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A Compendium of Gas Phase Basicity and Proton Affinity Measurements

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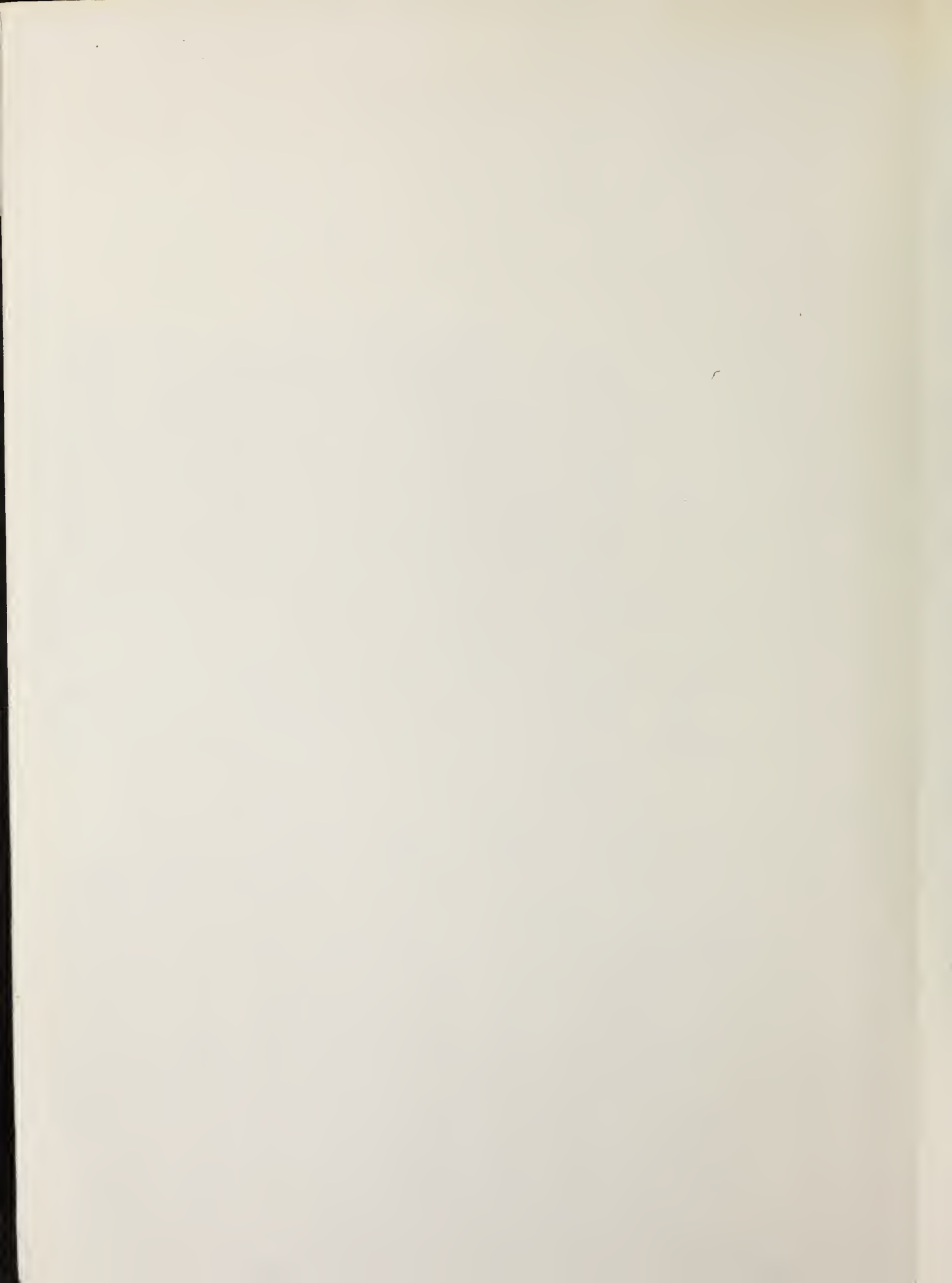
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Bethesda, MD 20205

April 1979

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U.S. DEPARTMENT OF COMMERCE, Juanita M. Kreps, Secretary
Jordan J. Baruch, Assistant Secretary for Science and Technology
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MEMORANDUM FOR THE RECORD

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FOREWORD

The National Standard Reference Data System was established in 1963 for the purpose of promoting the critical evaluation and dissemination of numerical data of the physical sciences. The program is coordinated by the Office of Standard Reference Data of the National Bureau of Standards, but involves the efforts of many groups in universities, government laboratories, and private industry. The primary aim of the program is to provide compilations of critically evaluated numerical data. These tables are published in the Journal of Physical and Chemical Reference Data, the various publication series of the National Bureau of Standards, and through other appropriate channels.

The present report consists of tables of data on gas phase basicity and proton affinity of molecules. It represents a contribution from the Ion Energetics Data Center, prepared in collaboration with staff of NHLBI, NIH and Fein-Marquart Associates. Support for the preparation of these tables has been provided by the National Heart, Lung, and Blood Institute and the Office of Standard Reference Data.

David R. Lide, Jr.
Chief, Office of Standard
Reference Data

ABSTRACT

Numerical values of experimental measurements, calculations and estimations of gas phase basicities and proton affinities are presented. Where appropriate they are recalculated to common values for the proton affinity of ammonia and the heat of formation of the proton. The annotated information is ordered by molecular formula following the Hill System. Indices are given to permit location of information by numerical value of the measurement(s), the compound formula, name and synonym, and CAS Registry Number. The literature coverage is essentially complete through 1977.

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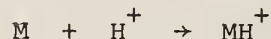
1. INTRODUCTION

1.1 The Data Base

The present compendium tabulates all experimental measurements of gas phase basicities and measurements or derived values of proton affinities available up to the end of 1977. This compilation was carried out for the NIH-EPA CIS project which is developing a comprehensive chemical data base for the use of workers concerned with research on environmental and health problems and related areas. The numerical information presented here is also accessible and searchable by computer through the NIH/EPA Chemical Information System (CIS)(1).

1.2 Definitions and units

The gas phase basicity (GB) of a molecule (M) is defined as the negative of the Gibbs free energy change for the process



and the proton affinity (PA) is defined as the negative of the enthalpy change for the same process.

$$PA(M) = \Delta H_f(M) + \Delta H_f(H^+) - \Delta H_f(MH^+)$$

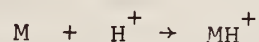
For completeness, the temperature has to be specified. It is generally desired to evaluate the quantity at room temperature. Occasionally experiments are carried out at high temperatures (e.g. 600 K or at undefined temperatures (threshold measurements)), and for these it is necessary to apply the appropriate thermochemical corrections or threshold interpretations.

From the relation $\Delta G = \Delta H - T\Delta S$ the proton affinity can be determined from the gas phase basicity if the temperature and the entropy change of the process are known or can be estimated.

The unit in most widespread use is the kcal/mol and this unit is adopted throughout. It is related to the recommended SI unit by $1 \text{ kcal} = 4.1840 \text{ kJ}$, exactly.

1.3 Standard states, conventions, and reference values

The process



makes no reference to an electron and no difficulties arise if the heats and free energies of formation of all species are defined with the same ionic standard state. Unfortunately this has not always been the case.

Historically, the community determining ion heats of formation by threshold measurements have assumed the convention that the electron is at rest (as it surely is at threshold) and that it remains at rest even when deducing finite (or room) temperature heats of formation of the ions. This convention is also adopted in the two major compilations of gaseous ion thermochemistry (2,3).

The two principal compilations of neutral thermochemistry (4,5) assign to the electron a classical heat capacity, C_p , of $5/2 R$. Thus at room temperature the heats of formation of all ions will be larger than those in, for example Energetics of Gaseous Ions (GIE) (3) by an amount equal to

$$\int_0^{298.15} C_p dT = \frac{5}{2} RT = 1.481 \text{ kcal/mol}$$

Calculations of proton affinities using room temperature ion heats of formation from threshold measurements as compiled and evaluated in Energetics of Gaseous Ions (3) and the proton heat of formation as given in the NBS Tech Note 270 series (4) or the JANAF tables (5) will be in error (too large) by this amount. Wherever the original reference quoted proton affinity values were in error for this reason, we have made the appropriate correction. When the heat of formation of the ion M^+ , is defined according to the GIE convention, the value for the heat of formation of the proton at 298.15 K is 365.7 kcal/mol. This subject is discussed in detail in a recent review article (6).

A major part of the measurement base consists of relative measurements which can be put on an absolute basis by relating to a small number of absolute values. Unfortunately, the magnitude of some of the absolute values is still in doubt. For instance, many of the extensive scales of proton affinity ladders which have been published (7,8) have ultimately been related to the heat of formation of $t\text{-C}_4\text{H}_9^+$ as a primary standard, although the values are usually cited relative to the proton affinity of a secondary standard, ammonia. At the time the present compilation was carried out, the latter value was considered to be established at 202.3 kcal/mol (6), and it is this number which is used as the standard for the values cited here. More recent redeterminations of the heat of formation (9,10) and ionization potential (11) of the *t*-butyl radical, as well as additional information on the entropy change associated with the deprotonation of $t\text{-C}_4\text{H}_9^+$ (12), have resulted in a revised estimate that the proton affinity of ammonia is

greater than or equal to 207.0 kcal/mol (6). Thus, the absolute values of proton affinities given here based on relative ΔG measurements and expressed "relative to ammonia" are, according to the most recent information, too low by at least 5 kcal/mol. In this and other cases we have indicated the species to which the relative measurement is referred, so that readjustment can be made as additional information becomes available.

1.4 References

1. S. R. Heller, G. W. A. Milne, and R. J. Feldmann, "A Computer Based Chemical Information System," *Science* 195, 253 (1977).
2. J. L. Franklin, J. G. Dillard, H. M. Rosenstock, J. T. Herron, K. Draxl, and F. H. Field, "Ionization Potentials, Appearance Potentials, and Heats of Formation of Gaseous Positive Ions," NSRDS-NBS-26, June 1969.
3. H. M. Rosenstock, K. Draxl, B. W. Steiner, and J. T. Herron, "Energetics of Gaseous Ions," *J. Phys. Chem. Ref. Data* 6 Supplement 1 (1977).
4. D. D. Wagman, et al, "Selected Values of Chemical Thermodynamics Properties," NBS Technical Note 270-3, January 1968, and subsequent Tech Notes in this series.
5. D. R. Stull and H. Prophet, "JANAF Thermochemical Tables," Second Edition, NSRDS-NBS-37, June 1971 and supplements published in *J. Phys. Chem. Ref. Data*.
6. S. Lias, "Thermochemistry of Polyatomic Cations," in "Kinetics of Ion-Molecule Reactions," (P. Ausloos, ed.) Plenum Press, New York, pg. 233.
7. J. F. Wolf, R. H. Staley, I. Koppel, M. Taagepera, R.

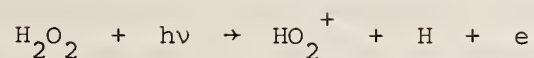
- T. McIver, Jr., J. L. Beauchamp, and R. W. Taft, "Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements," J. Am. Chem. Soc. 99, 5417 (1977).
8. R. Yamdagni, and P. Kebarle, "Gas Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements," J. Am. Chem. Soc. 98, 1320 (1976).
9. W. Tsang, "Evidence for Strongly Temperature-Dependent A-factors in Alkane Decomposition and High Heats of Formation for Alkyl Radicals," Int. J. Chem. Kinetics 11, 820 (1978).
10. M. Rossi and D. M. Golden, J. Am. Chem. Soc. submitted for publication.
11. F. A. Houle and J. L. Beauchamp, "Photoelectron Spectroscopy of Methyl, Ethyl, Isopropyl, and Tert-Butyl Radicals. Implications for the Thermochemistry and Structures of the Radicals and their Corresponding Carbonium Ions," J. Am. Chem. Soc., in press.
12. P. Ausloos and S. G. Lias "Entropy Changes for the Protonation of Alkenes," J. Am. Chem. Soc. 100, 1953 (1978).

2. THE MEASUREMENT TECHNIQUES

2.1 Absolute measurements

These are generally based on measurement of the heat of formation of a proton-containing species by a threshold

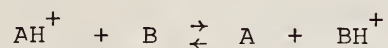
process, such as



From the threshold energy of this process and the heats of formation of the neutral atomic and molecular species one can deduce heat of formation of HO_2^+ , and by further straightforward calculation the proton affinity of molecular oxygen. In actual practice considerable care has to be exercised to establish the temperature to which the heat of formation refers. Threshold measurements leading to more or less accurate absolute values have been carried out by photoionization (PI), monoenergetic electron impact (EM) and conventional electron impact (EI) techniques. The accuracy of these techniques has been comprehensively discussed in a recent review article (1).

2.2 Equilibrium measurements

From a determination of the proton transfer equilibrium constant for



one can determine the Gibbs free energy change of the reaction. This gives the basicity difference between the two compounds. In order to determine the proton affinity difference it is necessary to determine the entropy change of the reaction. The most direct and unambiguous method is to measure the equilibrium constant as a function of temperature, which yields the proton affinity directly from the Van't Hoff relation

$$\frac{d \ln K_{\text{eq}}}{d(1/T)} = \frac{-\Delta H}{R}$$

So far for proton transfer equilibria this has only been performed in a few instances, with varying degrees of success (2). Most estimates of the relative proton affinity are based on assumptions about the entropy change. These range from consideration of symmetry changes in the reaction, to reasoning by analogy, to the assumption that the entropy change is zero. The method or the assumptions made for obtaining a value for ΔS are indicated in this compendium for each determination.

Equilibrium constant measurements are carried out in three quite distinct experimental systems operating at rather different pressures. These are the high pressure ion source coupled to a mass spectrometer (MS), the flowing afterglow tube (FAG) whose equilibrium ion composition is sampled by a quadrupole mass spectrometer, and ions trapped for finite time in a cyclotron field (ICR) with subsequent ejection and analysis by rf absorption. These techniques have been discussed in detail in a number of reviews (2-6).

2.3 Bracketing measurements

The same techniques described immediately above can be used to examine the occurrence or non-occurrence of a proton transfer reaction, and applying the criterion that occurrence implies a negative free energy change and non-occurrence implies a positive free energy change. Accepting these assumptions, one could in principle bracket the range which the gas phase basicity of a molecule lies (7). Using different reagent ions many authors have reported such relative basicities as relative "proton affinities". Results

obtained from this approach should be used only with great caution; it is now well known that many endoergic reactions may occur with a rate constant high enough that they can easily be observed under the experimental conditions described above (3). Furthermore, many proton transfer reactions which are clearly exothermic are not observed to occur if more favorable reaction channels exist (8).

2.4 Calculations and estimates

In principle, proton affinities or ion heats of formation can be calculated quantum mechanically. We include here only the very high quality calculations carried out on H_3^+ (see Tables). Another type of calculation deals with the evaluation of the lattice energy of an ionic crystal (CLE) (9). For an ammonium halide, for example, this gives the energy of the crystal relative to the gas phase ammonium and halide ions. These can then be related to gas phase neutral species via a Born-Haber cycle, and will yield the proton affinity of $\text{NH}_3(\text{gas})$. Lastly, there are a number of empirical correlations of proton affinities with other physical parameters such as core ionization potentials (10).

2.5 References

1. H. M. Rosenstock, "The Measurement of Ionization and Appearance Potentials," *Int. J. Mass Spectrom. Ion Phys.* 20, 139 (1976).
2. S. G. Lias, "Thermodynamic Information from Ion-Molecule Equilibrium Constant Determinations," in "Ion Cyclotron Resonance Spectrometry" (H. Hartmann and K.-P. Wanczek, eds.), Springer-Verlag, Berlin (1978).

3. S. Lias, "Thermochemistry of Polyatomic Cations," in "Kinetics of Ion Molecule Reactions," (P. Ausloos, Ed.), Plenum Press, New York (1979), pg. 233.
4. P. Kebarle, "Ion Thermochemistry and Solvation from Gas Phase Ion Equilibria," Ann. Rev. Phys. Chem. 28, 445 (1977).
5. D. H. Aue and M. T. Bowers, "Stabilities of Positive Ions from Equilibrium Gas Phase Basicity Measurements," in "Gas Phase Ion Chemistry," (M. T. Bowers, ed.), Academic Press, New York (1979).
6. D. K. Bohme, "The Kinetics and Energetics of Proton Transfer," in "Interactions between Ions and Molecules," (P. Ausloos, ed.), Plenum Press, New York (1975).
7. J. Long and B. Munson, "Proton Affinities of some Oxygenated Compounds," J. Am. Chem. Soc. 95, 2427 (1973).
8. P. Ausloos and S. G. Lias, "Proton Affinity of Dichlorocarbene," J. Am. Chem. Soc. 100, 4594 (1978).
9. J. Sherman, "Crystal Energies of Ionic Compounds and Thermochemical Applications," Chem. Rev. 11, 93 (1932).
10. J. A. Jen and T. D. Thomas, "Core Ionization Potentials in Dimethyl Ether and Methylamine," J. Electron Spectrosc. 4, 43 (1974).

3. ORGANIZATION OF THE INFORMATION

3.1 A typical measurement entry is shown below:

C ₈ H ₁₀	CAS REGN : 108-38-3
Benzene, 1,3-dimethyl- (9CI) m-Xylene (8CI)	
GB (exp) : 182+/-3 kcal/mol	Temperature : 340 K
PA (exp) : 189.7+/-3 kcal/mol	Temperature : 340 K
Chong, S. L., and Franklin, J. L., Proton Affinities of Benzene, Toluene, and the Xylenes, J. Am. Chem. Soc. 94, 6630 (1972).	
Method used : MS Equilibrium relative to CH ₃ SH and (CH ₃) ₂ O Entropy change assumed zero	
GB (exp) : 187.2+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 194.6+/-2 kcal/mol	Temperature : 298 K
Devlin, J. L., III, Wolf, J. F., Taft, R. W., and Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to C ₆ H ₆ (Benzene)	

The entry gives successively the following information:

- a) The empirical formula in Hill System order.
- b) The Chemical Abstracts Service (CAS) Registry Number.
- c) The structural formula (see discussion below).
- d) The Chemical Abstracts Service (CAS) Name, as given in the 8th Collective Index (8CI) and the 9th Collective Index (9CI). If it is the same in both it is denoted with (8CI9CI).
- e) The gas phase basicity, GB, in kcal/mol.
- f) The proton affinity, PA, in kcal/mol.
- g) The temperature at which the measurement was carried out.
- h) The literature citation.
- i) The method used (see discussion below).
- j) Additional comments on the nature of the measurement.

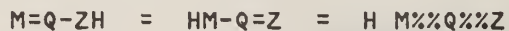
Where there are several measurements on the same species, the numerical value, literature reference, method and associated comments are listed successively.

The structural diagrams used in this publication have been generated from connection tables by the Structure and Nomenclature Search System (SANSS), one of the components of the CIS. The following symbols have been used to represent the different types of chemical bonds:

- * - single bond
- + - double bond
- # - triple bond
- . - ring alternating bond (e.g., benzene)
- % - tautomeric bond (e.g., O% C% O in carboxylic acids)

Hydrogen atoms are not explicitly included in the diagrams but are understood to occupy any otherwise available bonds.

Tautomeric structures are recognized as equivalent and the percent sign used in the structural diagrams under the following conditions.



when:

- a). Q = C, N, S, P, Sb, As, Se, Te, Br, Cl, or I with any allowed valence for the individual elements.
- b). M and Z = any combination of trivalent N and/or bivalent O, S, Se or Te atoms.
- c). The bonds which are involved in the tautomerization may be in an acyclic chain, a ring system, or partly in each.
- d). The end points, M and Z, may be in adjacent rings of a fused ring system. However, a nitrogen atom at a fusion point in a fused ring system can not be involved in tautomerization.
- e). A deuterium or tritium may replace the migrating hydrogen atom.
- f). If more than one of the systems described above are linked through a common atom, the hydrogen may be free to migrate along the chain defining a larger tautomeric system.

The experimental methods were discussed in the preceding section. They are abbreviated as follows:

CLE - Crystal lattice energy
EI - Threshold measurement by non-monoenergetic electron impact
EM - Threshold measurement by monoenergetic electron impact
FAG - Flowing afterglow
FI - Field ionization threshold
ICR - Ion cyclotron resonance
MS - High pressure mass spectrometry
PI - Threshold measurement by photoionization
TC - Theoretical calculation

Following the table of measurements in molecular formula order, Section 4, there are a number of indexes:

- a). The gas phase basicity index in which the file is ordered in increasing order of gas phase basicity, with numerical values arbitrarily given to four significant figures for purposes of ordering. The page number refers to the main body of information, Section 4.
- b). The proton affinity index, structured in the same fashion.
- c,d,e). Additional indices are provided for molecular formula, CAS Registry Number and compound name. The compound name index includes a number of synonyms in addition to the names adopted in the 8th and 9th collective indices.



Ar	CAS REGN : 7440-37-1
AR	
Argon (8CI9CI)	
PA (exp) : <100.+/-0.5 kcal/mol	Temperature :
Roche, A. E., Sutton, M. M., Bohme, D. K., and Schiff, H. I., Determination of Proton Affinity from the Kinetics of Proton Transfer Reactions. I. Relative Proton Affinities, J. Chem. Phys. 55, 5480 (1971).	
Method used : FAG Bracketing relative to 02.	

AsH3	CAS REGN : 7784-42-1
AS	
Arsine (8CI9CI)	
GB (exp) : 172.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

BF2H	CAS REGN : 13709-83-6
F**B**F	
Borane, difluoro- (8CI9CI)	
PA (exp) : 115+/-14 kcal/mol	Temperature : 85 K
Pierce, R. C., and Porter, R. F., Ion-Molecule Chemistry of BF3 and HBF2 in Hydrogen, Inorg. Chem. 14, 1087 (1975).	
Method used : MS Bracketing relative to CH4 and H2.	

BF3	CAS REGN : 7637-07-2
F**B**F * * F	
Borane, trifluoro- (9CI) Boron fluoride (BF3) (8CI)	
PA (exp) : 115+/-14 kcal/mol	Temperature : 85 K
Pierce, R. C., and Porter, R. F., Ion-Molecule Chemistry of BF3 and HBF2 in Hydrogen, Inorg. Chem. 14, 1087 (1975).	
Method used : MS Bracketing relative to CH4 and H2.	

B2H6	CAS REGN : 19287-45-7
H**B * * * * B**H	
Diborane(6) (8CI9CI)	
PA (exp) : 147+/-4 kcal/mol	Temperature : 79-86 K
Pierce, R. C., and Porter, R. F., Low-Temperature Chemical Ionization Mass Spectrometry of Boron Hydrides. The Proton Affinities of Diborane and Tetraborane(10), J. Am. Chem. Soc. 95, 3849 (1973).	
Method used : MS Observed reaction $C_2H_9^+ + B_2H_6 \rightarrow 2CH_4 + B_2H_7^+$. Reaction $B_2H_7^+ \rightarrow B_2H_5^+ + H_2$ has delta H formation = 3.0+/-0.3. Based on delta H formation($B_2H_5^+$) = 232.	

