hydrogen azide
 2.803   1 0 0 1   13.60 1788.9   438.68   % CN   %
BcT/se3
 2.255   1 1 0 1   12.50 1359.05   191.908 % HNC   %
BcT, hydrogen isocyanide
 2.126   1 1 0 1   13.60 1448.748 129.799 % HCN   %
BcT, hydrogen cyanide
 2.595   1 2 0 1   9.40 1171.87   238.569 % H2CN   % BcT
 2.933   1 2 0 1   0.00 0.   0.   % CNH2   % BcT
 2.832   1 2 0 1   0.00 0.   0.   % HCNH   % BcT
 2.943   1 3 0 1   9.97 1039.34   88.701   % CH2NH   %
BcT, methanimine
 3.390   1 5 0 1   8.90 859.387 -19.380   % CH3NH2   %
BcT, methyl amine
 2.679   1 0 1 1   11.76 1517.94   390.02   % NCO   %
BcT, isocyanato radical
 2.863   1 1 1 1   11.60 1006.582 -118.60   % HNCO   %
BcT, isocyanic acid
 2.826   1 1 1 1   0.00 0.   0.   % HOCN   %
BcT, cyanic acid
 3.226   1 1 1 1   10.83 1218.89   167.603 % HCNO   %
BcT, fulminic acid
 2.984   1 3 1 1   10.16 0.   0.   % CHONH2   %
TPSSh, 6-31G*, formamide
 3.554   1 3 1 1   0.00 0.   0.   % HOCHNH   %
BcT, hydroxymethylimine
 4.193   1 3 2 1   11.08 0.   0.   % CH3NO2   %
methane,nitro-
 4.418   1 3 2 1   10.44 0.   0.   % CH3ONO   %
methyl nitrite
 5.043   1 3 3 1   11.53 0.   0.   % CH3NO3   %
methyl nitrate
 3.170   1 0 0 2   0.00 0.   0.   % NCN   % BcT
 2.801   1 0 0 2   0.00 0.   0.   % CN2   %
BcT, 3H-diazirin-3-ylidene
 3.721   1 2 0 2   0.00 0.   0.   % HNCNH   %
BcT, diiminomethane
 3.966   1 2 0 2   10.30 0.   0.   % CH2NN   %
BcT, diazomethane
 3.390   1 2 0 2   10.40 0.   0.   % NH2CN   %
BcT, cynamamide
 4.638   1 6 0 2   0.00 0.   0.   % NH2CH2NH2   %
diaminomethane
 4.573   1 4 1 2   9.70 0.   0.   % NH2CONH2   %
urea
 5.365   1 5 0 3   9.10 0.   0.   % CH5N3   %
guanidine
 5.096   1 2 0 4   10.95 0.   0.   % CH2N4   % 1H-

```
tetrazole
 6.413    1  3  0  5    0.00  0.        0.       % CH3N5         % 5-
Aminotetrazole
 3.963    2  3  0  1   12.20  0.        0.       % CH3CN         %
BcT, acetonitrile
 4.194    2  3  0  1   11.53  0.        0.       % CH3NC         %
BcT, methyl isocyanide
 4.430    2  4  0  1    0.00  0.        0.       % CH3CHN        %
BcT, methylmethaniminyl radical
 4.494    2  5  0  1    9.20  0.        0.       % C2H5N         %
aziridine
 4.959    2  5  0  1    0.00  0.        0.       % CH2CHNH2      %
aminoethene
 4.946    2  5  0  1    9.30  0.        0.       % CH2NCH3       % N-
methylmethanimine
 4.848    2  5  0  1    8.10  0.        0.       % CH3CHNH       %
ethanimine
 5.240    2  7  0  1    8.90  0.        0.       % CH3CH2NH2     %
Ethylamine
 5.269    2  7  0  1    8.24  0.        0.       % CH3NHCH3      %
Dimethylamine
 5.204    2  5  1  1    9.69  0.        0.       % CH3CONH2      %
acetamide
 5.694    2  5  1  1   10.00  0.        0.       % CH3CHNOH      %
acetaldoxime
 5.698    2  5  2  1    8.90  0.        0.       % H2NCH2COOH    %
glycine
 6.930    2  5  3  1   11.22  0.        0.       % C2H5NO3       %
nitric acid, ethyl ester
 5.725    2  3  3  1   10.51  0.        0.       % C2H3NO3       %
oxamic acid
 4.393    2  0  0  2   13.37  1606.684  309.28   % C2N2          %
BcT, cyanogen
 6.386    2  8  0  2    8.60  0.        0.       % C2H8N2        %
ethylenediamine
 6.450    2  8  0  2    0.00  0.        0.       % CH3NHNHCH3    %
dimethyl hydrazine
 6.382    2  6  1  2    9.66  0.        0.       % C2H6N2O       %
urea,methyl-
 6.363    2  4  2  2    9.41  0.        0.       % C2H4N2O2      %
oxalamide