B3H5N3	CAS REGN : Not available
<pre> B**N * * * * N B * * * * * * * * B**N</pre>	
.beta.-Borazinyl radical	
PA (exp) : 193+/-2 kcal/mol	Temperature :
DeStefano, A. J., and Porter, R. F. Ion-Molecule Reactions of Cyclic Borazine Cations. Thermodynamic and Kinetic Considerations, J. Phys. Chem. 80, 2818 (1976).	
Method used : MS Bracketing relative to HCO2C2H5 and (CH3)2CO. The reactant ions are generated by photon impact	

B3H6N3	CAS REGN : 6569-51-3
<pre> B**N * * * * N * B * * * * B**N</pre>	
Borazine (8CI9CI)	
PA (exp) : 199+/-4 kcal/mol	Temperature :
Betowski, L. D., Solmon, J. J., and Porter, R. F., The Proton Affinity of Borazine, Inorg. Chem. 11, 424 (1972).	
Method used : MS Bracketing relative to C4H6(2-Butyne) and NH3	

B4H8	CAS REGN : 12007-71-5
B***B * * * * B***B	
Tetraborane(8)	
PA (exp) : 187+/-7 kcal/mol	Temperature : 375 K
Solmon, J. J., and Porter, R. F., Chemical Ionization Mass Spectrometry of Selected Boron Hydrides, J. Am. Chem. Soc. 94, 1443 (1972).	
Method used : MS Bracketing relative to C3D6 and (CH3)2CO.	

B4H10	CAS REGN : 18283-93-7
<pre>H*****B*****H * * * * * * * * B*****B * * * * * * * * H*****B*****H</pre>	
Tetraborane(10) (8CI9CI)	
PA (exp) : 144+/-5 kcal/mol	Temperature : 140-300 K
<p>Pierce, R. C., and Porter, R. F., Low-Temperature Chemical Ionization Mass Spectrometry of Boron Hydrides. The Proton Affinities of Diborane and Tetraborane(10), J. Am. Chem. Soc. 95, 3849 (1973).</p>	
<p>Method used : MS Based on delta H formation(B2H5+) and estimating delta S. Equilibrium of B2H5+ + B2H6 -> B4H11+.</p>	

B5H9	CAS REGN : 19624-22-7
H*****B*****H * *** * * * * * * B**B**B * * * * * * *** * H*****B*****H	
Pentaborane(9) (8CI9CI)	
PA (exp) : 172+/-2 kcal/mol	Temperature : 373~3 K
Solmon, J. J., and Porter, R. F., Chemical Ionization Mass Spectrometry of Selected Boron Hydrides, J. Am. Chem. Soc. 94, 1443 (1972).	
Method used : MS Based PA (H2O) = 170.3. Bracketing relative to H2O and H2S.	

BrH	CAS REGN : 10035-10-6
BR	
Hydrobromic acid (8CI9CI)	
PA (exp) : 141+/-3 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Absolute PA value estimated by assuming that for reaction $RH^+ + RH \rightarrow RH_2^+ + R$; the $\Delta H \sim 5X TC$. TC = measured translational energy of the products.	

CBrN	CAS REGN : 506-68-3
N##C**BR	
Cyanogen bromide (8CI9CI)	
PA (exp) : 179+/-3 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to AsH3, HCO2H and F2CHCH2OH	

CCIN	CAS REGN : 506-77-4
N##C**CL	
Cyanogen chloride (8CI9CI)	
PA (exp) : 177+/-3 kcal/mol	Temperature : 300 K
<p>Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).</p>	
<p>Method used : ICR Equilibrium relative to F2CH2CH, OH and HCHO</p>	
GB (exp) : 169.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 177.4+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

CC12	CAS REGN : 1605-72-7
CL*C**CL	
Methylene, dichloro- (8CI9CI)	
PA (exp) : 194.7+/-4 kcal/mol	Temperature : 325 K
Ausloos, P., and Lias, S. G. The Proton Affinity of Dichlorocarbene, To be published in J. Am. Chem. Soc.	
Method used : ICR Bracketing relative to Me2O and Et2O; scale based on PA (NH3) = 202.8	
PA (exp) : 200.4+/-1.5 kcal/mol	Temperature : 300 K
Lias, S. G., and Ausloos, P. Reactions of CC12H+ and CF2H+ with Organic and Inorganic Compounds: Proton Affinities and Heats of Formation of CC12 and CF2, Intern. J. Mass Spectrom. Ion Phys. 22, 135 (1976).	
Method used : ICR Bracketing relative to NH3 and (CH3)2S	

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GB not calculated for this reference	
PA (exp) : 208.3+/-2 kcal/mol	Temperature : 300 K
Levi, B. A., Taft, R. W., and Hehre, W. J. Dichlorocarbene, J. Am. Chem. Soc. 99, 8454 (1977).	
Method used : ICR Calculated entropy Bracketing relative to CF ₃ CH ₂ CH ₂ NH ₂ and C ₆ H ₅ NH ₂ ; scale based on NH ₃	
PA (exp) : 209+/-2 kcal/mol	Temperature : 300 K
Levi, B. A., Taft, R. W., and Hehre, W. J. Dichlorocarbene, J. Am. Chem. Soc. 99, 8454 (1977).	
Method used : ICR Calculated entropy The deuterium affinity determined by bracketing techniques relative to 2-CF ₃ Pyridine and CF ₃ (CH ₂) ₂ NH ₂ ; scale based on NH ₃	

CF2	CAS REGN : 2154-59-8
F**C**F	
Methylene, difluoro- (8CI9CI)	
PA (exp) : 178.5+/-1 kcal/mol	Temperature : 300 K
Lias, S. G., and Ausloos, P. Reactions of CCl ₂ H ⁺ and CF ₂ H ⁺ with Organic and Inorganic Compounds: Proton Affinities and Heats of Formation of CCl ₂ and CF ₂ , Intern. J. Mass Spectrom. Ion Phys. 22, 135 (1976).	
Method used : ICR Bracketing relative to H ₂ S and HCOOH and also observing the following: CD ₅ ⁺ + CF ₂ HCl -> CD ₄ + DCI + CF ₂ H ⁺ and CD ₅ ⁺ + CF ₃ H -> CD ₄ + DF + CF ₂ H ⁺ . Scale based on PA (H ₂ O) = 170.1 kcal/mol	

CF4	CAS REGN : 75-73-0
<pre> F * * F**C**F * * F </pre>	
Methane, tetrafluoro- (9CI) Carbon tetrafluoride (8CI)	
PA (exp) : 121+/-4 kcal/mol	Temperature : 300 K
Roche, A. E., Sutton, M. M., Bohme, D. K., and Schiff, H. I., Determination of Proton Affinity from the Kinetics of Proton Transfer Reactions. I. Relative Proton Affinities, J. Chem. Phys. 55, 5480 (1971).	
Method used : FAG Bracketing relative to CH4 and N2.	
PA (exp) : 121+/-5 kcal/mol	Temperature : 298 K
Blint, R. J., McMahon, T. B., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Fluoromethanes by Ion Cyclotron Resonance Spectroscopy. New Techniques for the Determination of Carbonium Ion Stabilities, J. Am. Chem. Soc. 96, 1269 (1974).	
Method used : ICR Bracketing relative to CH4. Using IP of H and CF4 and also HA of CF4+.	

CHF3	CAS REGN : 75-46-7
F**C**F * * F	
Methane, trifluoro- (8CI9CI)	
PA (exp) : 147+/-5 kcal/mol	Temperature : 298 K
Blint, R. J., McMahon, T. B., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Fluoromethanes by Ion Cyclotron Resonance Spectroscopy. New Techniques for the Determination of Carbonium Ion Stabilities, J. Am. Chem. Soc. 96, 1269 (1974).	
Method used : ICR Bracketing relative to CH3F. Using IP of H and CH3F, also HA (CH3F+).	

CHN	CAS REGN : 74-90-8
C##N	
Hydrocyanic acid (8CI9CI)	
GB (exp) : 166.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 174.5+/-2 kcal/mol	Temperature : 300 K
<p>Freeman, C. G., Harland, P. W., and McEwan, M. J. The Equilibrium $H_3S^+ + HCN = H_2CN^+ + H_2S$ and the Relative Proton Affinities of HCN and H₂S, Intern. J. Mass Spectrom. Ion Phys. 27, 77 (1978).</p>	
<p>Method used : FAG Equilibrium relative to H₂S; scale based on NH₃</p>	
PA (exp) : 139 kcal/mol	Temperature :
<p>Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).</p>	
<p>Method used : MS Estimated delta H = 5X translational energy of the product of reaction $RH^+ + RH \rightarrow RH_2^+ + R$</p>	

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GB (exp) : 166.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 174.5+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

CH2F2	CAS REGN : 75-10-5
F**C**F	
Methane, difluoro- (8CI9CI)	
PA (exp) : 147+/-5 kcal/mol	Temperature : 298 K
<p>Blint, R. J., McMahon, T. B., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Fluoromethanes by Ion Cyclotron Resonance Spectroscopy. New Techniques for the Determination of Carbonium Ion Stabilities, J. Am. Chem. Soc. 96, 1269 (1974).</p>	
<p>Method used : ICR Bracketing relative to CH3F and CO. Using IP of H and CH2F2, also HA (CH2F2+).</p>	

CH2N2	CAS REGN : 334-88-3
N++N++C	
Methane, diazo- (8CI9CI)	
PA (exp) : 207+/-5 kcal/mol	Temperature : 300 K
Foster, M. S., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Azomethane by Ion Cyclotron Resonance, J. Am. Chem. Soc. 94, 2425 (1972).	
Method used : ICR Bracketing relative to NH3 and CH3NH2	

CH2O	CAS REGN : 50-00-0
C++O	
Formaldehyde (8CI9CI)	
PA (exp) : 162+/-3 kcal/mol	Temperature :
Harrison, A. G., Ivko, A., and Van Raalte, D., Energetics of Formation of Some Oxygenated Ions and the Proton Affinities of Carbonyl Compounds, Can. J. Chem. 44, 1625 (1966).	
Method used : EI Electron impact fragmentation (various molecules).	

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PA (exp) : 169+/-1 kcal/mol	Temperature : 298 K
<p>Refaey, K. M. A., and Chupka, W. A., Photoionization of the Lower Aliphatic Alcohols with Mass Analysis, J. Chem. Phys. 48, 5205 (1968).</p>	
<p>Method used : PI Appearance potential by IP fragmentation of CH₃OH</p>	
PA (exp) : 170 kcal/mol	Temperature :
<p>Lossing, F. P. Heats of Formation of Some Isomeric [C_nH_{2n} + 10]⁺ Ions. Substitutional Effects on Ion Stability, J. Am. Chem. Soc. 99, 7526 (1977).</p>	
<p>Method used : EM Electron impact fragmentation (various molecules) using EM. $\Delta H_f(H^+) = 365.7$</p>	
GB (exp) : 167.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 174.6+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH₃</p>	

CH2O2	CAS REGN : 64-18-6
O=C=O	
Formic acid (8CI9CI)	
PA (exp) : 178+/-4 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to CH3OH and H2S.	
PA (exp) : 186.8 kcal/mol	Temperature :
Goldenfeld, I. V., Korostyshevsky, I. Z., and Mischanchuk, B. G., Analysis of Field Ion Energies in a Mass Spectrometer, Int. J. Mass Spectrom. Ion Phys. 13, 297 (1974).	
Method used : FI PA derived from field appearance potential. Correction for neutral particles potential energy	

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PA (exp) : 179+/-3 kcal/mol	Temperature : 340 K
Chong, S. L., and Franklin, J. L., Heats of Formation of Protonated Cyclopropane, Methylcyclopropane, and Ethane, J. Am. Chem. Soc. 94, 5347 (1972).	
Method used : MS Correction for path degeneracy. Equilibrium; scale based on CH3CH=CH2.	
GB (exp) : 162.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 178.9+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

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GB (exp) : 171.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.1+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

CH3Br	CAS REGN : 74-83-9
BRxC	
Methane, bromo- (8CI9CI)	
PA (exp) : 163 kcal/mol	Temperature : 300 K
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Bracketing and using also IP's of H and CH3Br and HA(CH3BR+).	

CH3Cl	CAS REGN : 74-87-3
C**CL	
Methane, chloro- (8CI9CI)	
PA (exp) : <170.3 kcal/mol	Temperature :
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to H2O.	
PA (exp) : 164+/-3 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Absolute PA value estimated by assuming that for reaction $RH^+ + RH \rightarrow R + RH_2^+$ the $\Delta H \sim 5X TC$. TC = measured translational energy of the products	

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PA (exp) : ~160 kcal/mol	Temperature : 300 K
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Bracketing and using also IP's of H and CH ₃ Cl and HA(CH ₃ Cl ⁺).	

CH ₃ F	CAS REGN : 593-53-3
C**F	
Methane, fluoro- (8CI9CI)	
PA (exp) : 151+/-5 kcal/mol	Temperature : 298 K
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Using also the IP's of H and CH ₃ F and HA of CH ₃ F ⁺ .	

CH3I	CAS REGN : 74-88-4
C**I	
Methane, iodo- (8CI9CI)	
PA (exp) : 174+/-3 kcal/mol	Temperature : 300 K
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Bracketing and using also IP's of H and CH3I and HA(CH3I+).	

CH3NO2	CAS REGN : 75-52-5
O++N**C + + 0	
Methane, nitro- (8CI9CI)	
PA (exp) : ~182 kcal/mol	Temperature : 300 K
McAllister, T., and Pitman, P. Ion-Molecule Reactions and Proton Affinities of Methyl Nitrite and Nitromethane, Intern. J. Mass Spectrom. Ion Phys. 19, 241 (1976).	
Method used : ICR Bracketing relative to CH3OH and (CH3)2CO	
PA (exp) : 182+/-2 kcal/mol	Temperature : 300 K
Kriemler, P., and Buttrill, S. E., Jr., Ion-Molecule Reactions and the Proton Affinities of the Nitroalkanes. I. Nitro methane and nitroethane, J. Am. Chem. Soc. 95, 1365 (1973).	
Method used : ICR Bracketing relative to CH3OH.	

CH3NO2	CAS REGN : 624-91-9
O++N**O**C	
Nitrous acid, methyl ester (8CI9CI) .	
PA (exp) : 190.3+/-3 kcal/mol	Temperature : 300 K
<p>McAllister, T., and Pitman, P. Ion-Molecule Reactions and Proton Affinities of Methyl Nitrite and Nitromethane, Intern. J. Mass Spectrom. Ion Phys. 19, 241 (1976).</p>	
<p>Method used : ICR Bracketing relative to C2H5OH and (CH3)2CO</p>	

CH4	CAS REGN : 74-82-8
C	
Methane (8CI9CI)	
PA (exp) : 127+/-2 kcal/mol	Temperature : 78,300 K
<p>Chupka, W. A., and Berkowitz, J., Photoionization of Methane: Ionization Potential and Proton Affinity of CH4, J. Chem. Phys. 54, 4256 (1971).</p>	
<p>Method used : PI From PI-efficiency curve of CH5+ in CH4.</p>	

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PA (exp) : 126+/-1 kcal/mol	Temperature : 483+/-10 K
<p>Munson, M. S. B., and Field, F. H., Reactions of Gaseous Ions. XV. Methane + 1% Ethane and Methane + 1% Propane, J. Am. Chem. Soc. 87, 3294 (1965).</p>	
<p>Method used : MS Observed reactions: CH₄⁺ + CH₄ -> CH₅⁺ + CH₃, CH₅⁺ + C₂H₆ -> C₂H₅⁺ + H₂ + CH₄.</p>	
PA (exp) : 131.4 kcal/mol	Temperature : 298 K
<p>Schiff, H. I., and Bohme, D. K., Flowing Afterglow Studies at York University, Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975).</p>	
<p>Method used : FAG Equilibrium relative to N₂O, delta S estimated. Based on PA (N₂O) which is derived from calculated PA (CO).</p>	
PA (exp) : 130.5 kcal/mol	Temperature : 340 K
<p>Kasper, S. F., and Franklin, J. L., Ion-Molecule Reactions in the System CO₂-CH₄, J. Chem. Phys. 56, 1156 (1972).</p>	
<p>Method used : MS Entropy change assumed zero Equilibrium relative to CO₂; found delta G = -1.35 Kcal/mol. Based on CO₂ with PA = 129.1. (Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975)).</p>	

CH4O	CAS REGN : 67-56-1
C**O	
Methanol (8CI9CI)	
PA (exp) : 182+/-3 kcal/mol	Temperature :
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to CH3CHO and HCOOH.	
PA (exp) : 179.0+/-2 kcal/mol	Temperature : 299-329 K
Wei, L. Y., and Bone, L. I., Ion-Molecule Reactions in Methanol and Hydrogen Sulfide, J. Phys. Chem. 78, 2527 (1974).	
Method used : MS Equilibrium relative to H2S Van't Hoff plot	

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PA (exp) : 182 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Delta H estimated = 5X total translational energy of the products of $RH^+ + RH \rightarrow RH_2^+ + R$	
GB (exp) : 166.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.1+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

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GB (exp) : 174.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 182.2+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

CH4S	CAS REGN : 74-93-1
C**S	
Methanethiol (8CI9CI)	
GB (exp) : 177.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 185.3+/-2 kcal/mol	Temperature : 300 K
<p>Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).</p>	
<p>Method used : MS Equilibrium; scale based on CH3CHO Entropy change assumed zero</p>	

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PA (exp) : 199+/-10 kcal/mol	Temperature :
Hobrock, B. G. and Kiser, R. W., Electron Impact Investigations of Sulfur Compounds. II. 3-Methyl-2-Thiabutane, 4-Thia-1-Pentene, and 3,4-Dithiahexane, J. Phys. Chem. 67, 648 (1963).	
Method used : EI Appearance potential by electron impact of sulfur compounds.	
GB (exp) : 178.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 185.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

CH5N	CAS REGN : 74-89-5
C**N	
Methanamine (9CI) Methylamine (8CI)	
GB (exp) : 202.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 211 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Estimated delta H = 5X translational energy of the product of reaction $RH^+ + RH \rightarrow RH_2^+ + R$	

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GB (exp) : 205.7+/-3 kcal/mol	Temperature : 298 K
PA (exp) : 213.7+/-3 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T. Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 195.9+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 213.1+/-2 kcal/mol	Temperature : 600 K
Briggs, J. P., Yamdagni, R., and Kebarle, P., Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton- Exchange Equilibria, J. Am. Chem. Soc. 94, 5128 (1972).	
Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero	

CH5P	CAS REGN : 593-54-4
C**P	
Phosphine, methyl- (8CI9CI)	
GB (exp) : 193.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 201.8+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

CO	CAS REGN : 630-08-0
C##0	
Carbon monoxide (8CI9CI)	
PA (exp) : 143+/-2 kcal/mol	Temperature :
Matthews, C. S., and Warneck, P., Heats of Formation of CH0+ and C3H3+ by Photoionization, J. Chem. Phys. 51, 854 (1969).	
Method used : PI Appearance potential by photoionization. PA value derived from delta H formation(HCO+).	
PA (exp) : 142.7+/-3 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Excess Energies in Mass Spectra of some Oxygen- Containing Organic Compounds, Trans. Faraday Soc. 65, 1794 (1969).	
Method used : MS Appearance potential by electron impact from HCOOH, CH3CHO and C2H3CHO. Correction for excess energy.	

C02	CAS REGN : 124-38-9
0++C++0	
Carbon dioxide (8CI9CI)	
PA (exp) : 130.7+/-1 kcal/mol	Temperature :
Warneck, P. Heat of Formation of the HCO Radical, Z. Naturforsch. 29, 350 (1974).	
Method used : PI Appearance potential by photoionization. $\Delta H_f(H^+)$ = 365.7	
PA (exp) : 129.1 kcal/mol	Temperature : 298 K
Schiff, H. I., and Bohme, D. K., Flowing Afterglow Studies at York University, Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975).	
Method used : FAG Calculated entropy. Equilibrium; scale based on CO VALUE	

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PA (exp) : 124+/-2 kcal/mol	Temperature : 300 K
Meot-Ner (Mautner), M., and Field, F. Proton Affinities and Cluster Ion Stabilities in CO ₂ and CS ₂ . Applications in Martian Ionspheric Chemistry, J. Chem. Phys. 66, 4527 (1977).	
Method used : MS Van't Hoff plot Equilibrium; scale based on PA (CH ₄) = 126.8	
GB (exp) : 123+/-3 kcal/mol	Temperature : 300 K
PA (exp) : 124+/-3 kcal/mol	Temperature : 300 K
Meot-Ner (Mautner), M., and Field, F. H. Proton Affinities and Cluster Ion Stabilities in CO ₂ and CS ₂ . Application in Martian Ionspheric Chemistry, J. Chem. Phys. 66, 4527 (1977).	
Method used : MS Calculated entropy The measurements done in the temperature range of 400-650K. Using the Hoff plot the delta H and delta S at 300K were derived. Using PA (CH ₄)-126.8	

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PA (exp) : 123+/-3 kcal/mol	Temperature : 800 K
<p>Fehsenfeld, F. C., Lindinger, W., Schiff, H. I., Hemsworth, R. S., and Bohne, D. K. Determination of the Proton Affinity from the Kinetics of Proton Transfer Reactions. VI. The Relative Proton Affinities of N₂, Xe, and CO₂, J. Chem. Phys. 64, 4887 (1976).</p>	
<p>Method used : FAG Van't Hoff plot Equilibrium relative to N₂ and Xe; scale based on PA (N₂) = 112.6 Van't Hoff plot</p>	

CS ₂	CAS REGN : 75-15-0
S++C++S	
Carbon disulfide (8CI9CI)	
GB (exp) : 165.7+/-2.5 kcal/mol	Temperature : 300 K
PA (exp) : 168+/-2.5 kcal/mol	Temperature : 300 K
<p>Meot-Ner (Mautner), M., and Field, F. H. Proton Affinities and Cluster Ion Stabilities in CO₂ and CS₂. Applications in Martian Ionospheric Chemistry, J. Chem. Phys. 66, 4527 (1977).</p>	
<p>Method used : MS Calculated entropy The measurements done in the temperature range of 400-650K. Using the Hoff plot the delta H and delta S at 300K were derived. Equilibrium, scale based on NH₃</p>	

C2C13N	CAS REGN : 545-06-2
CL * * CL*C**C##N * * CL	
Acetonitrile, trichloro- (8CI9CI)	
GB (exp) : 169.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 177.5+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2D6O	CAS REGN : 17222-37-6
C**O**C	
Methane-d3, oxybis- (9CI) (Methyl ether)-d6 (8CI)	
GB (exp) : ~186 kcal/mol	Temperature : 374 K
Blair, A. S., and Harrison, A. G., Bimolecular Reactions of Trapped Ions. V. Ionic Chemistry of Simple Oxygen-containing Molecules, Can. J. Chem. 51, 703 (1972).	
Method used : MS Equilibrium relative to CH3CHO. Found delta G ~3.	

C2HF3	CAS REGN : 359-11-5
F**C**C**F * * F	
Ethene, trifluoro- (9CI) Ethylene, trifluoro- (8CI)	
PA (exp) : 172+/-2 kcal/mol	Temperature : 300 K
Ridge, D. P., Gas Phase Proton Affinities of Several Fluoroethylenes, J. Am. Chem. Soc. 97, 5670 (1975).	
Method used : ICR Bracketing relative to H2O and H2S.	

C2HF3O2	CAS REGN : 76-05-1
<p>F * * F**C**C%O * % * % F O</p>	
Acetic acid, trifluoro- (8CI9CI)	
PA (exp) : 172+/-2 kcal/mol	Temperature : 323-373 K
<p>Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).</p>	
<p>Method used : MS Bracketing relative to H2S and H2O</p>	
GB (exp) : 154.7+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 171.9+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero</p>	

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GB (exp) : 165.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 173.3+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C2H2C1N	CAS REGN : 107-14-2
CLXC**C##N	
Acetonitrile, chloro- (8CI9CI)	
GB (exp) : 173.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C2H2F2	CAS REGN : 75-38-7
F*xC++C * * F	
Ethene, 1,1-difluoro- (9CI) Ethylene, 1,1-difluoro- (8CI)	
PA (exp) : 178+/-4 kcal/mol	Temperature : 300 K
Ridge, D. P., Gas Phase Proton Affinities of several Fluoroethylenes, J. Am. Chem. Soc. 97, 5670 (1975).	
Method used : ICR Bracketing relative to C2H5I and CH3OH	
PA (exp) : 174.8 kcal/mol	Temperature : 298 K
Williamson, A. D., LeBrenton, P. R., and Beauchamp, J. L., Photoionization Mass Spectrometry of 2-Fluoropropane and 2,2-Difluoropropane. A Novel Determination of the Proton Affinity of Vinyl Fluoride and 1,1-Difluoro- ethylene, J. Am. Chem. Soc. 98, 2705 (1976).	
Method used : PI Appearance potential by phototization of (CH3)2CF2.	

C2H2F2	CAS REGN : 1630-77-9
F**C++C**F	
Ethene, 1,2-difluoro-, (Z)- (9CI) Ethylene, 1,2-difluoro-, (Z)- (8CI)	
PA (exp) : 166+/-4 kcal/mol	Temperature : 300 K
Ridge, D. P., Gas Phase Proton Affinities of several Fluoroethylenes, J. Am. Chem. Soc. 97, 5670 (1975).	
Method used : ICR Bracketing relative to C2H5F and H2O.	

C2H2F2	CAS REGN : 1630-78-0
F**C++C**F	
Ethene, 1,2-difluoro-, (E)- (9CI) Ethylene, 1,2-difluoro-, (E)- (8CI)	
PA (exp) : 167+/-4 kcal/mol	Temperature : 300 K
Ridge, D. P., Gas Phase Proton Affinities of several Fluoroethylenes, J. Am. Chem. Soc. 97, 5670 (1975).	
Method used : ICR Bracketing relative to C2H5F and H2O.	

C2H2O	CAS REGN : 463-51-4
O++C++C	
Ethenone (9CI) Ketene (8CI)	
PA (exp) : 194.1+/-1 kcal/mol	Temperature : 350 K
Ausloos, P., and Lias, S. G. The Proton Affinity of Ketene and the Heat of Formation of CH3CO+, Chem. Phys. Letters 51, 53 (1977).	
Method used : ICR Equilibrium; scale based on PA (iso-C4H8) = 193.5+/-1	
PA (exp) : 195.9+/-2 kcal/mol	Temperature : 300 K
Vogt, J., Williamson, A. D., and Beauchamp, J. L. Properties and Reactions of Ketene in the Gas Phase by Ion Cyclotron Resonance Spectroscopy and Photoionization Mass Spectrometry. Proton Affinity, Site Specificity of Protonation, and Heat of Formation of Ketene, J. Am. Chem. Soc. 100, 3478 (1978).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H3ClO2	CAS REGN : 79-11-8
O=C*Cl % % 0	
Acetic acid, chloro- (8CI9CI)	
GB (exp) : 166.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 184+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero	

C2H3Cl3	CAS REGN : 115-20-8
CL * * CL* C**C**O * * CL	
Ethanol, 2,2,2-trichloro- (8CI9CI)	
GB (exp) : 171.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 179+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H3F	CAS REGN : 75-02-5
F**C++C	
Ethene, fluoro- (9CI) Ethylene, fluoro- (8CI)	
PA (exp) : 174+/-1 kcal/mol	Temperature : 300 K
Ridge, D. P., Gas Phase Proton Affinities of several Fluoroethylenes, J. Am. Chem. Soc. 97, 5670 (1975).	
Method used : ICR Bracketing relative to H2S and CH2O.	
PA (exp) : 173.6 kcal/mol	Temperature : 298 K
Williamson, A. D., LeBreton, P. R., and Beauchamp, J. L., Photoionization Mass Spectrometry of 2-Fluoro- propane and 2,2-Difluoropropane. A Novel Determination of Vinyl Fluoride and 1,1-Difluoro- ethylene, J. Am. Chem. Soc. 98, 2705 (1976).	
Method used : PI Appearance potential by photoionization of (CH3)2CHF.	

C2H3F02	CAS REGN : 144-49-0
O%XC**C**F % % 0	
Acetic acid, fluoro- (8CI9CI)	
GB (exp) : 167.3+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 184.5+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero	

C2H3F3O	CAS REGN : 75-89-8
F * * F**C**C**O * * F	
Ethanol, 2,2,2-trifluoro- (8CI9CI)	
GB (exp) : 164.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 172.2+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H3N	CAS REGN : 75-05-8
N##C**C	
Acetonitrile (8CI9CI)	
PA (exp) : 189.5+/-4.5 kcal/mol	Temperature : 298 K
Gray, G. A., Study of Ion-Molecule Reactions and Reaction Mechanisms in Acetonitrile by Ion Cyclotron Resonance, J. Am. Chem. Soc. 90, 6002 (1968).	
Method used : ICR Bracketing relative to CH3CHO and (CH3)2CO	
PA (exp) : 186+/-1 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Translational energy of RH2+ has been measured assuming $\Delta H = 5X$ translational energy for reaction $RH^+ + RH \rightarrow RH_2^+ + R$	

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GB (exp) : 179.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 171.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 187.4+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

C2H3NS	CAS REGN : 556-61-6
S++C++N**C	
Methane, isothiocyanato- (9CI) Isothiocyanic acid, methyl ester (8CI)	
PA (exp) : 189+/-6 kcal/mol	Temperature : 300 K
<p>McAllister, T., Ion-Molecule Reactions and Proton Affinities of Methyl Thio- and Isothiocyanate, Int. J. Mass Spectrom. Ion Phys. 15, 303 (1974).</p>	
<p>Method used : ICR Bracketing relative to (CH3)2CO and 1-C4H8.</p>	

C2H3NS	CAS REGN : 556-64-9
N##C**S**C	
Thiocyanic acid, methyl ester (8CI9CI)	
PA (exp) : 189+/-6 kcal/mol	Temperature : 300 K
<p>McAllister, T., Ion-Molecule Reactions and Proton Affinities of Methyl Thio- and Isothiocyanate, Int. J. Mass Spectrom. Ion Phys. 15, 303 (1974).</p>	
<p>Method used : ICR Bracketing relative to (CH3)2CO and 1-C4H8.</p>	

C2H4	CAS REGN : 74-85-1
C++C	
Ethene (9CI) Ethylene (8CI)	
PA (exp) : 160.6 kcal/mol	Temperature : 298 K
Lossing F. P., and Semeluk, G. P., Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals, Can. J. Chem. 48, 955 (1970).	
Method used : EM Appearance potential of C2H5+ using EM.	

C2H4F2O	CAS REGN : 359-13-7
F**C**C**O * * F	
Ethanol, 2,2-difluoro- (8CI9CI)	
GB (exp) : 170.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 177.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H4F3N	CAS REGN : 753-90-2
F * * F**C**C**N * * F	
Ethanamine, 2,2,2-trifluoro- (9CI) Ethylamine, 2,2,2-trifluoro- (8CI)	
GB (exp) : 188.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 197.9+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

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GB (exp) : 191.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.3+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

C2H4N2	CAS REGN : 540-61-4
N**C**C##N	
Acetonitrile, amino- (8CI9CI)	
PA (exp) : ~197 kcal/mol	Temperature : 300 K
<p>Taagepera, M., Hehre, W. J., Topsom, R. D., and Taft, R. W. Calculation of Polar Substituent Parameters by ab initio Molecular Orbital Methods. Proton Affinities of Substituted Primary Amines, J. Am. Chem. Soc. 98, 7438 (1976).</p>	
<p>Method used : ICR Equilibrium; scale based on NH3</p>	

C2H4O	CAS REGN : 75-07-0
O++C**C	
Acetaldehyde (8CI9CI)	
PA (exp) : 184+/-3 kcal/mol	Temperature :
Harrison, A. G., Ivko, A., and Van Raalte, D., Energetics of Formation of Some Oxygenated Ions and the Proton Affinities of Carbonyl Compounds, Can. J. Chem. 44, 1625 (1966).	
Method used : EI Electron impact fragmentation	
PA (exp) : 186+/-1 kcal/mol	Temperature : 298 K
Refaey, K. M. A., and Chupka, W. A., Photoionization of the Lower Aliphatic Alcohols with Mass Analysis, J. Chem. Phys. 48, 5205 (1968).	
Method used : PI Appearance potential by IP fragmentation of C2H5OH.	

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PA (exp) : 189.4 kcal/mol	Temperature : 298 K
<p>Lossing, F. P. Heats of Formation of Some Isomeric $[C_nH_{2n+10}]^+$ Ions. Substitutional Effects on Ion Stability, J. Am. Chem. Soc. 99, 7526 (1977).</p>	
<p>Method used : EM Electron impact fragmentation (various molecules) using EM. $\Delta H_f(H^+) = 365.7$</p>	
GB (exp) : 177.2 \pm 2 kcal/mol	Temperature : 300 K
PA (exp) : 185 \pm 2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH₃</p>	

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GB (exp) : 169.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 185.4+/-2 kcal/mol	Temperature : 600 K
<p>Yamdaqni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on NH3</p>	

C2H4O	CAS REGN : 75-21-8
<pre> 0 * * * * C*****C </pre>	
<p>Oxirane (9CI) Ethylene oxide (8CI)</p>	
PA (exp) : 185+/-4 kcal/mol	Temperature :
<p>Beauchamp, J. L., and Dunbar, R. C., Identification of C2H5O+ Structural Isomers by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 92, 1477 (1970).</p>	
<p>Method used : ICR Bracketing relative to CH3OH and (CH3)2O</p>	

C2H4O2	CAS REGN : 64-19-7
O%*C**C % % 0	
Acetic acid (8CI9CI)	
PA (exp) : 188+/-3 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Equilibrium; scale based on NH3	
GB (exp) : 171.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 188.2+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

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GB (exp) : 179.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H4O2	CAS REGN : 107-31-3
O++C**O**C	
Formic acid, methyl ester (8CI9CI)	
PA (exp) : 188+/-3 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to (CH3)2O and CH3CHO	

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GB (exp) : 179.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187+/-2 kcal/mol	Temperature : 300 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on CH3CHO Entropy change assumed zero	
GB (exp) : 179.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

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GB (exp) : 172.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 187.8+/-2 kcal/mol	Temperature : 600 K
<p>Yamdaqni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on NH3</p>	

C2H5Br	CAS REGN : 74-96-4
C**C**BR	
Ethane, bromo- (8CI9CI)	
PA (exp) : 171+/-2 kcal/mol	Temperature : 300 K
<p>Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).</p>	
<p>Method used : ICR Bracketing and using also IP's of H and C2H5BR and assuming HA(CH3BR+)=HA(C2H5BR+).</p>	

C2H5Cl	CAS REGN : 75-00-3
CL*C**C	
Ethane, chloro- (8CI9CI)	
PA (exp) : 170+/-2 kcal/mol	Temperature :
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Bracketing and using also IP's of H and C2H5Cl and HA(CH3CL+)=HA(C2H5CL+).	

C2H5F	CAS REGN : 353-36-6
F**C**C	
Ethane, fluoro- (8CI9CI)	
PA (exp) : 165+/-5 kcal/mol	Temperature : 300 K
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Bracketing and using also the IP's of H and C2H5F and assuming HA(CH3F+) = HA(C2H5F+).	

C2H5F2N	CAS REGN : 430-67-1
F**C**C**N * * F	
Ethanamine, 2,2-difluoro- (9CI) Ethylamine, 2,2-difluoro- (8CI)	
GB (exp) : 197.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 205.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H5I	CAS REGN : 75-03-6
I**C**C	
Ethane, iodo- (8CI9CI)	
PA (exp) : 175 kcal/mol	Temperature : 300 K
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Bracketing and using also IP's of H and assuming HA(CH3I+)=HA(C2H5I+).	

C2H5N	CAS REGN : 151-56-4
<pre> N * * * * C*****C </pre>	
Aziridine (9CI) Ethylenimine (8CI)	
GB (exp) : 204.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 212.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 204.9+/-2 kcal/mol	Temperature : 298 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	

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PA (exp) : 213+/-2 kcal/mol	Temperature : 300 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Nitrogen and Oxygen Bases. Hybridization Effects, J. Am. Chem. Soc. 97, 4137 (1975).	
Method used : ICR Equilibrium; scale based on CH3NH2 Van't Hoff plot	

C2H5NO	CAS REGN : 60-35-5
N% % % 0	
Acetamide (8CI9CI)	
GB (exp) : 188.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 205.7+/-2 kcal/mol	Temperature : 600 K
Yamdaqui, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).	
Method used : MS Equilibrium; scale based on CH3NH2 Entropy change assumed zero	

C2H5NO	CAS REGN : 123-39-7
O% C% N* *C	
Formamide; N-methyl- (8CI9CI)	
GB (exp) : 195+/-4 kcal/mol	Temperature : 300 K
PA (exp) : 202.8+/-4 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H5NO2	CAS REGN : 79-24-3
O++NXXCXXC + + 0	
Ethane, nitro- (8CI9CI)	
PA (exp) : 186+/-2 kcal/mol	Temperature : 300 K
Kriemler, P., and Buttrill, S. E., Jr., Ion-Molecule Reactions and the Proton Affinities of the Nitroalkanes, J. Am. Chem. Soc. 95, 1365 (1973).	
Method used : ICR Bracketing relative to CH3CN and CH3CHO.	

C2H5NO3	CAS REGN : 625-58-1
C**C**O**N**+0 + + 0	
Nitric acid, ethyl ester (8CI9CI)	
PA (exp) : 181+/-3 kcal/mol	Temperature : 300 K
Kriemler, P., and Buttrill, S. E., Jr., Positive and Negative Ion-Molecule Reactions and the Proton Affinity of Ethyl Nitrate, J. Am. Chem. Soc. 92, 1123 (1970).	
Method used : ICR Bracketing relative to cyclo-C6H10 and CH3NO2.	

C2H6	CAS REGN : 74-84-0
C**C	
Ethane (8CI9CI)	
PA (exp) : 128+/-1 kcal/mol	Temperature :
Chong, S. L., and Franklin, J. L., Heats of Formation of Protonated Cyclopropane, Methylcyclopropane, and Ethane, J. Am. Chem. Soc. 94, 6347 (1972).	
Method used : MS By applying path degeneracy correction found delta H formation (C2H7+) = 218.8 Equilibrium relative to CH4; assume delta S = 0.	
PA (exp) : 139.6 (1) kcal/mol	Temperature : 300 K
Hiraoka, K., and Kebarle, P., Stabilities and Energetics of Pentacoordinated Carbonium Ions. The Isomeric C2H7+ Ions and Some Higher Analogues: C3H9+ and C4H11+, J. Am. Chem. Soc. 98, 6119 (1976).	
Method used : MS Based on delta H formation(C2H5+) = 219. Equilibrium of reaction: C2H5+ + H2 -> C2H7+(C-C protonation) (1).	

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PA (exp) : 131.8 (2) kcal/mol	Temperature :
<p>Hiraoka, K., and Kebarle, P., Stabilities and Energetics of Pentacoordinated Carbonium Ions. The Isomeric C₂H₇⁺ Ions and Some Higher Analogues: C₃H₉⁺ and C₄H₁₁⁺, J. Am. Chem. Soc. 98, 6119 (1976).</p>	
<p>Method used : MS Based on delta H formation(C₂H₅⁺) = 219 Equilibrium of reaction: C₂H₅⁺ + H₂ + H₂ → C₂H₇⁺ + H₂(CH protonation) (2).</p>	

C ₂ H ₆ FN	CAS REGN : 406-34-8
F**C**C**N	
<p>Ethanamine, 2-fluoro- (9CI) Ethylamine, 2-fluoro- (8CI)</p>	
GB (exp) : 201.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 210.2+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH₃</p>	

C2H6N2	CAS REGN : 4143-41-3
C**N++N**C	
Diazene, dimethyl-, (E)- (9CI) Azomethane, (E)- (8CI)	
GB (exp) : 197.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204.5+/-2 kcal/mol	Temperature : 300 K
Foster, M. S., Williamson, A. D., and Beauchamp, J. L., Photoionization Mass Spectrometry of trans-Azomethane, Int. J. Mass Spectrom. Ion Phys. 15, 429 (1974).	
Method used : MS Calculated entropy Equilibrium relative to NH3	
PA (exp) : 206.8+/-5 kcal/mol	Temperature : 300 K
Foster, M. S., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Azomethane by Ion Cyclotron Resonance, J. Am. Chem. Soc. 94, 2425 (1972).	
Method used : ICR Bracketing between NH3 and CH3NH2	

C2H6O	CAS REGN : 64-17-5
O**C**C	
Ethanol (9CI) Ethyl alcohol (8CI)	
PA (exp) : 186+/-2 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to CH3COOH and CH3CHO	
GB (exp) : 178.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 186.2+/-2 kcal/mol	Temperature : 300 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on CH3CHO Entropy change assumed zero	

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GB (exp) : 171.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 186.8+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 178.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 186.7+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C2H6O	CAS REGN : 115-10-6
C**O**C	
Methane, oxybis- (9CI) Methyl ether (8CI)	
PA (exp) : 190+/-4 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to I-C4H8 and CH3CHO; Scale based on NH3	
PA (exp) : 189 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Delta H assume = 5X translational energy of the products of reaction $RH + RH^+ \rightarrow RH_2^+ + R$.	

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GB (exp) : 181.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 189.1+/-2 kcal/mol	Temperature : 298 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on MECHO Entropy change assumed zero	
GB (exp) : 174.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 189.3+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

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GB (exp) : 182.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.1+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 193.3 kcal/mol	Temperature : 300 K
Hiraoka, K., Grimsrud, E. P., and Kebarle, P., Gas Phase Ion Equilibria Studies of the Hydrogen Ion in Water-Dimethyl Ether and Methanol-Dimethyl, J. Am. Chem. Soc. 96, 3359 (1974).	
Method used : MS Van't Hoff plot Equilibrium relative to H2O. Delta G determined by means of thermodynamic cycles involving mixed clusters.	

C2H6OS	CAS REGN : 67-68-5
C**S**C + + 0	
Methane, sulfinylbis- (9CI) Methyl sulfoxide (8CI)	
GB (exp) : 200.9+/-2.5 kcal/mol	Temperature : 300 K
PA (exp) : 208.3+/-2.5 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 184+/-3 kcal/mol	Temperature : 300 K
McAllister, T. Ion Cyclotron Resonance Mass Spectroscopy of Dimethyl Sulfoxide, Intern. J. Mass Spectrom. Ion Phys. 25, 353 (1977).	
Method used : ICR Bracketing relative to CH3OH and EtOH.	

C2H6S	CAS REGN : 75-08-1
S**C**C	
Ethanethiol (8CI9CI)	
GB (exp) : 180.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H6S	CAS REGN : 75-18-3
C**S**C	
Methane, thiobis- (9CI) Methyl sulfide (8CI)	
GB (exp) : 190.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.6+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H7N	CAS REGN : 75-04-7
N**C**C	
Ethanamine (9CI) Ethylamine (8CI)	
GB (exp) : 205.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.0+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 205.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 214.3+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C2H7N	CAS REGN : 124-40-3
C×N×C	
Methanamine, N-methyl- (9CI) Dimethylamine (8CI)	
GB (exp) : 209.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 217.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 209.5+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 217.7+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

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GB (exp) : 203.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 220.6+/-2 kcal/mol	Temperature : 600 K
Briggs, J. P., Yamdagni, R., and Kebarle, P., Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton- Exchange Equilibria, J. Am. Chem. Soc. 94, 5128 (1972).	
Method used : MS Entropy change assumed zero Equilibrium; scale based on NH3	

C2H7P	CAS REGN : 676-59-5
C**P**C	
Phosphine, dimethyl- (8CI9CI)	
GB (exp) : 205.6+/-2 kcal/mol	Temperature : 298 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	

C2H8N2	CAS REGN : 57-14-7
C**N**C * * N	
Hydrazine, 1,1-dimethyl- (8CI9CI)	
GB (exp) : 209.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 217.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H8N2	CAS REGN : 107-15-3
N**C**C**N	
1,2-Ethanediamine (9CI) Ethylenediamine (8CI)	
GB (exp) : 213.60+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.50+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	
GB (exp) : 215.50+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 227.50+/-2 kcal/mol	Temperature : 298 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).	
Method used : MS Equilibrium; scale based on (CH3)3N Van't Hoff plot	

C3D9N	CAS REGN : 13960-80-0
C**N**C * * C	
Methan-d3-amine, N,N-di(methyl-d3)- (9CI) Trimethylamine-d9. (8CI)	
GB (exp) : 214.00+/-2 kcal/mol	Temperature : 298 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	

C3H2N2	CAS REGN : 109-77-3
N##C**C**C##N	
Propanedinitrile (9CI) Malononitrile (8CI)	
GB (exp) : 169.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 177.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H3F3O2	CAS REGN : 431-47-0
F * * C**O**C**C**F + * + * O F	
Acetic acid, trifluoro-, methyl ester (8CI9CI)	
GB (exp) : 172.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.3+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H3F3O2	CAS REGN : 32042-38-9
F * * F**C**C**O**C++O * * F	
Ethanol, 2,2,2-trifluoro-, formate (9CI)	
GB (exp) : 173+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.8+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H3N	CAS REGN : 107-13-1
C++C**C##N	
2-Propenenitrile (9CI) Acrylonitrile (8CI)	
GB (exp) : 180.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187.9+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
PA (exp) : 188.3+/-2.5 kcal/mol	Temperature : 300 K
<p>Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium relative to C3H6O2(1,3-Dioxolane) with its PA value = 189.8; relative to Et CHO and MeCN</p>	

C3H4	CAS REGN : 74-99-7
C##C**C	
1-Propyne (9CI) Propyne (8CI)	
PA (exp) : 176+/-2 kcal/mol	Temperature : 300 K
Aue, D. H., Davidson, W. R., and Bowers, M. T., Heats of Formation of C3H5+ Ions. Allyl, Vinyl, and Cyclopropyl Cations in Gas-Phase Proton-Transfer Reactions, J. Am. Chem. Soc. 98, 6700 (1976).	
Method used : ICR Entropy change assumed zero Equilibrium; scale based on H2S.	

C3H4	CAS REGN : 463-49-0
C++C++C	
1,2-Propadiene (9CI) Allene (8CI)	
PA (exp) : 176+/-2 kcal/mol	Temperature : 300 K
Aue, D. H., Davidson, W. R., and Bowers, M. T., Heats of Formation of C3H5+ Ions. Allyl, Vinyl, and Cyclopropyl Cations in Gas-Phase Proton-Transfer Reactions, J. Am. Chem. Soc. 98, 6700 (1976).	
Method used : ICR Equilibrium; scale based on H2S. Entropy change assumed zero.	