 7.374    2  6  2  2    9.53  0.        0.       % C2H6N2O2      %
dimethylnitroamine
 5.701    2  3  0  3    9.80  0.        0.       % C2H3N3        %
1H-1,2,4-Triazole
 6.591    2  2  0  4    9.14  0.        0.       % C2H2N4        %
sym-tetrazine
 6.957    2  4  0  4   10.30  0.        0.       % C2H4N4        % 1H-
tetrazole,5-methyl-
 5.334    3  1  0  1   11.62  0.        0.       % HCCCN         %
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BcT, cyanoacetylene
 5.695    3  3  0  1   10.91  0.        0.       % C3H3N         %
acrylonitrile
 5.664    3  5  0  1   11.85  0.        0.       % C2H5CN        %
ethyl cyanide, B3LYP,TZVP
 6.346    3  7  0  1    8.80  0.        0.       % C3H7N         %
cyclopropylamine
 5.820    3  3  1  1    9.96  0.        0.       % C3H3NO        %
isoxazole
 7.807    3  5  1  1    9.50  0.        0.       % CH2CHCONH2    %
acrylamide, B3LYP,aug-cc-pVDZ
 6.330    3  5  1  1   10.75  0.        0.       % CH3OCH2CN     %
methoxyacetonitrile
 7.207    3  7  1  1    9.13  0.        0.       % C3H7NO        %
dimethylformamide
 6.032    3  2  0  2   12.80  0.        0.       % C3H2N2        %
imidazolyl radical
 6.448    3  4  0  2    9.38  0.        0.       % C3H4N2        % 1H-
pyrazole
 7.029    3  6  0  2    0.00  0.        0.       % C3H6N2        % 3-
aminopropionitrile
 7.018    3  3  0  3    9.80  0.        0.       % C3H3N3        %
1,3,5-Triazine
 6.801    4  4  0  1    0.00  0.        0.       % C4H4N         %
pyrrolide radical
 7.141    4  5  0  1    8.21  1083.0    306.085  % C4H5N         %
pyrrole
 7.508    4  7  0  1   11.30  0.        0.       % CH3CH(CH3)CN  %
propanenitrile,2-methyl-
 7.566    4  7  0  1   11.20  0.        0.       % CH3CH2CH2CN   %
butaneitrile
 7.776    4  5  1  1    9.61  0.        0.       % C4H5NO        %
isoxazole,5-methyl-
 8.720    4  0  0  2   11.81  0.        0.       % C4N2          %
BcT, 2-butynedinitrile
 8.409    4  2  0  2   11.16  0.        0.       % C4H2N2        %
fumaronitrile
 7.591    4  4  0  2   12.10  0.        0.       % C4H4N2        %
succinonitrile
 8.412    4  6  0  2    8.50  0.        0.       % C4H6N2        % 1H-
imidazole,2-methyl-
 9.412    4  4  2  2    0.00  0.        0.       % C4H4N2O2      %
uracil, B3LYP,TZVP
 8.601    5  5  0  1    9.26  0.        0.       % C5H5N         %
pyridine
 10.597   5  0  0  4    0.00  0.        0.       % C(CN)4        %
BLYP,aug-cc-pVDZ, tetracyanomethane
 9.458    5  5  1  1    9.50  0.        0.       % C5H5NO        % 3-
pyridinol, B3LYP,TZVP
 13.156   6  0  0  4   11.77  0.        0.       % C6N4          %
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tetracyanoethylene

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 0.897    0  3  1  0   24.7   0.        0.       % H3O+
 1.356    1  1  1  0   26.7   0.        0.       % HCO+
 1.281    1  3  0  0   25.6   0.        0.       % CH3+
 1.937    1  3  1  0   21.7   0.        0.       % CH3O+
 2.462    1  5  1  0   18.3   0.        0.       % CH5O+
 3.141    2  3  1  0   26.1   0.        0.       % C2H3O+
 1.424    0  0  2  0   0.45   0.        0.       % O2-
 1.258    0  1  1  0   1.83   0.        0.       % OH-
 2.677    1  0  3  0   2.69   0.        0.       % CO3-
 3.345    1  1  2  0   3.50   0.        0.       % CHO2-
 3.712    1  1  3  0   3.69   0.        0.       % CHO3-
 1.424    0  0  1  0   1.46   0.        0.       % O-
```