C3H4	CAS REGN : 2781-85-3
C * + * + C*****C	
Cyclopropene (8CI9CI)	
PA (exp) : 194+/-3 kcal/mol	Temperature : 300 K
Aue, D. H., Davidson, W. R., and Bowers, M. T., Heats of Formation of C3H5+ Ions. Allyl, Vinyl, and Cyclopropyl Cations in Gas-Phase Proton-Transfer Reactions, J. Am. Chem. Soc. 98, 6700 (1976).	
Method used : ICR Bracketing relative to (CH3)2O and (C2H5)2O.	

C3H4C1N	CAS REGN : 542-76-7
N##C**C**C**CL	
Propanenitrile, 3-chloro- (9CI) Propionitrile, 3-chloro- (8CI)	
PA (exp) : 181.1+/-2 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to MeCN	
GB (exp) : 178.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 186.1+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H5N	CAS REGN : 107-12-0
C**C**C##N	
Propanenitrile (9CI) Propionitrile (8CI)	
GB (exp) : 182.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.2+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
PA (exp) : 190.2+/-2.5 kcal/mol	Temperature : 300 K
<p>Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium relative to n-PrCN, HCO2Et, i-PrCHO, Me2O, EtCHO and relative to 1,3-Dioxane using its PA = 189.8</p>	

C3H5N	CAS REGN : 2450-71-7
C##C**C**N	
2-Propyn-1-amine (9CI) 2-Propynylamine (8CI)	
GB (exp) : 200.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 209.0+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H6	CAS REGN : 75-19-4
<pre> C * * * * C*****C </pre>	
Cyclopropane (8CI9CI)	
PA (exp) : 180.6+/-4 kcal/mol	Temperature : 340 K
<p>Chong, S. L., and Franklin, J. L., Heats of Formation of Protonated Cyclopropane, Methylcyclopropane, and Ethane, J. Am. Chem. Soc. 94, 6347 (1972).</p>	
<p>Method used : MS $\text{HC(OH)}_2^+ + \text{C-C}_3\text{H}_6 \rightarrow \text{HC(OH)} + \text{C-C}_3\text{H}_7^+$. Equilibrium of reactions: $\text{CH}_3\text{OH}_2^+ + \text{C-C}_3\text{H}_6 \rightarrow \text{CH}_3\text{OH} + \text{C-C}_3\text{H}_7^+$; Apply correction for path degeneracy. Assuming $\Delta S = 0$.</p>	

C3H6	CAS REGN : 115-07-1
C++C**C	
1-Propene (9CI) Propene (8CI)	
PA (exp) : 180 kcal/mol	Temperature : 298 K
Lossing F. P., and Semeluk, G. P. Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals, Can. J. Chem. 48, 955 (1970).	
Method used : EM Appearance potential of C3H7+.	
PA (exp) : 182.2+/-2 kcal/mol	Temperature : 340 K
Chong, S. L., and Franklin, J. L., Heats of Formation of Protonated Cyclopropane, Methylcyclopropane, and Ethane, J. Am. Chem. Soc. 94, 6347 (1972).	
Method used : MS Correction for path degeneracy. Equilibrium relative to CH3OH; assuming delta S = 0.	

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GB (exp) : 165.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.6+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero</p>	

C3H6F3N	CAS REGN : 460-39-9
<pre> F * * N**C**C**C**F * * F </pre>	
<p>1-Propanamine, 3,3,3-trifluoro- (9CI) Propylamine, 3,3,3-trifluoro- (8CI)</p>	
GB (exp) : 200.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 209.0+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C3H6F3N	CAS REGN : 677-41-8
F C * * * * F**C**N**C * * F	
Methanamine, 1,1,1-trifluoro-N,N-dimethyl-	
PA (exp) : 192+/-3 kcal/mol	Temperature : 300 K
Staley, R. H., Taagepera, M., Henderson, W. G., Koppel, I., Beauchamp, J. L., and Taft, R. W. Effects of Alkyl and Fluoroalkyl Substitution on the Heterolytic and Homolytic Bond Dissociation Energies of Protonated Amines, J. Am. Chem. Soc. 99, 326 (1977).	
Method used : ICR Calculated entropy Equilibrium scale based on NH3	

C3H6F3N	CAS REGN : 2730-67-8
F x x C*x*N*x*C*x*C*x*F x x F	
Ethanamine, 2,2,2-trifluoro-N-methyl- (9CI) Ethylamine, 2,2,2-trifluoro-N-methyl- (8CI)	
GB (exp) : 199.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 207.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H6N2	CAS REGN : 151-18-8
N##C**C**C**N	
Propanenitrile, 3-amino- (9CI) Propionitrile, 3-amino- (8CI)	
GB (exp) : 196.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H6N2	CAS REGN : 5616-32-0
C**N**C**C##N	
Acetonitrile, (methylamino)- (8CI9CI)	
GB (exp) : 196.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H6O	CAS REGN : 67-64-1
C**C**C + + 0	
2-Propanone (9CI) Acetone (8CI)	
PA (exp) : 195.7+/-2 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to (C2H5)2O and CH2CO	
PA (exp) : 193.6+/-1 kcal/mol	Temperature : 350 K
Ausloos, P., and Lias, S. G. The Proton Affinity of Ketene and the Heat of Formation of CH3CO+, Chem. Phys. Letters 51, 53 (1977).	
Method used : ICR Equilibrium; scale based on PA (iso-C4H8) = 193.5+/-1	

Continued on next page

GB not calculated for this reference	
PA (exp) : 188 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Delta H estimated equal 5 times translational energy of the products.	
PA (exp) : 196 kcal/mol	Temperature : 298 K
Heats of Formation of Some Isomeric $[C_nH_{2n+10}]^+$ Ions. Substitutional Effects on Ion Stability, J. Am. Chem. Soc. 99, 7526 (1977).	
Method used : EM Electron impact fragmentation (various molecules) using EM. $\Delta H_f(H^+) = 365.7$ Lossing, F. P.	

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GB (exp) : 179+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 193.8+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 186.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 193.9+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C3H6O	CAS REGN : 123-38-6
C**C**C++O	
Propanal (9CI) Propionaldehyde (8CI)	
PA (exp) : 190+/-3 kcal/mol	Temperature :
Harrison, A. G., Ivko, A., and Van Raalte, D., Energetics of Formation of Some Oxygenated Ions and the Proton Affinities of Carbonyl Compounds, Can. J. Chem. 44, 1625 (1966).	
Method used : EI Electron impact fragmentation of various molecules.	
PA (exp) : 187 kcal/mol	Temperature : 298 K
Lossing, F. P. Heats of Formation of Some Isomeric [C _n H _{2n} + 10] ⁺ Ions. Substitutional Effects on Ion Stability, J. Am. Chem. Soc. 99, 7526 (1977).	
Method used : EM Electron impact fragmentation (various molecules) using EM. $\Delta H_f(H^+) = 365.7$	

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GB (exp) : 172.3+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 187.9+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 180.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C3H6O	CAS REGN : 503-30-0
C**O * * * * C**C	
Oxetane (9CI) Trimethylene oxide (8CI)	
PA (exp) : 194+/-1 kcal/mol	Temperature : 300 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Nitrogen and Oxygen Bases. Hybridization Effects, J. Am. Chem. Soc. 97, 4137 (1975).	
Method used : ICR Semiquantitative. Absolute value assign relative to CH3CHO and (CH3)2C=CH2.	

C3H6OS	CAS REGN : 1534-08-3
C**C**S**C + + 0	
Ethanethioic acid, S-methyl ester (9CI) Acetic acid, thio-, S-methyl ester (8CI)	
PA (exp) : ~197+/-2 kcal/mol	Temperature : 300 K
Grunwell, J. R., Foerst, D. L., Kaplan, F., and Siddiqui, J. The Relative Basicity of Sulfur containing Esters, Tetrahedron 33, 2781 (1977).	
Method used : ICR Bracketing relative to MeCOOMe and MeCONHCH3. Also found the reactions of Me2S with MeCOOMe and MeCOSMe are both thermoneutral concluded PA (CH3COSCH3) is within 2 kcal of that of PA (MeCOOMe)	

C3H6O2	CAS REGN : 79-09-4
O=C*O	
Propanoic acid (9CI) Propionic acid (8CI)	
GB (exp) : 173.9+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 191.1+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero	

C3H6O2	CAS REGN : 79-20-9
C**C**O**C + + 0	
Acetic acid, methyl ester (8CI9CI)	
PA (exp) : 194+/-2 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to ME2CO and CH2CO	
GB (exp) : 186.7+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 194.1+/-2 kcal/mol	Temperature : 298 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on (CH3)2CO Entropy change assumed zero	

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GB (exp) : 187.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 195.4+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 179.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 195.4+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

C3H6O2	CAS REGN : 109-94-4
O++C**O**C**C	
Formic acid, ethyl ester (8CI9CI)	
PA (exp) : 194+/-2 kcal/mol	Temperature : 323-373 K
<p>Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).</p>	
<p>Method used : MS Bracketing relative to CH2CO AND I-C4H8; scale based on NH3.</p>	
GB (exp) : 183.7+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 191.1+/-2 kcal/mol	Temperature : 298 K
<p>Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).</p>	
<p>Method used : MS Equilibrium; scale based on (CH3)2CO Entropy change assumed zero</p>	

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GB (exp) : 175.6+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 191.2+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on NH₃</p>	
GB (exp) : 183.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 191.2+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH₃</p>	

C3H6O3	CAS REGN : 616-38-6
C**O**C**O**C + + O	
Carbonic acid, dimethyl ester (8CI9CI)	
GB (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.2+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H6S2	CAS REGN : 2168-84-5
S + + C**S****C**C	
Ethane(dithioic)acid, methyl ester	
PA (exp) : >197+/-2 kcal/mol	Temperature : 300 K
Grunwell, J. R., Forest, D. L., Kaplan, F., and Siddiqui, J. The Relative Basicity of Sulfur Containing Esters, Tetrahedron 33, 2781 (1977).	
Method used : ICR Double resonance technique shows PA (MeCSSMe) > PA (the COSMe)	

C3H7N	CAS REGN : 107-11-9
C++C**C**N	
2-Propen-1-amine (9CI) Allylamine (8CI)	
GB (exp) : 205.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 213.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H7N	CAS REGN : 503-29-7
C**N * * * * C**C	
Azetidine (8CI9CI)	
GB (exp) : 211.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 220.1+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 212.2+/-2 kcal/mol	Temperature : 290 K
PA (exp) : 220.+/-2 kcal/mol	Temperature : 290 K
Bowers, M. T., Aue, D. H., and Webb, H. M., Equilibrium Constants for Gas-Phase Ionic Reactions. Accurate Determination of Relative Proton Affinities, J. Am. Chem. Soc. 93, 4314 (1971).	
Method used : ICR Entropy change assumed zero Equilibrium; scale based on (CH3)3N	

C3H7N	CAS REGN : 1072-44-2
<pre> C * * * * N*****C * * C</pre>	
Aziridine, 1-methyl- (8CI9CI)	
PA (exp) : 219.4+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Nitrogen and Oxygen Bases. Hybridization Effects, J. Am. Chem. Soc. 97, 4137 (1975).</p>	
<p>Method used : ICR Equilibrium; scale based on CH3NH2</p>	

C3H7NO	CAS REGN : 68-12-2
C**N**C++O * * C	
Formamide, N,N-dimethyl- (8CI9CI)	
GB (exp) : 201.2+/-3 kcal/mol	Temperature : 300 K
PA (exp) : 209.0+/-3 kcal/mol	Temperature : 300 K
· Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H8	CAS REGN : 74-98-6
C**C**C	
Propane (8CI9CI)	
PA (exp) : 148.2 kcal/mol	Temperature : 163-213 K
<p>Hiraoka, K., and Kebarle, P., Information on the Proton Affinity and Protolysis of Propane from Measurement of the Ion Cluster, Equilibrium: $C_2H_5^+ + CH_4 = C_3H_9^+$. Can. J. Chem. 53, 970 (1975).</p>	
<p>Method used : MS Equilibrium of reaction $C_2H_5^+ + 2CH_4 \rightarrow C_3H_9^+ + CH_4$ Van't Hoff plot</p>	
PA (exp) : 143 kcal/mol	Temperature : 170 K
<p>Field, F. H., and Beggs, D. P., Reversible Reactions of Gaseous Ions. III. Studies with Methane at 0.1-1.0 Torr and 77-300 K, J. Am. Chem. Soc. 93, 1585 (1971).</p>	
<p>Method used : MS Equilibrium of reaction: $C_2H_5^+ + CH_4 \rightarrow C_3H_9^+$. Based on delta H formation($C_2H_5^+$). Calculated entropy</p>	

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GB not calculated for this reference	
PA (exp) : <152.8 kcal/mol	Temperature : -170 K
<p>Hiraoka, K., and Kebarle, P., Stabilities and Energetics of Pentacoordinated Carbonium Ions. The Isomeric C₂H₇⁺ Ions and Some Higher Analogues: C₃H₉⁺ and C₄H₁₁⁺, J. Am. Chem. Soc. 98, 6119 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium of reaction Sec-C₃H₇⁺ + H₂ -> C₃H₉⁺ Based on delta H formation(C₃H₇⁺); C-H protonation</p>	

C3H8O	CAS REGN : 67-63-0
<p>C**C**C * * 0</p>	
<p>2-Propanol (9CI) Isopropyl alcohol (8CI)</p>	
PA (exp) : 192+/-2 kcal/mol	Temperature : 323-373 K
<p>Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).</p>	
<p>Method used : MS Bracketing relative to I-C₄H₈ and (CH₃)₂O</p>	

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GB not calculated for this reference	
PA (exp) : 190 kcal/mol	Temperature :
<p>Hiraoka, K., and Kebarle, P. Condensation Reactions Involving Carbonium Ions and Lewis Bases in the Gas Phase. Hydration of the tert-Butyl Cation, J. Am. Chem. Soc. 99, 360 (1977).</p>	
<p>Method used : MS Equilibrium relative to known standard acids</p>	

C3H8O	CAS REGN : 71-23-8
C**C**C**O	
<p>1-Propanol (9CI) Propyl alcohol (8CI)</p>	
GB (exp) : 181.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188.8+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

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PA (exp) : 189+/-2 kcal/mol	Temperature : 323-373 K
<p>Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).</p>	
<p>Method used : MS Bracketing relative to C2H5OH and (CH3)2O</p>	

C3H8O	CAS REGN : 540-67-0
C**C**O**C	
<p>Ethane, methoxy- (9CI) Ether, ethyl methyl (8CI)</p>	
GB (exp) : 186.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 194+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C3H8S	CAS REGN : 75-33-2
C**C**C * * S	
2-Propanethiol (8CI9CI)	
GB (exp) : 184.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 192+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H8S	CAS REGN : 107-03-9
C**C**C**S	
1-Propanethiol (8CI9CI)	
GB (exp) : 181.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H8S	CAS REGN : 624-89-5
C**C**S**C	
Ethane, (methylthio)- (9CI) Sulfide, ethyl methyl (8CI)	
GB (exp) : 192.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H9As	CAS REGN : 593-88-4
C**AS*C * * C	
Arsine, trimethyl- (8CI9CI)	
PA (exp) : 210.6 kcal/mol	Temperature : 300 K
Hodges, R. V., and Beauchamp, J. L., Basicity and Ion-Molecule Reactions of Trimethylarsine in the Gas Phase Determined by Ion Cyclotron Resonance Spectroscopy, Inorg. Chem. 14, 2887 (1975).	
Method used : ICR Equilibrium relative to CH3NH2 and also to CF3(CH2)3NH2.	

C3H9N	CAS REGN : 75-31-0
C**C**C * * N	
2-Propanamine (9CI) Isopropylamine (8CI)	
GB (exp) : 208.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 216.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 208.2+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.6+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C3H9N	CAS REGN : 75-50-3
C**N**C * * C	
Methanamine, N,N-dimethyl- (9CI) Trimethylamine (8CI)	
GB (exp) : 214.30+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 222.10+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 213.70+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 221.50+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

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GB (exp) : 208.40+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 225.60+/-2 kcal/mol	Temperature : 600 K
Briggs, J. P., Yamdagni, R., and Kebarle, P., Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton- Exchange Equilibria, J. Am. Chem. Soc. 94, 5128 (1972).	
Method used : MS Entropy change assumed zero Equilibrium; scale based on NH3	

C3H9N	CAS REGN : 107-10-8
C**C**C**N	
1-Propanamine (9CI) Propylamine (8CI)	
GB (exp) : 207.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 215.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

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GB (exp) : 207.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 215.7+/-2 kcal/mol	Temperature : 300 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C3H9N	CAS REGN : 624-78-2
C**C**N**C	
Ethanamine, N-methyl- (9CI) Ethylamine, N-methyl- (8CI)	
GB (exp) : 212.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 220.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

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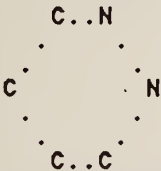
GB (exp) : 212+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 220.2+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C3H9NO	CAS REGN : 109-85-3
C**O**C**C**N	
Ethanamine, 2-methoxy- (9CI) Ethylamine, 2-methoxy- (8CI)	
GB (exp) : 209.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 221.0+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

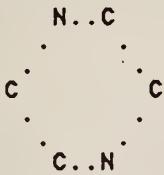
C3H9P	CAS REGN : 594-09-2
C**P**C * * C	
Phosphine, trimethyl- (8CI9CI)	
GB (exp) : 214.9+/-2 kcal/mol	Temperature : 298 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	
PA (exp) : 223.3+/-2 kcal/mol	Temperature : 300 K
Staley, P. H., and Beauchamp, J. L. Basicities and Ion-Molecule Reactions of the Methylphosphines in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 96, 6252 (1974).	
Method used : ICR Bracketing relative to (CH3)3N and (CH3)2C2H5N	

C3H10N2	CAS REGN : -109-76-2
N**C**C**C**N	
1,3-Propanediamine (8CI9CI)	
GB (exp) : 219.10+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 231.60+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	
GB (exp) : 221.10+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 235.10+/-2 kcal/mol	Temperature : 298 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).</p>	
<p>Method used : MS Equilibrium; scale based on (CH3)3N Van't Hoff plot</p>	

C4H4F4O2	CAS REGN : 1683-88-1
F * * F**C**C**O**C**C**F * + * + F 0	
Acetic acid, trifluoro-, 2-fluoroethyl ester (8CI)	
GB (exp) : 172.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.1+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

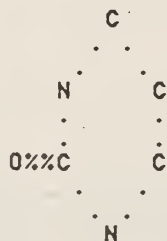
C4H4N2	CAS REGN : 289-80-5
	
Pyridazine (8CI9CI)	
GB (exp) : 206.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 213.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H4N2	CAS REGN : 289-95-2
<pre> N..C . . C N . . C..C</pre>	
Pyrimidine (8CI9CI)	
GB (exp) : 201.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 208.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H4N2	CAS REGN : 290-37-9
	
Pyrazine (8CI9CI)	
GB (exp) : 199.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H4N2O

CAS REGN : 557-01-7



2(1H)-Pyrimidinone (8CI9CI)

PA (exp) : 207+/-5 kcal/mol

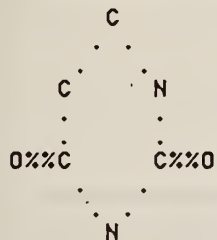
Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to NH3 and CH3NH2.

C4H4N2O2

CAS REGN : 66-22-8



2,4(1H,3H)-Pyrimidinedione (9CI)
Uracil (8CI)

PA (exp) : 207+/-5 kcal/mol

Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to NH3 and CH3NH2.

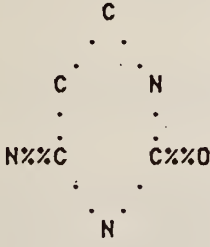
C4H4O	CAS REGN : 110-00-9
C*****O + * + * C C * + * + C	
Furan (8CI9CI)	
PA (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K
Chong, S. L., and Franklin, J. L., Proton Affinities of Benzene, Toluene, and the Xylenes, J. Am. Chem. Soc. 94, 6630 (1972).	
Method used : MS Entropy change assumed zero Equilibrium relative to (CH3)2O.	

C4H5F3O2	CAS REGN : 383-63-1
F * * F**C**C**O**C**C * + * + F O	
Acetic acid, trifluoro-, ethyl ester (8CI9CI)	
GB (exp) : 175.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 183.2+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H5N	CAS REGN : 109-97-7
<pre> C*****N + * + * C C * + * + C </pre>	
1H-Pyrrole (9CI) Pyrrole (8CI)	
GB (exp) : 197.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 205.9+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	
GB (exp) : 192.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 209.4+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).	
Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero	

C4H5N	CAS REGN : 5500-21-0
<pre> C * * * * * * C*****C * * N##C </pre>	
Cyclopropanecarbonitrile (8CI9CI)	
PA (exp) : 193.2+/-2 kcal/mol	Temperature : 300 K
<p>Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium relative to HCO2-n-C4H9</p>	
GB (exp) : 185.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 193.2+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C4H5NO2	CAS REGN : 623-49-4
N##C**C**O**C**C + + 0	
Carbonocyanidic acid, ethyl ester (9CI) Formic acid, cyano-, ethyl ester (8CI)	
GB (exp) : 173.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H5N3O	CAS REGN : 71-30-7
	
<p>2(1H)-Pyrimidinone, 4-amino- (9CI) Cytosine (8CI)</p>	
PA (exp) : 220+/-2 kcal/mol	Temperature :
<p>Wilson, M. S., and McCloskey, J. A., Chemical Ionization Mass Spectrometry of Nucleosides. Mechanisms of Ion Formation and Estimations of Proton Affinity, J. Am. Chem. Soc. 97, 3436 (1975).</p>	
<p>Method used : MS Bracketing relative to (CH3)2NH and (CH3)3N.</p>	

C4H6N2	CAS REGN : 616-47-7
<pre> C++++N * * * * C**N C * + * + C</pre>	
1H-Imidazole, 1-methyl- (9CI) Imidazole, 1-methyl- (8CI)	
GB (exp) : 217.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 225.1+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H7F3O	CAS REGN : 461-24-5
F * * F**C**C**O**C**C * * F	
Ethane, 2-ethoxy-1,1,1-trifluoro- (9CI) Ether, ethyl 2,2,2-trifluoroethyl (8CI)	
GB (exp) : 177.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 184.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H7N	CAS REGN : 78-82-0
CXXCXXC##N * * C	
Propanenitrile, 2-methyl- (9CI) Isobutyronitrile (8CI)	
PA (exp) : 192.2+/-2 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to HC02C2H5	
GB (exp) : 184.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 192.2+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H7N	CAS REGN : 109-74-0
N##C**C**C**C	
Butanenitrile (9CI) Butyronitrile (8CI)	
PA (exp) : 191.2+/-2.5 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to HC02Et, ME2O and EtCN	
GB (exp) : 183.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 191.4+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8	CAS REGN : 106-98-9
C**C**C++C	
1-Butene (8CI9CI)	
PA (exp) : 183.2 kcal/mol	Temperature : 298 K
Lossing F. P., and Semeluk, G. P. Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals, Can. J. Chem. 48, 955 (1970).	
Method used : EM Appearance potential of C4H9+ by EM	

C4H8	CAS REGN : 115-11-7
C××C××C + + C	
1-Propene, 2-methyl- (9CI) Propene, 2-methyl- (8CI)	
PA (exp) : 192.6+/-2 kcal/mol	Temperature : 363-553 K
Goren, A., and Munson, B. Thermochemistry of Alkyl Ions, J. Phys. Chem. 80, 2848 (1976).	
Method used : MS Using $\Delta H_f(t-C_4H_9^+)$ = 169+/-1.8 derived from, $\Delta H_f(t-C_4H_9)$ = 9.3 and $IP(t-C_4H_9)$ = 159.9	
PA (exp) : 193.7 kcal/mol	Temperature :
Lossing F. P., and Semeluk, G. P. Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals, Can. J. Chem. 48, 955 (1970).	
Method used : EM Appearance potential of C4H9+	

Continued on next page

GB (exp) : 177.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 194.2+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 185.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 193.5+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8	CAS REGN : 590-18-1
C**C++C**C	
2-Butene, (Z)- (8CI9CI)	
PA (exp) : 181.9 kcal/mol	Temperature : 298 K
Lossing F. P., and Semeluk, G. P. Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals, Can. J. Chem. 48, 955 (1970).	
Method used : EM Appearance potential of C4H9+	

C4H8	CAS REGN : 594-11-6
<pre> C * * * * C*****C * * C</pre>	
Cyclopropane, methyl- (8CI9CI)	
.PA (exp) : 181+/-2 kcal/mol	Temperature :
Chong, S. L., and Franklin, J. L., Heats of Formation of Protonated Cyclopropane, Methylcyclopropane, and Ethane, J. Am. Chem. Soc. 94, 6347 (1972).	
Method used : MS Equilibrium relative to HCOOH based on PA(HCOOH)=180.1+/-2 assuming delta S=0 Correction for path degeneracy.	

C4H8	CAS REGN : 624-64-6
C**C++C**C	
2-Butene, (E)- (8CI9CI)	
PA (exp) : 180.9 kcal/mol	Temperature : 298 K
Lossing F. P., and Semeluk, G. P. Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals, Can. J. Chem. 48, 955 (1970).	
Method used : EM Appearance potential of C4H9+	

C4H8F3N	CAS REGN : 819-06-7
F * * C**N**C**C**F * * * * C F	
Ethanamine, 2,2,2-trifluoro-N,N-dimethyl- (9CI) Ethylamine, 2,2,2-trifluoro-N,N-dimethyl- (8CI)	
GB (exp) : 204.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 212.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8F3N	CAS REGN : 819-46-5
F * * F**C**C**C**C**N * * F	
1-Butanamine, 4,4,4-trifluoro- (9CI) Butylamine, 4,4,4-trifluoro- (8CI)	
GB (exp) : 203.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 212.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8N2	CAS REGN : 926-64-7
N##C**C**N**C * * C	
Acetonitrile, (dimethylamino)- (8CI9CI)	
GB (exp) : 200.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 208.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8O	CAS REGN : 78-84-2
C**C**C++O * * C	
Propanal, 2-methyl- (9CI) Isobutyraldehyde (8CI)	
GB (exp) : 182.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.6+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Tæagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8O	CAS REGN : 78-93-3
C**C**C**C + + 0	
2-Butanone (8CI9CI)	
GB (exp) : 189.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 193.7+/-1 kcal/mol	Temperature : 293 K
Lossing, F. P. Heats of Formation of Some Isomeric [C _n H _{2n} + 10] ⁺ Ions. Substitutional Effects on Ion Stability, J. Am. Chem. Soc. 99, 7526 (1977).	
Method used : EM Electron impact fragmentation (various molecules) using EM. delta Hf(H+) = 365.7	

C4H8O	CAS REGN : 109-99-9
C*****O * * * * C C * * * * C	
Furan, tetrahydro- (8CI9CI)	
GB (exp) : 189+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 196.4+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8O	CAS REGN : 123-72-8
O++C**C**C**C	
Butanal (9CI) Butyraldehyde (8CI)	
GB (exp) : 181.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8O2	CAS REGN : 110-74-7
C**C**C**O**C**+	
Formic acid, propyl ester (8CI9CI)	
PA (exp) : 194+/-2 kcal/mol	Temperature : 323-373 K
<p>Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).</p>	
<p>Method used : MS Bracketing relative to CH2CO AND I-C4H8; scale based on NH3.</p>	
GB (exp) : 184.7+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 192.1+/-2 kcal/mol	Temperature : 298 K
<p>Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).</p>	
<p>Method used : MS Equilibrium; scale based on (CH3)2CO Entropy change assumed zero</p>	

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GB (exp) : 184.5 kcal/mol	Temperature : 300 K
PA (exp) : 192.3+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 176.1+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 191.7+/-2 kcal/mol	Temperature : 600 K
Yamdaqni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

C4H8O2	CAS REGN : 123-91-1
<pre> O**C * * * * C C * * * * C**O</pre>	
1,4-Dioxane (9CI) p-Dioxane (8CI)	
GB (exp) : 183.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8O2	CAS REGN : 141-78-6
<p>C**C**O**C**C + + O</p>	
Acetic acid ethyl ester (8CI9CI)	
PA (exp) : 197+/-2 kcal/mol	Temperature : 323-373 K
<p>Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).</p>	
<p>Method used : MS Bracketing relative to (C2H5)2O and CH3CO2ME.</p>	
GB (exp) : 188.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 196+/-2 kcal/mol	Temperature : 300 K
<p>Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).</p>	
<p>Method used : MS Equilibrium; scale based on (CH3)2CO Entropy change assumed zero</p>	

Continued on next page

GB (exp) : 190.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.1+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 182.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 198+/-2 kcal/mol	Temperature : 600 K
Yamdaqui, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

C4H8O2	CAS REGN : 554-12-1
C**O**C**C**C + + 0	
Propanoic acid, methyl ester (9CI) Propionic acid, methyl ester (8CI)	
GB (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 197+/-2 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to (C2H5)2O and CH3COOMe	

C4H8O2	CAS REGN : 625-55-8
O++C**O**C**C * * C	
Formic acid, 1-methylethyl ester (9CI) Formic acid, isopropyl ester (8CI)	
GB (exp) : 185.8+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 193.2+/-2 kcal/mol	Temperature : 298 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on (CH3)2CO Entropy change assumed zero	

C4H8O2S	CAS REGN : 38103-96-7
C**O**C**S**C**C + + O	
Carbonylthioic acid, S-ethyl O-methyl ester (9CI)	
GB (exp) : 190.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8O3	CAS REGN : 623-53-0
C**O**C**O**C**C + + O	
Carbonic acid, ethyl methyl ester (8CI9CI)	
GB (exp) : 192.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 199.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H9N	CAS REGN : 123-75-1
<pre> C*****N * * * * C C * * * * C </pre>	
Pyrrolidine (8CI9CI)	
GB (exp) : 213.70+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 221.90+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 213.30+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 221.50+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

C4H9N	CAS REGN : 1190-79-0
C**C++N**C**C	
Ethanamine, N-ethylidene- (9CI) Ethylamine, N-ethylidene- (8CI)	
PA (exp) : 220.5+/-2 kcal/mol	Temperature :
Aue, D. H., Webb, H. M., and Bowers, M. T., Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Nitrogen and Oxygen Bases. Hybridization Effects, J. Am. Chem. Soc. 97, 4137 (1975).	
Method used : ICR Equilibrium; scale based on CH3NH2	

C4H9NO	CAS REGN : 110-91-8
<pre> O**C * * * * C * C * * * * C**N</pre>	
Morpholine (8CI9CI)	
GB (exp) : 208.6+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.8+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

C4H9NO	CAS REGN : 127-19-5
C**C**N**C + * + * O C	
Acetamide, N,N-dimethyl- (8CI9CI)	
GB (exp) : 205.4+/-2.5 kcal/mol	Temperature : 300 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	

C4H9NO	CAS REGN : 563-83-7
C**C**C**N * % * % C 0.	
Propanamide, 2-methyl- (9CI) Isobutyramide (8CI)	
GB (exp) : 206.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 213.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H10	CAS REGN : 106-97-8
C**C**C**C	
Butane (8CI9CI)	
PA (exp) : 166.8 (2) kcal/mol	Temperature : 291 K
<p>Hiraoka, K., and Kebarle, P., Stabilities and Energetics of Pentacoordinated Carbonium Ions. The Isomeric C₂H₇⁺ Ions and Some Higher Analogues: C₃H₉⁺ and C₄H₁₁⁺, J. Am. Chem. Soc. 98, 6119 (1976).</p>	
<p>Method used : MS Van't Hoff plot C-H protonation (2) Equilibrium of reaction t-C₄H₉⁺ + H₂ -> C₄H₁₁⁺ (2)</p>	
PA (exp) : 164 (1) kcal/mol	Temperature : 291 K
<p>Hiraoka, K., and Kebarle, P., Stabilities and Energetics of Pentacoordinated Carbonium Ions. The Isomeric C₂H₇⁺ Ions and Some Higher Analogues: C₃H₉⁺ and C₄H₁₁⁺, J. Am. Chem. Soc. 98, 6119 (1976).</p>	
<p>Method used : MS Van't Hoff plot C-C protonation (1) Equilibrium of reaction C₃H₇⁺ + CH₄ -> C₄H₁₁⁺ (1)</p>	

C4H10N2	CAS REGN : 110-85-0
<pre> NxC * * * * C C * * * * C*xN </pre>	
Piperazine (8CI9CI)	
GB (exp) : 210.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 218.9+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

C4H100	CAS REGN : 60-29-7
C**C**O**C**C	
Ethane, 1,1'-oxybis- (9CI) Ethyl ether (8CI)	
PA (exp) : 198+/-4 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to (CH3)2CO and NH3.	
GB (exp) : 188.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 196.1+/-2 kcal/mol	Temperature : 300 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on (CH3)2CO Entropy change assumed zero	

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GB (exp) : 182.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 197.3+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 190+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.4+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taaqepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C4H100	CAS REGN : 71-36-3
O**C**C**C**C	
1-Butanol (9CI) Butyl alcohol (8CI)	
GB (exp) : 181.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H100	CAS REGN : 75-65-0
<pre> O * * C**C**C * * C </pre>	
<p>2-Propanol, 2-methyl- (9CI) tert-Butyl alcohol (8CI)</p>	
PA (exp) : 194+/-1 kcal/mol	Temperature :
<p>Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).</p>	
<p>Method used : MS Bracketing relative to CH2CO and I-C5H10</p>	
PA (exp) : 192 kcal/mol	Temperature :
<p>Hiraoka, K., and Kebarle, P. Condensation Reactions Involving Carbonium Ions and Lewis Bases in the Gas Phase. Hydration of the tert-Butyl Cation, J. Am. Chem. Soc. 99, 360 (1977).</p>	
<p>Method used : MS Equilibrium relative to known standard acids</p>	

C4H10S	CAS REGN : 75-66-1
S * * C**C**C * * C	
2-Propanethiol, 2-methyl- (8CI9CI)	
GB (exp) : 186.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 194.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H10S	CAS REGN : 352-93-2
C**C**S**C**C	
Ethane, 1,1'-thiobis- (9CI) Ethyl sulfide (8CI)	
GB (exp) : 195.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 202.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H11N	CAS REGN : 75-64-9
<pre> N * * C**C**C * * C </pre>	
2-Propanamine, 2-methyl- (9CI) tert-Butylamine (8CI)	
GB (exp) : 210.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 218.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 210.2+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 218.6+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on CH3NH2	

C4H11N	CAS REGN : 78-81-9
C**C**C**N * * C	
1-Propanamine, 2-methyl- (9CI) Isobutylamine (8CI)	
GB (exp) : 207.7+/-2 kcal/mol	Temperature : 298 K
Taft, R. W., Proton-Transfer Reactions, Ed, E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	
GB (exp) : 208.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.7+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C4H11N	CAS REGN : 109-73-9
N**C**C**C**C	
1-Butanamine (9CI) Butylamine (8CI)	
GB (exp) : 207.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 216+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 207.8+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.2+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C4H11N	CAS REGN : 109-89-7
C**C**N**C**C	
Ethanamine, N-ethyl- (9CI) Diethylamine (8CI)	
GB (exp) : 214.50+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 222.70+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 214.10+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 222.30+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C4H11N	CAS REGN : 598-56-1
C**N**C**C * * C	
Ethanamine, N,N-dimethyl- (9CI) Ethylamine, N,N-dimethyl- (8CI)	
GB (exp) : 216.70+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 224.50+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 216.00+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 223.80+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

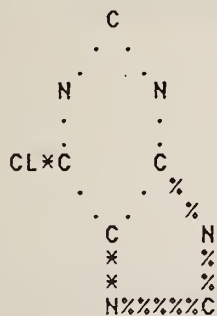
C4H11N	CAS REGN : 13952-84-6
C**C**C**C * * N	
2-Butanamine (9CI) sec-Butylamine (8CI)	
GB (exp) : 208.9 kcal/mol	Temperature : 300 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	
GB (exp) : 209.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 217.7+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C4H12N2	CAS REGN : 110-60-1
N**C**C**C**C**N	
1,4-Butanediamine (8CI9CI)	
GB (exp) : 221.70+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 236.60+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C5Fe05	CAS REGN : 13463-40-6
<pre> O # # C C##O * * ** O##C**FE*C##O * * C # # O </pre>	
<p>Iron carbonyl (Fe(CO)5), (TB-5-11)- (9CI) Iron carbonyl (Fe(CO)5) (8CI)</p>	
PA (exp) : 200+/-3 kcal/mol	Temperature : 300 K
<p>Foster, M. S., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Iron Pentacarbonyl by Ion Cyclotron Resonance Spectroscopy. New Insights into the Properties and Reactions of Transition Metal Complexes in the Absence of Complicating Solvation Phenomena, J. Am. Chem. Soc. 97, 4808 (1975).</p>	
<p>Method used : ICR Bracketing relative to (CH3O)2CO and NH3.</p>	

C5H3ClN4

CAS REGN : 87-42-3



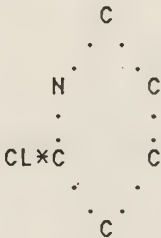
1H-Purine, 6-chloro- (9CI)
 Purine, 6-chloro- (8CI)

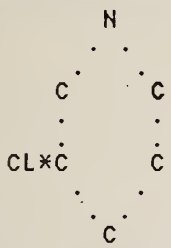
PA (exp) : 207+/-5 kcal/mol

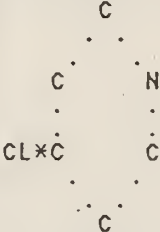
Temperature :

Wilson, M. S., and McCloskey, J. A.,
 Chemical Ionization Mass Spectrometry of Nucleosides.
 Mechanisms of Ion Formation and Estimations of
 Proton Affinity,
 J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
 Bracketing relative to NH3 and CH3NH2.

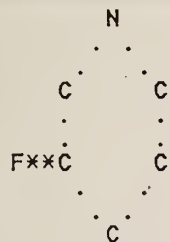
C5H4ClN	CAS REGN : 109-09-1
	
Pyridine, 2-chloro- (8CI9CI)	
GB (exp) : 204.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H4ClN	CAS REGN : 626-60-8
	
Pyridine, 3-chloro- (8CI9CI)	
GB (exp) : 204.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 212.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H4ClN	CAS REGN : 626-61-9
	
Pyridine, 4-chloro- (8CI9CI)	
GB (exp) : 207.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 215+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C5H4FN

CAS REGN : 372-47-4



Pyridine, 3-fluoro- (8CI9CI)

GB (exp) : 203.7+/-2 kcal/mol

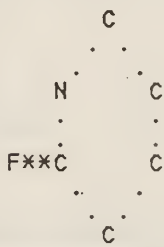
Temperature : 300 K

PA (exp) : 211.5+/-2 kcal/mol

Temperature : 300 K

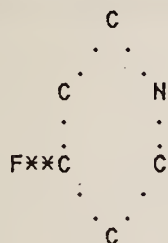
Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H4FN	CAS REGN : 372-48-5
	
Pyridine, 2-fluoro- (8CI9CI)	
GB (exp) : 200.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 208.4+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C5H4FN

CAS REGN : 694-52-0



Pyridine, 4-fluoro- (8CI9CI)

GB (exp) : 206.4+/-2 kcal/mol

Temperature : 300 K

PA (exp) : 214.2+/-2 kcal/mol

Temperature : 300 K

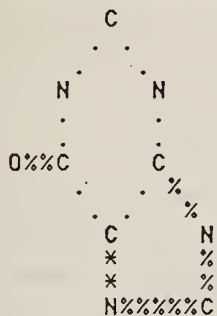
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H4N2O2	CAS REGN : 1122-61-8
<pre> C . . . C N . . O++N**C C + . + . O C </pre>	
Pyridine, 4-nitro- (8CI9CI)	
GB (exp) : 198.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.2+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
PA (exp) : 201+/-2 kcal/mol	Temperature : 300 K
<p>Taagepera, M., Henderson, W. G., Brownlee, R. T. C., Beauchamp, J. L., Holtz, D., and Taft, R. W., Gas-Phase Basicities and Pyridine Substituent Effects. J. Am. Chem. Soc. 94, 1369 (1972).</p>	
<p>Method used : ICR Equilibrium; scale based on Pyridine</p>	

C5H4N4O

CAS REGN : 68-94-0



6H-Purin-6-one, 1,7-dihydro- (9CI)
Hypoxanthine (8CI)

PA (exp) : 215+/-4 kcal/mol

Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to CH3NH2 and (CH3)2NH.

C5H5N	CAS REGN : 110-86-1
Pyridine (8CI9CI)	
GB (exp) : 210.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 218.1+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : >209.7 kcal/mol	Temperature : 423-473 K
<p>Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).</p>	
<p>Method used : MS Bracketing relative to (CH3)2NH</p>	

Continued on next page

GB (exp) : 209.8+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 217.6+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	
GB (exp) : 203.7+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 220.9+/-2 kcal/mol	Temperature : 600 K
<p>Briggs, J. P., Yamdagni, R., and Kebarle, P., Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton-Exchange Equilibria, J. Am. Chem. Soc. 94, 5128 (1972).</p>	
<p>Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero</p>	

C5H5N5	CAS REGN : 73-24-5
<pre> C . . . N N . . N%%C C% C N * % * % N%%%%C </pre>	
<p>1H-Purin-6-amine (9CI) Adenine (8CI)</p>	
PA (exp) : 220+/-2 kcal/mol	Temperature :
<p>Wilson, M. S., and McCloskey, J. A., Chemical Ionization Mass Spectrometry of Nucleosides. Mechanisms of Ion Formation and Estimations of Proton Affinity, J. Am. Chem. Soc. 97, 3436 (1975).</p>	
<p>Method used : MS Bracketing relative to (CH3)2NH and (CH3)3N</p>	

C5H5N5O	CAS REGN : 73-40-5
<pre>C%%N % % % % % C..N % . % . N**C . C%%N . . . C..N . % . % . 0</pre>	
6H-Purin-6-one, 2-amino-1,7-dihydro- (9CI) Guanine (8CI)	
PA (exp) : 220+/-2 kcal/mol	Temperature :
Wilson, M. S., and McCloskey, J. A., Chemical Ionization Mass Spectrometry of Nucleosides. Mechanisms of Ion Formation and Estimations of Proton Affinity, J. Am. Chem. Soc. 97, 3436 (1975).	
Method used : MS Bracketing relative to (CH3)2NH and (CH3)3N.	

C5H6N2O2	CAS REGN : 65-71-4
<pre> C..N . . C**C C%%O . . C..N % % O</pre>	
2,4(1H,3H)-Pyrimidinedione, 5-methyl- (9CI) Thymine (8CI)	
PA (exp) : 207+/-5 kcal/mol	Temperature :
Wilson, M. S., and McCloskey, J. A., Chemical Ionization Mass Spectrometry of Nucleosides. Mechanisms of Ion Formation and Estimations of Proton Affinity, J. Am. Chem. Soc. 97, 3436 (1975).	
Method used : MS Bracketing relative to NH3 and CH3NH2	

C5H7F3O2	CAS REGN : 383-66-4
F * * F**C**C**O**C**C**C * + * + F 0	
Acetic acid, trifluoro-, propyl ester (8CI9CI)	
GB (exp) : 176.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 184.2+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taqapera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

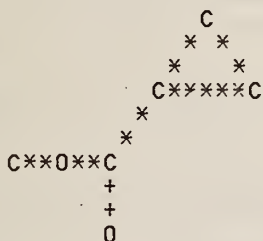
C5H8	CAS REGN : 693-86-7
<pre> C * * * * C*****C * * C++C </pre>	
Cyclopropane, ethenyl- (9CI) Cyclopropane, vinyl- (8CI)	
GB (exp) : 187.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 195.2+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C5H8O	CAS REGN : 765-43-5
<pre> C * * * * * * C*****C * * C**C + + 0 </pre>	
Ethanone, 1-cyclopropyl- (9CI) Ketone, cyclopropyl methyl (8CI)	
GB (exp) : 194.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 202.2+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H8O2	CAS REGN : 123-54-6
C**C**C**C**C + + + + 0 0	
2,4-Pentanedione (8CI9CI)	
GB (exp) : 197.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204.6+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia From Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H8O2

CAS REGN : 2868-37-3



Cyclopropanecarboxylic acid, methyl ester (8CI9CI)

GB (exp) : 192.3+/-2 kcal/mol

Temperature : 300 K

PA (exp) : 200.1+/-2 kcal/mol

Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H9N	CAS REGN : 110-59-8
C**C**C**C**C**C##N	
Pentanenitrile (9CI) Valeronitrile (8CI)	
PA (exp) : 191.9+/-2 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to HC02C2H5	
GB (exp) : 184.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 191.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H10	CAS REGN : 513-35-9
C**C++C**C * * C	
2-Butene, 2-methyl- (8CI9CI)	
PA (exp) : 194.4+/-2 kcal/mol	Temperature : 363-553 K
Goren, A., and Munson, B. Thermochemistry of Alkyl Ions, J. Phys. Chem. 80, 2848 (1976).	
Method used : MS Van't Hoff plot Equilibrium of hydride transfer reaction between (t-C4H9+) + Me2CHEt. This delta H of the reaction was determined from van't Hoff plot. PA (M) derived from the obtained delta Hf(NH+); scale based on delta Hf(t-C4H9+) = 169	

C5H10	CAS REGN : 563-46-2
C**C**C**C + + C	
1-Butene, 2-methyl- (8CI9CI)	
PA (exp) : 193.5+/-2 kcal/mol	Temperature :
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to Iso-C4H8	
PA (exp) : 197.32 kcal/mol	Temperature : 300 K
Solomon, J. J., and Field, F. H., Reversible Reactions of Gaseous Ions. IX. The Stability of C4-C7 Tertiary Alkyl Carbonium Ions, J. Am. Chem. Soc. 97, 2625 (1975).	
Method used : MS Equilibrium scale Based on delta H formation(T-C4H9+) = 169 Kcal/mol.	

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GB not calculated for this reference	
PA (exp) : 195.9+/-2 kcal/mol	Temperature : 363-553 K
Goren, A., and Munson, B. Thermochemistry of Alkyl Ions, J. Phys. Chem. 80, 2848 (1976).	
Method used : MS Equilibrium of hydride transfer reaction between (t-C4H9+) + Me2CHEt. This delta H of the reaction was determined from van't Hoff plot. PA (M) derived from the obtained delta Hf(MH+); scale based on delta Hf(t-C4H9+) = 169	

C5H10O	CAS REGN : 96-22-0
C**C**C**C**C + + O	
3-Pentanone (8CI9CI)	
GB (exp) : 191.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H100	CAS REGN : 96-47-9
<pre>O*****C * * * * C**C C * * * * C</pre>	
Furan, tetrahydro-2-methyl- (8CI9CI)	
GB (exp) : 192.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H100	CAS REGN : 110-62-3
C**C**C**C**C**C++0	
Pentanal (9CI) Valeraldehyde (8CI)	
GB (exp) : 182.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.6+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H100	CAS REGN : 142-68-7
<pre> C**O * * * * C * C * * * * C**C </pre>	
2H-Pyran, tetrahydro- (8CI9CI)	
GB (exp) : 189.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.1+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C5H100	CAS REGN : 563-80-4
C**C**C**C * + * + C 0	
2-Butanone, 3-methyl- (8CI9CI)	
GB (exp) : 190.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H10O2	CAS REGN : 109-60-4
C**C**O**C**C**C + + O	
Acetic acid, propyl ester (8CI9CI)	
PA (exp) : 200+/-3 kcal/mol	Temperature :
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to NH3 and CH3COOC2H5.	
GB (exp) : 182.9+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 200.1+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds Between Water and Ammonia and Substituted Benzenes from A Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero	

C5H1002	CAS REGN : 547-63-7
C**O**C**C**C + * + * O C	
Propanoic acid, 2-methyl-, methyl ester (9CI) Isobutyric acid, methyl ester (8CI)	
GB (exp) : 191.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H10O2	CAS REGN : 592-84-7
O=C*O*O*O*O*O*O*O	
Formic acid, butyl ester (8CI9CI)	
GB (exp) : 184.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 192.5+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H11N	CAS REGN : 110-89-4
<pre> C**N * * * * C * C * * * * * * C**C </pre>	
Piperidine (8CI9CI)	
GB (exp) : 214.90+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 223.10+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 214.40+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 222.60+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

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GB (exp) : 209.60+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 226.80+/-2 kcal/mol	Temperature : 600 K
<p>Yamdaqni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).</p>	
<p>Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero</p>	

C5H11N	CAS REGN : 120-94-5
<pre> CxxxxxC * * * * C**N C * * * * C </pre>	
<p>Pyrrolidine, 1-methyl- (8CI9CI)</p>	
GB (exp) : 217.80+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 225.60+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

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GB (exp) : 217.30+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 225.10+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C5H11N02	CAS REGN : 687-48-9
C**N**C**O**C**C * + * + C 0	
Carbamic acid, dimethyl-, ethyl ester (8CI9CI)	
GB (exp) : 203.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.2+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H12O	CAS REGN : 625-54-7
C**C**O**C**C * * C	
Propane, 2-ethoxy- (9CI) Ether, ethyl isopropyl (8CI)	
GB (exp) : 192.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H120	CAS REGN : 1634-04-4
C * * C**C**O**C * * C	
Propane, 2-methoxy-2-methyl- (9CI) Ether, tert-butyl methyl (8CI)	
GB (exp) : 191.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 199.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H13N	CAS REGN : 110-58-7
C**C**C**C**C**N	
1-Pentanamine (9CI) Pentylamine (8CI)	
GB (exp) : 208+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.4+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C5H13N	CAS REGN : 594-39-8
<pre> N * * C**C**C**C * * C </pre>	
2-Butanamine, 2-methyl- (9CI) tert-Pentylamine (8CI)	
GB (exp) : 211.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 220.1+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 211.1+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 219.5+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C5H13N	CAS REGN : 616-39-7
C**C**N**C**C * * C	
Ethanamine, N-ethyl-N-methyl- (9CI) Diethylamine, N-methyl- (8CI)	
GB (exp) : 218.90+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.70+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 218.40+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 226.20+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C5H13N	CAS REGN : 996-35-0
C**C**N**C * * * * C C	
2-Propanamine, N,N-dimethyl- (9CI) Ethylamine, N,N,1-trimethyl- (8CI)	
GB (exp) : 218.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H13N	CAS REGN : 5813-64-9
<p>C * * C**C**C**N * * C</p>	
<p>1-Propanamine, 2,2-dimethyl- (9CI) Neopentylamine (8CI)</p>	
GB (exp) : 208.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 217.2+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 209.0+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 217.4+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

C5H13N	CAS REGN : 19961-27-4
C**C**N**C**C * * C	
2-Propanamine, N-ethyl- (9CI) Diethylamine, 1-methyl- (8CI)	
GB (exp) : 216+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 224.2+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H14N2	CAS REGN : 109-55-7
C**N**C**C**C**N * * C	
1,3-Propanediamine, N,N-dimethyl- (8CI9CI)	
GB (exp) : 225.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Equilibrium; scale based on NH3	

C5H14N2	CAS REGN : 462-94-2
N**C**C**C**C**C**N	
1,5-Pentanediamine (8CI9CI)	
GB (exp) : 220.00+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 234.60+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	
GB (exp) : 221.40+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 235.10+/-2 kcal/mol	Temperature : 298 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).	
Method used : MS Equilibrium; scale based on (CH3)3N Van't Hoff plot	

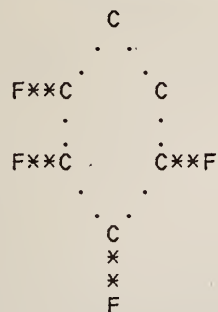
C6F6	CAS REGN : 392-56-3
<pre> F F * * * * C..C . . F**C C**F . . C..C * * * * F F </pre>	
Benzene, hexafluoro- (8CI9CI)	
GB (exp) : 171.2 kcal/mol	Temperature : 373 K
PA (exp) : 178.5+/-2 kcal/mol	Temperature : 373 K
<p>Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on C6H6</p>	

C6HF5	CAS REGN : 363-72-4
<pre> C . . . F**C C**F . . F**C C**F C * * F</pre>	
Benzene, pentafluoro- (8CI9CI)	
GB (exp) : 172.7+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 180.3+/-2 kcal/mol	Temperature : 373 K
Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).	
Method used : ICR Calculated entropy Equilibrium; scale based on C6H6	

C6H2F4	CAS REGN : 327-54-8
<pre> F * * * C..C . . F**C C**F . . C..C * * * * F </pre>	
Benzene, 1,2,4,5-tetrafluoro- (8CI9CI)	
GB (exp) : 173.1+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 180.3+/-2 kcal/mol	Temperature : 373 K
<p>Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on C6H6</p>	

C6H2F4

CAS REGN : 551-62-2



Benzene, 1,2,3,4-tetrafluoro- (8CI9CI)

GB (exp) : 173.4+/-2 kcal/mol

Temperature : 373 K

PA (exp) : 180.4+/-2 kcal/mol

Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

C6H2F4	CAS REGN : 2367-82-0
<pre> C F**C C**F F**C C C * * F </pre>	
Benzene, 1,2,3,5-tetrafluoro- (8CI9CI)	
GB (exp) : 173.4+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 180.5+/-2 kcal/mol	Temperature : 373 K
<p>Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on C6H6</p>	

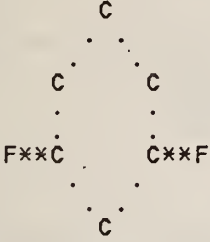
C6H3F3	CAS REGN : 367-23-7
<pre> C..C F**C C**F C..C * * F</pre>	
Benzene, 1,2,4-trifluoro- (8CI9CI)	
GB (exp) : 173.7+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 181.35+/-2 kcal/mol	Temperature : 373 K
Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).	
Method used : ICR Calculated entropy Equilibrium; scale based on C6H6	

C6H3F3	CAS REGN : 372-38-3
<pre> F x x C . . C C . . FxxC CxxF . . C </pre>	
Benzene, 1,3,5-trifluoro- (8CI9CI)	
GB (exp) : 174.1+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 181.15+/-2 kcal/mol	Temperature : 373 K
<p>Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on C6H6</p>	

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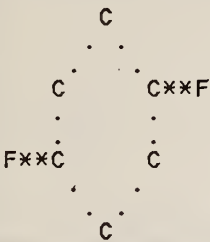
GB (exp) : 165.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 179.8+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

C6H4F2	CAS REGN : 367-11-3
<pre> C..C . . F**C C . . C..C * * F</pre>	
Benzene, 1,2-difluoro- (9CI) Benzene, o-difluoro- (8CI)	
GB (exp) : 174.36+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 181.35+/-2 kcal/mol	Temperature : 373 K
Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).	
Method used : ICR Calculated entropy Equilibrium; scale based on C6H6	

C6H4F2	CAS REGN : 372-18-9
	
Benzene, 1,3-difluoro- (9CI) Benzene, m-difluoro- (8CI)	
GB (exp) : 174.42+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 171.67+/-2 kcal/mol	Temperature : 373 K
Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).	
Method used : ICR Calculated entropy Equilibrium; scale based on C6H6	

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GB (exp) : 165.9+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 181.6+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

C6H4F2	CAS REGN : 540-36-3
	
Benzene, 1,4-difluoro- (9CI) Benzene, p-difluoro- (8CI)	
GB (exp) : 173.9+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 180.6+/-2 kcal/mol	Temperature : 373 K
Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).	
Method used : ICR Calculated entropy Equilibrium; scale based on C6H6	

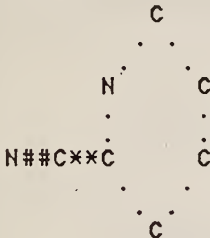
C6H4F3N	CAS REGN : 368-48-9
<pre> C F N . C * . . . * . . . F**C**C . C * . . . * . . . F . . C </pre>	
Pyridine, 2-(trifluoromethyl)- (8CI9CI)	
GB (exp) : 201.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 209.0+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

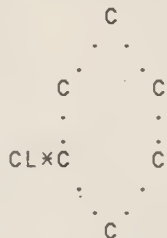
C6H4F3N	CAS REGN : 3796-23-4
<pre> N . . F C C * . . * . . F**C**C C * . . * . . F C </pre>	
Pyridine, 3-(trifluoromethyl)- (8CI)	
GB (exp) : 202.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 210.0+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C6H4F3N	CAS REGN : 3796-24-5
<pre> C . . F C . N * . . * . . F * C * * C * . . * . . F . C </pre>	
Pyridine, 4-(trifluoromethyl)- (8CI9CI)	
GB (exp) : 202.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 210.3+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
PA (exp) : 207.1+/-2 kcal/mol	Temperature : 298 K
<p>Taagepera, M., Henderson, W. G., Brownlee, R. T. C., Beauchamp, J. L., Holtz, D., and Taft, R. W., Gas-Phase Basicities and Pyridine Substituent Effects, J. Am. Chem. Soc. 94, 1369 (1972).</p>	
<p>Method used : ICR Equilibrium; scale based on C5H5N(Pyridine)</p>	

C6H4N2	CAS REGN : 100-48-1
<pre> C . . . C N . . N##C**C C C </pre>	
4-Pyridinecarbonitrile (9CI) Isonicotinonitrile (8CI)	
GB (exp) : 199.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 207.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

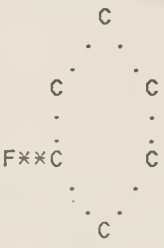
C6H4N2	CAS REGN : 100-54-9
<pre> N . . . C C . . N##C**C C . . C C . C </pre>	
3-Pyridinecarbonitrile (9CI) Nicotinonitrile (8CI)	
GB (exp) : 199.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H4N2	CAS REGN : 100-70-9
	
2-Pyridinecarbonitrile (9CI) Picolinonitrile (8CI)	
GB (exp) : 197.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 205.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H5Cl	CAS REGN : 108-90-7
	
Benzene, chloro- (8CI9CI)	
GB (exp) : 174.24+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 181.9+/-2 kcal/mol	Temperature : 373 K
Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).	
Method used : ICR Calculated entropy Equilibrium; scale based on C6H6	

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GB (exp) : 166.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.3+/-2 kcal/mol	Temperature : 600 K
<p>Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium relative to C6H6. Using GB and PA values respectively 167.8+/-2 and 181.2+/-2 kcal/mol</p>	
GB (exp) : 166.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.5+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on NH3</p>	

C6H5F	CAS REGN : 462-06-6
	
Benzene, fluoro- (8CI9CI)	
GB (exp) : 174.5+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 182.2+/-2 kcal/mol	Temperature : 373 K
Hartman, K. G., and Lias, S. G. Proton Transfer Equilibria in Halobenzene Systems: Entropy Changes and Relative Proton Affinities, Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).	
Method used : ICR Calculated entropy Equilibrium; scale based on C6H6	

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GB (exp) : 167+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.5+/-2 kcal/mol	Temperature : 600 K
Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).	
Method used : MS Calculated entropy Equilibrium relative to C6H6. Using GB and PA values respectively 167.8+/-2 and 181.2+/-2 kcal/mol	
GB (exp) : 166.9+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.6+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

C6H5NO2	CAS REGN : 98-95-3
<pre> C . . . C . C . . O++N**C C + . . + . . O . C </pre>	
Benzene, nitro- (8CI9CI)	
GB (exp) : 176.7+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 192.2+/-2 kcal/mol	Temperature : 600 K
<p>Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2</p>	

C6H6		CAS REGN : 71-43-2	
Benzene (8CI9CI)			
GB (exp) : 172+/-2 kcal/mol		Temperature : 340 K	
PA (exp) : 180.1+/-2 kcal/mol		Temperature : 340 K	
<p>Chong, S. L., and Franklin, J. L., Proton Affinities of Benzene, Toluene, and the Xylenes, J. Am. Chem. Soc. 94, 6630 (1972).</p>			
<p>Method used : MS Equilibrium relative to HCOOH Entropy change assumed zero</p>			
GB (exp) : 174.7+/-2 kcal/mol		Temperature : 300 K	
PA (exp) : 181.4+/-2 kcal/mol		Temperature : 300 K	
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>			
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>			

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GB (exp) : 167.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 181.2+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

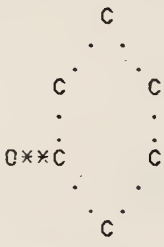
C6H6ClN	CAS REGN : 106-47-8
<pre> C C C**N . . CLxC C C </pre>	
Benzenamine, 4-chloro- (9CI) Aniline, p-chloro- (8CI)	
GB (exp) : 198.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H6ClN	CAS REGN : 108-42-9
<pre> C . . C C . . CL*C C*N . . C </pre>	
Benzenamine, 3-chloro- (9CI) Aniline, m-chloro- (8CI)	
GB (exp) : 197.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 205.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR. Calculated entropy Equilibrium; scale based on NH3	

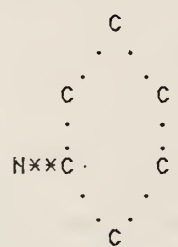
C6H6FN	CAS REGN : 371-40-4
<pre> C C . . C**N . . . F**C . C C</pre>	
Benzenamine, 4-fluoro- (9CI) Aniline, p-fluoro- (8CI)	
GB (exp) : 198.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H6FN		CAS REGN : 372-19-0	
<pre> C . C . C . . F**C C**N . . C</pre>			
Benzenamine, 3-fluoro- (9CI) Aniline, m-fluoro- (8CI)			
GB (exp) : 197.0+/-2 kcal/mol		Temperature : 300 K	
PA (exp) : 205.4+/-2 kcal/mol		Temperature : 300 K	
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.			
Method used : ICR Calculated entropy Equilibrium; scale based on NH3			

C6H6N4	CAS REGN : 2004-03-7
<pre> C . . . N N . . C**C C . . C N * % * % N****C</pre>	
1H-Purine, 6-methyl- (9CI) Purine, 6-methyl- (8CI)	
PA (exp) : 220+/-2 kcal/mol	Temperature :
Wilson, M. S., and McCloskey, J. A., Chemical Ionization Mass Spectrometry of Nucleosides. Mechanisms of Ion Formation and Estimations of Proton Affinity, J. Am. Chem. Soc. 97, 3436 (1975).	
Method used : MS Bracketing relative to (CH3)2NH and (CH3)3N	

C6H6O	CAS REGN : 108-95-2
	
Phenol (8CI9CI)	
PA (exp) : ~180 kcal/mol	Temperature :
<p>DeFrees, D. J. McIver, R. T., and Hehre, W. J. The Proton Affinities of Phenol, J. Am. Chem. Soc. 99, 3853 (1977).</p>	
<p>Method used : ICR Bracketing relative to various molecules. Oxygen protonation</p>	
GB (exp) : 179.1+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 194.6+/-2 kcal/mol	Temperature : 600 K
<p>Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2</p>	

C6H6O	CAS REGN : 6921-27-3
C##C**C**O**C**C##C	
1-Propyne, 3,3'-oxybis- (9CI) 2-Propynyl ether (8CI)	
GB (exp) : 181.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

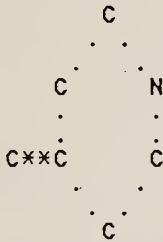
C6H7N	CAS REGN : 62-53-3
	
Benzenamine (9CI) Aniline (8CI)	
GB (exp) : 200.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 208.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 193.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 208.9+/-2 kcal/mol	Temperature : 600 K
Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).	
Method used : MS Calculated entropy Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2	

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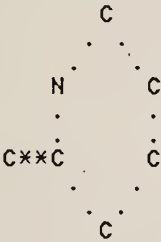
GB (exp) : >193.7 kcal/mol	Temperature : 423-473 K
Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).	
Method used : MS Bracketing relative to NH3	
GB (exp) : 194.0+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 211.2+/-2 kcal/mol	Temperature : 600 K
Briggs, J. P., Yamdagni, R., and Kebarle, P., Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton- Exchange Equilibria, J. Am. Chem. Soc. 94, 5128 (1972).	
Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero	

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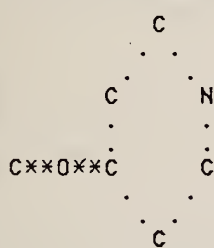
GB (exp) : 199.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 203.9+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

C6H7N	CAS REGN : 108-89-4
	
Pyridine, 4-methyl- (9CI) 4-Picoline (8CI)	
GB (exp) : 214.30+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 222.10+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppal, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

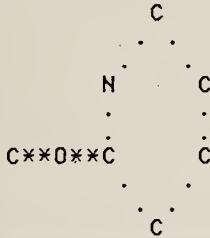
C6H7N	CAS REGN : 108-99-6
<pre> N . . C C . . C*x C . . C </pre>	
Pyridine, 3-methyl- (9CI) 3-Picoline (8CI)	
GB (exp) : 213+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 220.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H7N	CAS REGN : 109-06-8
	
Pyridine, 2-methyl- (9CI) 2-Picoline (8CI)	
GB (exp) : 213.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 221.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H7N	CAS REGN : 6921-28-4
C##C**C**N**C**C##C	
2-Propyn-1-amine, N-2-propynyl- (9CI) Di-2-propynylamine (8CI)	
GB (exp) : 205.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 213.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

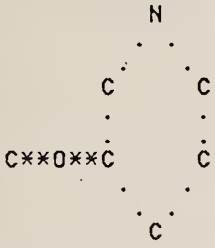
C6H7NO	CAS REGN : 620-08-6
	
Pyridine, 4-methoxy- (8CI9CI)	
GB (exp) : 217.00+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 224.80+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H7NO	CAS REGN : 694-85-9
<pre> C++C * * * * C**N * * C * * + * * + C**C + + O </pre>	
<p>2(1H)-Pyridinone, 1-methyl- (9CI) 2(1H)-Pyridone, 1-methyl- (8CI)</p>	
PA (exp) : 217.2+/-2 kcal/mol	Temperature :
<p>Cook, M. J., Katritzky, A. R., Taagepera, M., Singh, I. D., and Taft, R. W. Application of Ion Cyclotron Resonance Spectro- scopic Gas-Phase Basicities to the Study of Tautomeric Equilibria, J. Am. Chem. Soc. 98, 6048 (1976).</p>	
<p>Method used : ICR Equilibrium relative to pyridine. Use value of PA (pyridine) = 210.1 Entropy change assumed zero</p>	

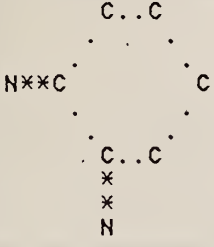
C6H7NO	CAS REGN : 1628-89-3
	
Pyridine, 2-methoxy- (8CI9CI)	
GB (exp) : 211.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 219.2+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

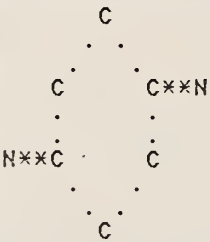
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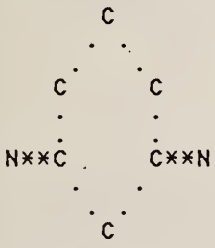
PA (exp) : 219.8+/-2 kcal/mol	Temperature :
Cock, M. J., Katritzky, A. R., Taagepera, M., Singh, T. D., and Taft, R. W. Application of Ion Cyclotron Resonance Spectro- scopic Gas-Phase Basicities to the Study of Tautomeric Equilibria, J. Am. Chem. Soc. 98, 6048 (1976).	
Method used : ICR Equilibrium relative to t-Butylamine. Use value of PA (t-C ₄ H ₉ NH ₂) = 218.3 Entropy change assumed zero	

C6H7NO	CAS REGN : 7295-76-3
	
Pyridine, 3-methoxy- (8CI9CI)	
GB (exp) : 213.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 221.1+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H7N5O	CAS REGN : 23662-75-1
<pre>C * * C%%N % % % % % % C..N % % N**C C%%N % C..N % % O</pre>	
6H-Purin-6-one, 2-amino-1,7-dihydro-8-methyl- (9CI) Guanine, 8-methyl- (8CI)	
PA (exp) : >222 kcal/mol	Temperature :
Wilson, M. S., and McCloskey, J. A., Chemical Ionization Mass Spectrometry of Nucleosides. Mechanisms of Ion Formation and Estimations of Proton Affinity, J. Am. Chem. Soc. 97, 3436 (1975).	
Method used : MS Bracketing relative to (CH3)3N	

C6H8N2	CAS REGN : 95-54-5
	
1,2-Benzenediamine (9CI) o-Phenylenediamine (8CI)	
GB (exp) : >193.7 kcal/mol	Temperature : 424-473 K
Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).	
Method used : MS Bracketing relative to NH3	

C6H8N2	CAS REGN : 106-50-3
	
1,4-Benzenediamine (9CI) p-Phenylenediamine (8CI)	
GB (exp) : >193.7 kcal/mol	Temperature : 424-473 K
Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).	
Method used : MS Bracketing relative to NH3	

C6H8N2	CAS REGN : 108-45-2
	
1,3-Benzenediamine (9CI) m-Phenylenediamine (8CI)	
GB (exp) : >202.9 kcal/mol	Temperature : 424-473 K
<p>Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).</p>	
Method used : MS Bracketing relative to CH3NH2	

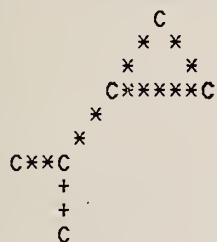
C6H9F3O2	CAS REGN : 367-64-6
<pre> F * * F**C**C**O**C**C**C**C * + * + F 0 </pre>	
Acetic acid, trifluoro-, butyl ester (8CI9CI)	
GB (exp) : 176.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 184.4+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C6H10	CAS REGN : 693-89-0
<pre>C*****C + * + * C**C C * * * * C</pre>	
Cyclopentene, 1-methyl- (8CI9CI)	
GB (exp) : 186.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 195+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H10	CAS REGN : 1528-30-9
<pre>C*****C * * * * C++C C * * * * * C</pre>	
Cyclopentane, methylene- (8CI9CI)	
GB (exp) : 190.7+/-2 kcal/mol	Temperature : 298 K
Pollack, S. K., Wolf, J. F., Levi, B. A., Taft, R. W., and Hehre W. J. Kinetic Detection of Common Intermediates in Gas Phase Ion-Molecule Reactions, J. Am. Chem. Soc. 99, 1350 (1977).	
Method used : ICR Equilibrium; scale based on NH3	

C6H10

CAS REGN : 4663-22-3



Cyclopropane, (1-methylethenyl)- (9CI)
Propene, 2-cyclopropyl- (8CI)

GB (exp) : 198.9+/-2 kcal/mol

Temperature : 300 K

PA (exp) : 207.1+/-2 kcal/mol

Temperature : 300 K

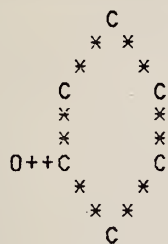
Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H10F3NO	CAS REGN : 400-59-9
<pre> F * * F**C**C**N**C**C**C**C * % * % F 0 </pre>	
Acetamide, N-butyl-2,2,2-trifluoro- (8CI9CI)	
GB (exp) : 193.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 201.7+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C6H100

CAS REGN : 108-94-1



Cyclohexanone (3CI9CI)

PA (exp) : 204 kcal/mol

Temperature :

Jelus, B. L., Murray, R. K., Jr., Munson, B.,
Studies in Chemical Ionization Mass Spectrometry.
Secondary Alcohols with Isobutane,
J. Am. Chem. Soc. 97, 2362 (1975).

Method used : MS
The (M-H)⁺ ion for cyclo-hexanol is assumed to
be the same as O-protonated cyclohexanone.

C6H100	CAS REGN : 557-40-4
C++C**C**O**C**C++C	
1-Propene, 3,3'-oxybis- (9CI) Allyl ether (8CI)	
GB (exp) : 190+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H11N	CAS REGN : 124-02-7
C++C**C**N**C**C++C	
2-Propen-1-amine, N-2-propenyl- (9CI) Diallylamine (8CI)	
GB (exp) : 213.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 221.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H11NO	CAS REGN : 931-20-4
<pre> C**C * * * * * C**N * C * * * * * * C**C + + 0 </pre>	
<p>2-Piperidinone, 1-methyl- (9CI) 2-Piperidone, 1-methyl- (8CI)</p>	
PA (exp) : 216.8+/-2 kcal/mol	Temperature :
<p>Cook, M. J., Katritzky, A. R., Taagepera, M., and Singh, T. D., and Taft, R. W. Application of Ion Cyclotron Resonance Spectroscopic Gas-Phase Basicities to the Study of Tautomeric Equilibria, J. Am. Chem. Soc. 98, 6048 (1976).</p>	
<p>Method used : ICR Equilibrium relative to i-C3H7NH2. Use value of PA (i-C3H7NH2) = 216.5 Entropy change assumed zero</p>	

C6H11NO	CAS REGN : 53687-79-9
<pre> N + * + * C C * * * * C**O***C C * * * * C </pre>	
Piperidine, 2-methoxy-	
PA (exp) : 226.3+/-2 kcal/mol	Temperature :
<p>Cook, M. J., Katritzky, A. R., Taagepera, M., and Singh, T. D., and Taft, R. W. Application of Ion Cyclotron Resonance Spectroscopic Gas-Phase Basicities to the Study of Tautomeric Equilibria, J. Am. Chem. Soc. 98, 6048 (1976).</p>	
<p>Method used : ICR Equilibrium relative to (i-C3H7)2NH. Use value of PA(i-C3H7)2NH = 266.6 Entropy change assumed zero</p>	

C6H12	CAS REGN : Not available
<p>C * * C * * C**C**C++C</p>	
1-Butene, 2-ethyl-	
PA (exp) : 197.7+/-2 kcal/mol	Temperature : 363-553 K
<p>Goren, A., and Munson, B. Thermochemistry of Alkyl Ions, J. Phys. Chem. 80, 2848 (1976).</p>	
<p>Method used : MS Equilibrium of hydride transfer reaction between (t-C4H9+) + Et2CHMe and between (t-C5H11+) + Et2CHMe. This delta H of the reaction was determined from van't Hoff plot. PA (M) derived from the obtained delta Hf(MH+); scale based on delta Hf(t-C4H9+) = 169</p>	

C6H12	CAS REGN : 616-12-6
C**C++C**C**C * * C	
2-Pentene, 3-methyl-, (E)- (8CI9CI)	
PA (exp) : 196.1+/-2 kcal/mol	Temperature : 363-553 K
Goren, A., and Munson, B. Thermochemistry of Alkyl Ions, J. Phys. Chem. 80, 2848 (1976).	
Method used : MS Equilibrium of hydride transfer reaction between (t-C4H9+) + Et2CHMe and between (t-C5H11+) + Et2CHMe. This delta H of the reaction was determined from van't Hoff plot. PA (M) derived from the obtained delta Hf(MH+); scale based on delta Hf(t-C4H9+) = 169	

C6H12	CAS REGN : 625-27-4
C**C**C++C**C * * C	
2-Pentene, 2-methyl- (8CI9CI)	
PA (exp) : 196.4+/-2 kcal/mol	Temperature : 363-553 K
Goren, A., and Munson, B. Thermochemistry of Alkyl Ions, J. Phys. Chem. 80, 2848 (1976).	
Method used : MS Equilibrium of hydride transfer Reaction between (t-C4H9+) + Me2CHC3H7 and between (t-C5H11+) + Me2CHC3H7. This delta H of the reaction was determined from van't Hoff plot. PA (M) derived from the obtained delta Hf(MH+); scale based on delta Hf(t-C4H9+) = 169	

C6H12	CAS REGN : 763-29-1
C**C**C**C**C + + C	
i-Pentene, 2-methyl- (8CI9CI)	
PA (exp) : 198.2+/-2 kcal/mol	Temperature : 363-553 K
Goren, A., and Munson, B. Thermochemistry of Alkyl Ions, J. Phys. Chem. 80, 2848 (1976).	
Method used : MS Equilibrium of hydride transfer reaction between (t-C4H9+) + Me2CHC3H7 and between (t-C5H11+) + Me2 CHC3H7. This delta H of the reaction was determined from van't Hoff plot. PA (M) derived from the obtained delta Hf(MH+); scale based on delta Hf(t-C4H9+) = 169	

C6H12N2	CAS REGN : 280-57-9
<pre> C**N * ** * C * C * C * C * * * * N**C </pre>	
1,4-Diazabicyclo[2.2.2]octane (8CI9CI)	
GB (exp) : 217.20+/-2 kcal/mol	Temperature :
<p>Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.</p>	
<p>Method used : ICR Equilibrium; scale based on NH3</p>	
GB (exp) : 217.90+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 225.90+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

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PA (exp) : 225.50+/-2 kcal/mol	Temperature :
<p>Staley, R., and Beauchamp, J. L., Relationship of Nitrogen Lone Pair Interactions to Thermodynamic Parameters Associated with Amine Basicities, J. Am. Chem. Soc. 96, 1604 (1974).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C6H12O	CAS REGN : 75-97-8
<pre> C * * C**C**C**C * + * + C 0 </pre>	
2-Butanone, 3,3-dimethyl- (8CI9CI)	
GB (exp) : 191.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 199.6+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C6H12O2	CAS REGN : 598-98-1
C * * * C**O**C**C**C + * + * O C	
Propanoic acid, 2,2-dimethyl-, methyl ester (9CI) Pivalic acid, methyl ester (8CI)	
GB (exp) : 192.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H13N	CAS REGN : 108-91-8
<pre> C * * * * * * * * * C * * * C * * * * * * * * N**C * * C * * * * * * * C </pre>	
Cyclohexanamine (9CI) Cyclohexylamine (8CI)	
GB (exp) : 210.10+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 218.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 210.1+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 218.5+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Dowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

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GB (exp) : 204.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 222+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).</p>	
<p>Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero</p>	

C6H13N	CAS REGN : 626-67-5
<pre> C * * * * C C * * * * C**N C * * * * C </pre>	
<p>Piperidine, 1-methyl- (8CI9CI)</p>	
GB (exp) : 218.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.6+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

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GB (exp) : 218.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 226.1+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C6H14O	CAS REGN : 108-20-3
C**C**O**C**C * * * * C C	
Propane, 2,2'-oxybis- (9CI) Isopropyl ether (8CI)	
GB (exp) : 195.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 203+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H14O	CAS REGN : 111-43-3
C**C**C**O**C**C**C	
Propane, 1,1'-oxybis- (9CI) Propyl ether (8CI)	
GB (exp) : 191.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 199.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H140	CAS REGN : 637-92-3
C * * C**C**O**C**C * * C	
Propane, 2-ethoxy-2-methyl- (9CI) Ether, tert-butyl ethyl (8CI)	
GB (exp) : 195.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 203.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H14S	CAS REGN : 111-47-7
C**C**C**S**C**C**C	
Propane, 1,1'-thiobis- (9CI) Propyl sulfide (8CI)	
GB (exp) : 196.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H14S	CAS REGN : 625-80-9
C**C**S**C**C * * * * C C	
Propane, 2,2'-thiobis- (9CI) Isopropyl sulfide (8CI)	
GB (exp) : 199.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H15N	CAS REGN : 108-18-9
<p>C**C**N**C**C * * * * C C</p>	
<p>2-Propanamine, N-(1-methylethyl)- (9CI) Diisopropylamine (8CI)</p>	
GB (exp) : 218.40+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.60+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 217.90+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 226.1+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

C6H15N	CAS REGN : 111-26-2
N**C**C**C**C**C**C	
1-Hexanamine (9CI) Hexylamine (8CI)	
GB (exp) : 208.1+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.5+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C6H15N	CAS REGN : 121-44-8
<p>C**C**N**C**C * * C * * C</p>	
<p>Ethanamine, N,N-diethyl- (9CI) Triethylamine (8CI)</p>	
GB (exp) : 221.20+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 229.00+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 220.60+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 228.40+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

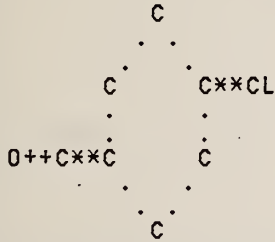
C6H15N	CAS REGN : 142-84-7
C**C**C**N**C**C**C	
1-Propanamine, N-propyl- (9CI) Dipropylamine (8CI)	
GB (exp) : 216.50+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 224.70+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 216.10+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 224.30+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C6H15N	CAS REGN : 918-02-5
C * * C**C**N**C * * * * C C	
2-Propanamine, N,N,2-trimethyl- (9CI) Ethylamine, N,N,1,1-tetramethyl- (8CI)	
GB (exp) : 220.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 228.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

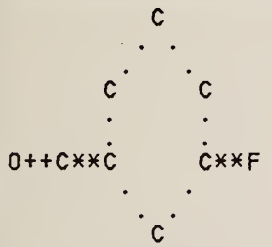
C6H16N2	CAS REGN : 110-18-9
C**N**C**C**N**C * * * * C C	
1,2-Ethanediamine, N,N,N',N'-tetramethyl- (9CI) Ethylenediamine, N,N,N',N'-tetramethyl- (8CI)	
GB (exp) : 224.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 232.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taaqepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 224+/-2 kcal/mol	Temperature : 298 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	

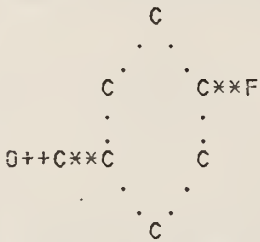
C6H16N2	CAS REGN : 124-09-4
N**C**C**C**C**C**C**N	
1,6-Hexanediamine (8CI9CI)	
GB (exp) : 220.00+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 235.40+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	
GB (exp) : 221.20+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 235.00+/-2 kcal/mol	Temperature : 298 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).	
Method used : MS Equilibrium; scale based on (CH3)3N Van't Hoff plot	

C6H17NSi	CAS REGN : 18182-40-6
<pre> C * * C**N**C**SI*C * * * * C C </pre>	
Methanamine, N,N-dimethyl-1-(trimethylsilyl)- (9CI) Trimethylamine, (trimethylsilyl)- (8CI)	
GB (exp) : 219.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 227.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C7H5ClO	CAS REGN : 104-88-1
	
Benzaldehyde, 4-chloro- (9CI) Benzaldehyde, p-chloro- (8CI)	
GB (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C7H5D3	CAS REGN : 1124-18-1
<pre> C D . * . * . * C C**C**D . * . * C C D . C</pre>	
Benzene, methyl-d3-	
GB (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188.7+/-2 kcal/mol	Temperature : 300 K
<p>Ausloos, P., and Lias, S. G. Equilibrium Isotope Effects on the Proton Transfer Reactions of Methylbenzenes, J. Am. Chem. Soc. 99, 4198 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C7H5FO	CAS REGN : 456-48-4
	
Benzaldehyde, 3-fluoro- (9CI) Benzaldehyde, m-fluoro- (8CI)	
GB (exp) : 186.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 194.1+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

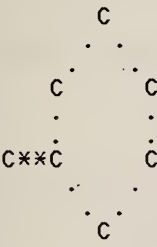
C7H5FO	CAS REGN : 459-57-4
	
Benzaldehyde, 4-fluoro- (9CI) Benzaldehyde, p-fluoro- (8CI)	
GB (exp) : 188.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 196.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C7H5N	CAS REGN : 100-47-0
<pre> C . . C C . . N##C**C C C </pre>	
Benzonitrile (8CI9CI)	
GB (exp) : 179.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 194.7+/-2 kcal/mol	Temperature : 600 K
<p>Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2</p>	

C7H60	CAS REGN : 100-52-7
<pre> C . . . C . C . . O++C**C C . . . C </pre>	
Benzaldehyde (8CI9CI)	
GB (exp) : 190.4 kcal/mol	Temperature : 300 K
PA (exp) : 198.2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 183.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 198.7+/-2 kcal/mol	Temperature : 600 K
<p>Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2</p>	

C7H7NO	CAS REGN : 350-03-8
<pre> N . . C C . . C**C**C C . . + . + . O C </pre>	
Ethanone, 1-(3-pyridinyl)- (9CI) Ketone, methyl 3-pyridyl (8CI)	
GB (exp) : 206.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C7H7NO	CAS REGN : 1122-54-9
<pre> C . . . C . N . . C**C**C + + O C </pre>	
Ethanone, 1-(4-pyridinyl)- (9CI) Ketone, methyl 4-pyridyl (8CI)	
GB (exp) : 206.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C7H8	CAS REGN : 108-88-3
	
Benzene, methyl- (9CI) Toluene (8CI)	
GB (exp) : 179.6+/-2 kcal/mol	Temperature : 340 K
PA (exp) : 187.5+/-2 kcal/mol	Temperature : 340 K
Chong, S. L., and Franklin, J. L., Proton Affinities of Benzene, Toluene, and the Xylenes, J. Am. Chem. Soc. 94, 6630 (1972).	
Method used : MS Equilibrium relative to CH3SH Entropy change assumed zero	
PA (exp) : 187.4+/-2 kcal/mol	Temperature : 300 K
Devlin, J. L., III., Wolf, J. F., Taft, R. W., Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).	
Method used : ICR Equilibrium relative to C6H6(Benzene) Protonation position 2	

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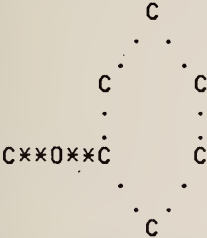
PA (exp) : 183.8+/-2 kcal/mol	Temperature : 300 K
Devlin, J. L., III., Wolf, J. F., Taft, R. W., Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).	
Method used : ICR Equilibrium relative to C6H6(Benzene) Protonation position 3	
PA (exp) : 182.6+/-2 kcal/mol	Temperature : 300 K
Devlin, J. L., III., Wolf, J. F., Taft, R. W., Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).	
Method used : ICR Equilibrium relative to C6H6(Benzene) Protonation position 1	
GB (exp) : 174.1+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 139.6+/-2 kcal/mol	Temperature : 600 K
Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).	
Method used : MS Calculated entropy Equilibrium relative to C6H6. Using GB and PA values respectively 167.8+/-2 and 181.2+/-2 kcal/mol	

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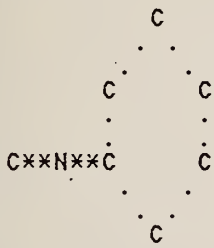
GB (exp) : 180.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188.6+/-2 kcal/mol	Temperature : 300 K
Devlin, J. L., III., Wolf, J. F., Taft, R. W., Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).	
Method used : ICR Protonation position 4 Calculated entropy Equilibrium relative to C6H6(Benzene)	
GB (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

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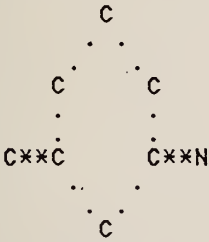
GB (exp) : 180.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187.9+/-2 kcal/mol	Temperature : 300 K
Yamdaqni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on C6H6(Benzene)	

C7H8O	CAS REGN : 100-66-3
	
Benzene, methoxy- (9CI) Anisole (8CI)	
GB (exp) : 183.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 199+/-2 kcal/mol	Temperature : 600 K
<p>Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).</p>	
<p>Method used : MS Calculated entropy . Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2</p>	

C7H9N	CAS REGN : 100-46-9
<pre> C . . . C C . . N**C**C C C </pre>	
Benzenemethanamine (9CI) Benzylamine (8CI)	
GB (exp) : 206.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

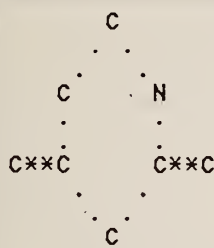
C7H9N	CAS REGN : 100-61-8
	
<p>Benzenamine, N-methyl- (9CI) Aniline, N-methyl- (8CI)</p>	
GB (exp) : 200.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 217.4+/-2 kcal/mol	Temperature : 600 K
<p>Briggs, J. P., Yamdagni, R., and Kebarle, P., Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton- Exchange Equilibria, J. Am. Chem. Soc. 94, 5128 (1972).</p>	
<p>Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero</p>	

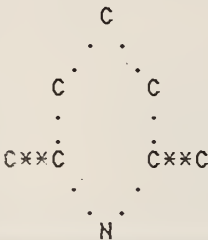
C7H9N	CAS REGN : 106-49-0
<pre> C . . . C C**N . . C**C C C </pre>	
Benzenamine, 4-methyl- (9CI) p-Toluidine (8CI)	
GB (exp) : 203.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C7H9N	CAS REGN : 108-44-1
	
Benzenamine, 3-methyl- (9CI) m-Toluidine (8CI)	
GB (exp) : 203.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 211.6+/-2 kcal/mol	Temperature : 298 K
Pollack, S. K., Devlin, J. L., III, Summerhays, K. D., Taft, R. W., and Hehre, W J. The Site of Protonation in Aniline, J. Am. Chem. Soc. 99, 4583 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3. Ring protonation	

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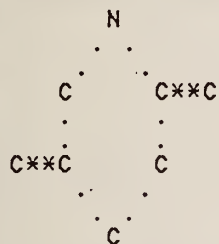
PA (exp) : 211.6+/-2 kcal/mol	Temperature : 300 K
Summerhays, K. D., Pollack, S. K., Taft, R. W., and Hehre, W. J. Gas-Phase Basicities of Substituted Anilines. Inferences about the Role of Solvent in Dictating Site of Protonation, J. Am. Chem. Soc. 99, 4585 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale base on NH3. Ring protonation	

C7H9N	CAS REGN : 108-47-4
	
Pyridine, 2,4-dimethyl- (9CI) 2,4-Lutidine (8CI)	
PA (exp) : 225.1+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., Bowers, M. T., Liotta, C. L., Alexander, C. J., and Hopkins, H. P., Jr. A Quantitative Comparison of Gas- and Solution-Phase Basicities of Substituted Pyridines, J. Am. Chem. Soc. 98, 854 (1976).	
Method used : ICR Calculated Entropy Equilibrium; scale based on NH3	

C7H9N	CAS REGN : 108-48-5
	
Pyridine, 2,6-dimethyl- (9CI) 2,6-Lutidine (8CI)	
PA (exp) : 226.1+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., Bowers, M. T., Liotta, C. L., Alexander, C. J., and Hopkins, H. P., Jr. A Quantitative Comparison of Gas- and Solution-Phase Basicities of Substituted Pyridines, J. Am. Chem. Soc. 98, 854 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C7H9N

CAS REGN : 589-93-5



Pyridine, 2,5-dimethyl- (9CI)
2,5-Lutidine (8CI)

PA (exp) : 224.5+/-2 kcal/mol

Temperature : 298 K

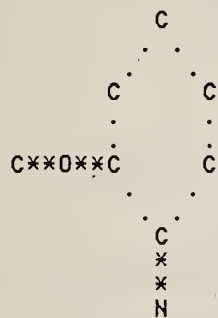
Aue, D. H., Webb, H. M., Bowers, M. T., Liotta, C. L.,
Alexander, C. J., and Hopkins, H. P., Jr.
A Quantitative Comparison of Gas- and Solution-Phase
Basicities of Substituted Pyridines,
J. Am. Chem. Soc. 98, 854 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H9N	CAS REGN : 591-22-0
<pre> N C C . . C**C C**C C </pre>	
Pyridine, 3,5-dimethyl- (9CI) 3,5-Lutidine (8CI)	
PA (exp) : 223.5 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., Bowers, M. T., Liotta, C. L., Alexander, C. J., and Hopkins, H. P., Jr. A Quantitative Comparison of Gas- and Solution-Phase Basicities of Substituted Pyridines, J. Am. Chem. Soc. 98, 854 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C7H9NO

CAS REGN : 90-04-0



Benzenamine, 2-methoxy- (9CI)
o-Anisidine (8CI)

GB (exp) : 200.2+/-2 kcal/mol

Temperature : 600 K

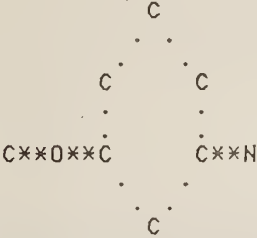
PA (exp) : 217.4+/-2 kcal/mol

Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities of Amines. Hydrogen Bonding
in Proton-Bound Amine Dimers and Proton-Induced
Cyclization of alpha,omega-Diamines,
J. Am. Chem. Soc. 95, 3504 (1973).

Method used : MS
Entropy change assumed zero
Equilibrium; scale based on CH3NH2

C7H9NO	CAS REGN : 104-94-9
<pre> C . . C . C**N . C**O**C . C . C </pre>	
Benzenamine, 4-methoxy- (9CI) p-Anisidine (8CI)	
GB (exp) : 203.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 212.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C7H9NO	CAS REGN : 536-90-3
	
Benzenamine, 3-methoxy- (9CI) m-Anisidine (8CI)	
PA (exp) : 214.0+/-2 kcal/mol	Temperature : 300 K
Summerhays, K. D., Pollack, S. K., Taft, R. W., and Hehre, W. J. Gas-Phase Basicities of Substituted Anilines. Inferences about the Role of Solvent in Dictating Site of Protonation, J. Am. Chem. Soc. 99, 4585 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale base on NH3. Ring protonation	

C7H10	CAS REGN : 498-66-8
C*****C * * * * C*C+C*C * * * * C	
Bicyclo[2.2.1]hept-2-ene (9CI) 2-Norbornene (8CI)	
PA (exp) : 198.8+/-2 kcal/mol	Temperature : 300 K
Staley, R. H., Wieting, R. D., and Beauchamp, J. L. Carbenium Ion Stabilities in the Gas Phase and Solution. An Ion Cyclotron Resonance Study of Bromide Transfer Reactions Involving Alkali Ions, Alkyl Carbenium Ions, Acyl Cations, and Cyclic Halonium Ions, J. Am. Chem. Soc. 99, 5964 (1977).	
Method used : ICR Calculated entropy Equilibrium relative to Et2O; scale based on NH3	

C7H10N2	CAS REGN : 1122-58-3
<pre> C . . . C N . . C**N**C C * . * . C C </pre>	
<p>4-Pyridinamine, N,N-dimethyl- (9CI) Pyridine, 4-(dimethylamino)- (8CI)</p>	
GB (exp) : 224.90+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 232.70+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH₃</p>	
GB (exp) : >209.7 kcal/mol	Temperature : 423-473 K
<p>Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).</p>	
<p>Method used : MS Bracketing relative to (CH₃)₂NH</p>	

C7H12		CAS REGN : 591-49-1	
<pre> C * * * * C C + * + * C**C C * * * * C</pre>			
Cyclohexene, 1-methyl- (8CI9CI)			
GB (exp) : 188.4+/-2 kcal/mol		Temperature : 300 K	
PA (exp) : 196.6+/-2 kcal/mol		Temperature : 300 K	
Unpublished work by Wolf, Staley, Koppel, Taagepera, Mciver, Beauchamp, and Taft.			
Method used : ICR Calculated entropy Equilibrium; scale based on NH3			

C7H12	CAS REGN : 765-47-9
<pre>C*****C * * * * C**C C + * + * C * * C</pre>	
Cyclopentene, 1,2-dimethyl- (8CI9CI)	
GB (exp) : 188.4+/-2 kcal/mol	Temperature : 298 K
<p>Pollack, S. K., Wolf, J. F., Levi, B. A., Taft, R. W., and Hehre, W. J. Kinetic Detection of Common Intermediates in Gas Phase Ion-Molecule Reactions, J. Am. Chem. Soc. 99, 1350 (1977).</p>	
Method used : ICR	

C7H13N	CAS REGN : 100-76-5
<pre> C**N * ** * C * C * C * C * * * * C**C </pre>	
1-Azabicyclo[2.2.2]octane (9CI) Quinuclidine (8CI)	
GB (exp) : 220.80+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 228.60+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 220.80+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 228.60+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

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GB (exp) : 209.7 kcal/mol	Temperature : 423-473 K
<p>Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).</p>	
<p>Method used : MS Bracketing relative to (CH₃)₂NH</p>	

C7H17N	CAS REGN : 111-68-2
<p>C**C**C**C**C**C**C**N</p>	
<p>1-Heptanamine (9CI) Heptylamine (8CI)</p>	
GB (exp) : 208.2+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.5+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH₃NH₂</p>	

C7H17N	CAS REGN : 4458-31-5
C**C**N**C**C**C * * C * * C	
1-Propanamine, N,N-diethyl- (9CI) Propylamine, N,N-diethyl- (8CI)	
GB (exp) : 221.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 229.1+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C7H17N	CAS REGN : 10076-31-0
C * * C**N**C**C**C * * * * C C	
1-Propanamine, N,N,2,2-tetramethyl- (9CI) Propylamine, N,N,2,2-tetramethyl- (8CI)	
GB (exp) : 218.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

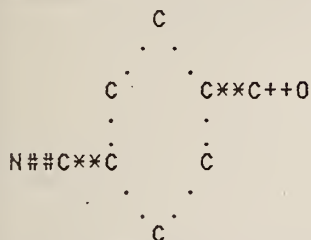
C7H18N2	CAS REGN : 110-95-2
C**N**C**C**C**N**C * * * * C C	
1,3-Propanediamine, N,N,N',N'-tetramethyl- (8CI9CI)	
GB (exp) : 227.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Equilibrium; scale based on NH3	

C8H4D6	CAS REGN : 25493-13-4
<pre> D C * . * . D**C**C C D * . * * . * D C C**C**D . * . * C D </pre>	
Benzene, 1,4-(dimethyl-d3)-	
GB (exp) : 182.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K
<p>Ausloos, P., and Lias, S. G. Equilibrium Isotope Effects on the Proton Transfer Reactions of Methylbenzenes, J. Am. Chem. Soc. 99, 4198 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C8H5F3O	CAS REGN : 455-19-6
<pre> C . . F C . . C**C++O * . . * . . F**C**C . C * . . * . . F . . C </pre>	
<p>Benzaldehyde, 4-(trifluoromethyl)- (9CI) p-Tolualdehyde, .alpha.,.alpha.,.alpha.-trifluoro- (8CI)</p>	
GB (exp) : 181.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.1+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C8H5NO

CAS REGN : 105-07-7



Benzonitrile, 4-formyl- (9CI)
Terephthalaldehydonitrile (8CI)

GB (exp) : 177.6+/-2 kcal/mol

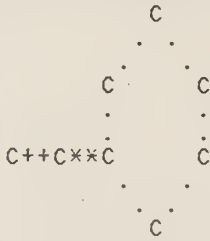
Temperature : 300 K

PA (exp) : 185.4+/-2 kcal/mol

Temperature : 300 K

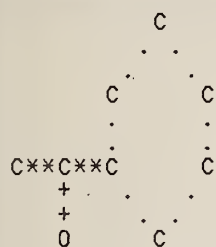
Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H8	CAS REGN : 100-42-5
	
Benzene, ethenyl- (9CI) Styrene (8CI)	
GB (exp) : 191.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 199.3+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C8H8O

CAS REGN : 98-86-2



Ethanone, 1-phenyl- (9CI)
Acetophenone (8CI)

GB (exp) : 195.3+/-2 kcal/mol

Temperature : 300 K

PA (exp) : 203.1+/-2 kcal/mol

Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H8O	CAS REGN : 104-87-0
<pre> C . . . C C**C . . O**C**C C C </pre>	
Benzaldehyde, 4-methyl- (9CI) p-Tolualdehyde (8CI)	
GB (exp) : 194+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 201.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C8H8O2	CAS REGN : 93-58-3
<pre> C . . . C C . . CxxOxxCxxC + + O C </pre>	
Benzoic acid, methyl ester (8CI9CI)	
GB (exp) : 193.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.9+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C8H8O2	CAS REGN : 123-11-5
<pre> C . . . C C**O**C . . O**C**C C . . C </pre>	
Benzaldehyde, 4-methoxy- (9CI) p-Anisaldehyde (8CI)	
GB (exp) : 203.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 210.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

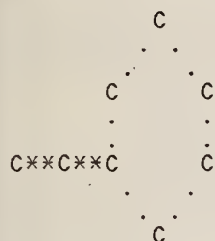
C8H10	CAS REGN : 95-47-6
<pre> C..C . . C**C . . C . . C..C * * C</pre>	
Benzene, 1,2-dimethyl- (9CI) o-Xylene (8CI)	
GB (exp) : 183+/-3 kcal/mol	Temperature : 340 K
PA (exp) : 190+/-3 kcal/mol	Temperature : 340 K
Chong, S. L., and Franklin, J. L., Proton Affinities of Benzene, Toluene, and the Xylenes, J. Am. Chem. Soc. 94, 6630 (1972).	
Method used : MS Equilibrium relative to CH3SH and (CH3)2O Entropy change assumed zero	

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GB (exp) : 183.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 191.1+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia From Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C8H10

CAS REGN : 100-41-4



Benzene, ethyl- (8CI9CI)

GB (exp) : 181.8+/-2 kcal/mol

Temperature : 300 K

Hehre, W. J., McIver, R. T., Jr., Pople, J. A.,
and Schleyer, P. v. R.,
Alkyl Substituent Effects on the Stability of
Protonated Benzene,
J. Am. Chem. Soc. 96, 7162 (1974).

Method used : ICR
Equilibrium; scale based on C6H5CH3(Toluene)

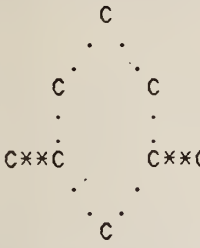
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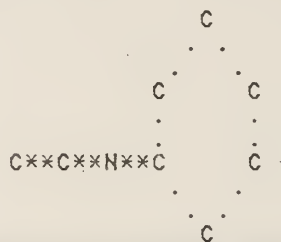
GB (exp) : 175.1+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 190.6+/-2 kcal/mol	Temperature : 600 K
<p>Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2</p>	
GB (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.1+/-2 kcal/mol	Temperature : 300 K
<p>Yamdaqni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on C6H6(Benzene)</p>	

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GB (exp) : 181.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.6+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C8H10	CAS REGN : 106-42-3
<pre> C . . . C C**C . . C**C C C </pre>	
Benzene, 1,4-dimethyl- (9CI) p-Xylene (8CI)	
GB (exp) : 182+/-3 kcal/mol	Temperature : 340 K
PA (exp) : 189+/-3 kcal/mol	Temperature : 340 K
Chong, S. L., and Franklin, J. L., Proton Affinities of Benzene, Toluene, and the Xylenes, J. Am. Chem. Soc. 94, 6630 (1972).	
Method used : MS Equilibrium; scale based on CH3SH and (CH3)2O Entropy change assumed zero	
GB (exp) : 182.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K
Devlin, J. L., III, Wolf, J. F., Taft, R. W., and Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to C6H6(Benzene)	

C8H10	CAS REGN : 108-38-3
	
Benzene, 1,3-dimethyl- (9CI) m-Xylene (8CI)	
GB (exp) : 182+/-3 kcal/mol	Temperature : 340 K
PA (exp) : 189.7+/-3 kcal/mol	Temperature : 340 K
Chong, S. L., and Franklin, J. L., Proton Affinities of Benzene, Toluene, and the Xylenes, J. Am. Chem. Soc. 94, 6630 (1972).	
Method used : MS Equilibrium relative to CH3SH and (CH3)2O Entropy change assumed zero	
GB (exp) : 187.2+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 194.6+/-2 kcal/mol	Temperature : 298 K
Devlin, J. L., III, Wolf, J. F., Taft, R. W., and Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to C6H6(Benzene)	

C8H11N	CAS REGN : 103-69-5
	
<p>Benzenamine, N-ethyl- (9CI) Aniline, N-ethyl- (8CI)</p>	
GB (exp) : 203.6+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 220.8+/-2 kcal/mol	Temperature : 600 K
<p>Yamdaqni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).</p>	
<p>Method used : ICR Equilibrium; scale based on NH3 Entropy change assumed zero</p>	

C8H11N	CAS REGN : 121-69-7
<pre> C . . . C C . . C**N**C * * * * C C </pre>	
Benzenamine, N,N-dimethyl- (9CI) Aniline, N,N-dimethyl- (8CI)	
GB (exp) : 212.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 220.1+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 220+/-2 kcal/mol	Temperature : 298 K
Pollack, S. K., Devlin, J. L., III, Summerhays, K. D., Taft, R. W., and Hehre, W. J. The Site of Protonation in Aniline, J. Am. Chem. Soc. 99, 4583 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3. Protonation on the nitrogen	

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GB (exp) : 206.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 224+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).</p>	
<p>Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero</p>	
GB (exp) : >209.7 kcal/mol	Temperature : 423-473 K
<p>Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).</p>	
<p>Method used : MS Bracketing relative to (CH3)2NH</p>	

C8H18S	CAS REGN : 107-47-1
C C * * * * C**C**S**C**C * * * * C C	
Propane, 2,2'-thiobis[2-methyl- (9CI) tert-Butyl sulfide (8CI)	
GB (exp) : 203.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 210.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C8H19N	CAS REGN : 110-96-3
<p>C**C**C**N**C**C**C</p> <p> * *</p> <p> * *</p> <p> C C</p>	
<p>1-Propanamine, 2-methyl-N-(2-methylpropyl)- (9CI) Diisobutylamine (8CI)</p>	
GB (exp) : 217.7+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 225.9+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

C8H19N	CAS REGN : 111-92-2
C**C**C**C**N**C**C**C**C	
1-Butanamine, N-butyl- (9CI) Dibutylamine (8CI)	
GB (exp) : 217.20+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 225.40+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C8H19N	CAS REGN : 626-23-3
C**C**C**N**C**C**C * * * * C C	
2-Butanamine, N-(1-methylpropyl)- (9CI) Di-sec-butylamine (8CI)	
GB (exp) : 219.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 228.1+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C8H19N	CAS REGN : 7087-68-5
C**C**N**C**C * * * * * * C C C * * C	
2-Propanamine, N-ethyl-N-(1-methylethyl)- (9CI) Triethylamine, 1,1'-dimethyl- (8CI)	
GB (exp) : 223.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 231.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C8H19N	CAS REGN : 21981-37-3
C C * * * * C**C**N**C**C * * * * C C	
2-Propanamine, N-(1,1-dimethylethyl)-2-methyl- (9CI) Di-tart-butylamine (8CI)	
GB (exp) : 221.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 229.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C8H20N2	CAS REGN : 111-51-3
C**N**C**C**C**C**N**C * * * * * * * * * * C * * * * C	
1,4-Butanediamine, N,N,N',N'-tetramethyl- (8CI9CI)	
GB (exp) : 229.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Equilibrium; scale based on NH3	

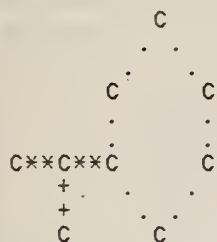
C9H9Cl	CAS REGN : 1712-70-5
<pre> C . . . C . C**CL . . C**C**C . C + . + . C . C </pre>	
Benzene, 1-chloro-4-(1-methylethenyl)- (9CI) Styrene, p-chloro-.alpha.-methyl- (8CI)	
GB (exp) : 195.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 203+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C9H9F	CAS REGN : 350-40-3
<pre> C / \ / \ C C**F / \ / \ C**C**C C / \ / \ + + C C </pre>	
Benzene, 1-fluoro-4-(1-methylethenyl)- (9CI) Styrene, p-fluoro-.alpha.-methyl- (8CI)	
GB (exp) : 196.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C9H9N	CAS REGN : 6921-29-5
C##C**C**N**C**C##C * * C * * C # # C	
2-Propyn-1-amine, N,N-di-2-propynyl- (9CI) Tri-2-propynylamine (8CI)	
GB (exp) : 209.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 217.1+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C9H10

CAS REGN : 98-83-9



Benzene, (1-methylethenyl)- (9CI)
Styrene, .alpha.-methyl- (8CI)

GB (exp) : 197.0+/-2 kcal/mol

Temperature : 300 K

PA (exp) : 205.2+/-2 kcal/mol

Temperature : 300 K

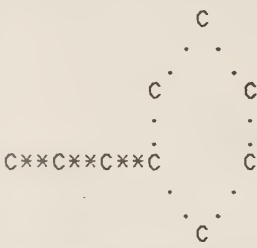
Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C9H12	CAS REGN : 98-82-8
<pre> C . . . C C . . C**C**C C * . . * . . C C</pre>	
Benzene, (1-methylethyl)- (9CI) Cumene (8CI)	
GB (exp) : 183+/-2 kcal/mol	Temperature : 300 K
Hehre, W. J., McIver, R. T., Jr., Pople, J. A., and Schleyer, P. v. R., Alkyl Substituent Effects on the Stability of Protonated Benzene, J. Am. Chem. Soc. 96, 7162 (1974).	
Method used : ICR Equilibrium; scale based on C6H5CH3(Toluene)	

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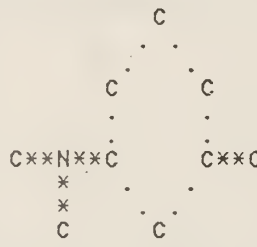
GB (exp) : 182.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.4+/-2 kcal/mol	Temperature : 300 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on C6H6(Benzene)	

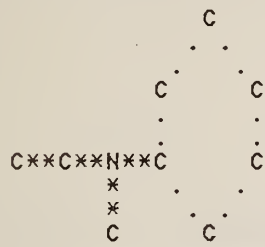
C9H12	CAS REGN : 103-65-1
	
Benzene, propyl- (8CI9CI)	
GB (exp) : 182.6+/-2 kcal/mol	Temperature : 300 K
Hehre, W. J., McIver, R. T., Jr., Pople, J. A., and Schleyer, P. v. R., Alkyl Substituent Effects on the Stability of Protonated Benzene, J. Am. Chem. Soc. 96, 7162 (1974).	
Method used : ICR Equilibrium; scale based on C6H5CH3(Toluene)	

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GB (exp) : 181.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190+/-2 kcal/mol	Temperature : 300 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on C6H6(Benzene)</p>	
GB (exp) : 182.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.4+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C9H12	CAS REGN : 108-67-8
<pre> C * * C . C . C . . C**C C**C . . C </pre>	
Benzene, 1,3,5-trimethyl- (9CI) Mesitylene (8CI)	
GB (exp) : 191.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.4+/-2 kcal/mol	Temperature : 300 K
<p>Devlin, J. L., III, Wolf, J. F., Taft, R. W., and Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium relative to benzene</p>	

C9H13N	CAS REGN : 121-72-2
	
Benzenamine, N,N,3-trimethyl- (9CI) m-Toluidine, N,N-dimethyl- (8CI)	
PA (exp) : 221+/-2 kcal/mol	Temperature : 298 K
Pollack, S. K., Devlin, J. L., III, Summerhays, K. D. Taft, R. W., and Hehre, W. J. The Site of Protonation in Aniline, J. Am. Chem. Soc. 99, 4583 (1977).	
Method used : ICR Equilibrium; scale based on NH3. Protonation on the nitrogen	

C9H13N	CAS REGN : 613-97-8
	
<p>Benzenamine, N-ethyl-N-methyl- (9CI) Aniline, N-ethyl-N-methyl- (8CI)</p>	
GB (exp) : 209.40+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 226.60+/-2 kcal/mol	Temperature : 600 K
<p>Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).</p>	
<p>Method used : MS Entropy change assumed zero Equilibrium; scale based on NH3</p>	

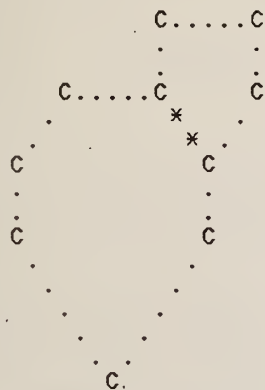
C9H15N	CAS REGN : 102-70-5
C++C**C**N**C**C++C * * C * * C + + C	
2-Propen-1-amine, N,N-di-2-propenyl- (9CI) Triallylamine (8CI)	
GB (exp) : 219+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C9H21N	CAS REGN : 102-69-2
<p>C**C**C**N**C**C**C</p> <p style="text-align: center;">* * C * * C * * C</p>	
<p>1-Propanamine, N,N-dipropyl- (9CI) Tripropylamine (8CI)</p>	
GB (exp) : 223.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 230.9+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 222.8+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 230.60+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

C9H21N	CAS REGN : 2085-66-7
C C * * * * C**C**N**C**C**C * * * * C C	
Propylamine, N-tert-butyl-1,1-dimethyl- (8CI)	
GB (exp) : 221.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 230.1+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C10H8

CAS REGN : 275-51-4



Azulene (8CI9CI)

GB (exp) : 215.9+/-2 kcal/mol

Temperature : 300 K

PA (exp) : 223.3+/-2 kcal/mol

Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C10H9F3	CAS REGN : 55186-75-9
<pre> C . . F C . C**C**C * . . . + * . . . + F**C**C . C C * . . . * . . . F . . C </pre>	
Benzene, 1-(1-methylethenyl)-4-(trifluoromethyl)- (9CI)	
GB (exp) : 189.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.1+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C10H10Fe	CAS REGN : 102-54-5
<pre>C+++C C+++C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * C+++C C+++C</pre>	
Ferrocene (8CI9CI)	
PA (exp) : 208+/-4 kcal/mol	Temperature : 300 K
Foster, M. S., and Beauchamp, J. L., Ion-Molecule Reactions and Gas-Phase Basicity of Ferrocene, J. Am. Chem. Soc. 97, 4814 (1975).	
Method used : ICR Bracketing relative to CH3N=NCH3 and CH3NH2.	

C10H12	CAS REGN : 1195-32-0
<pre> C . . C C**C . . C**C**C C + . + . C C </pre>	
Benzene, 1-methyl-4-(1-methylethenyl)- (9CI) Styrene, p,.alpha.-dimethyl- (8CI)	
GB (exp) : 200.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 208.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C10H12O	CAS REGN : 1712-69-2
<pre> C . . . C . C**O**C . . C**C**C C + + C C</pre>	
Benzene, 1-methoxy-4-(1-methylethenyl)- (9CI) Anisole, p-isopropenyl- (8CI)	
GB (exp) : 206.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

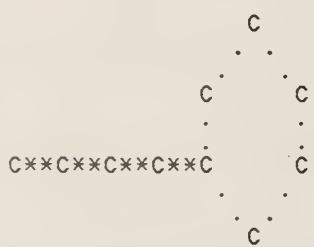
C10H13N	CAS REGN : 4096-21-3
<pre> C . . C C C*****C . . * * . . * * C C C*****N C . . * * . . * * C C</pre>	
Pyrrolidine, 1-phenyl- (8CI9CI)	
GB (exp) : 213.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 221.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C10H13N5O4	CAS REGN : 58-61-7
<pre> O * * * C * N N++C % * * % * * C..C * * O**C * * * * * * * * N C**N*****C * * * * * * * * * * * * * * C..N * * C**C * * * * O O </pre>	
Adenosine (8CI9CI)	
PA (exp) : >222 kcal/mol	Temperature :
<p>Wilson, M. S., and McCloskey, J. A., Chemical Ionization Mass Spectrometry of Nucleosides. Mechanisms of Ion Formation and Estimations of Proton Affinity, J. Am. Chem. Soc. 97, 3436 (1975).</p>	
<p>Method used : MS Bracketing relative to (CH3)3N.</p>	

C10H14	CAS REGN : 98-06-6
<pre> C C C C * . . * . . C**C**C C * . . * . . C C </pre>	
<p>Benzene, (1,1-dimethylethyl)- (9CI) Benzene, tert-butyl- (8CI)</p>	
GB (exp) : 183.2+/-2 kcal/mol	Temperature : 300 K
<p>Hahre, W. J., McIver, R. T., Jr., Pople, J. A., and Schleyer, P. v. R., Alkyl Substituent Effects on the Stability of Protonated Benzene, J. Am. Chem. Soc. 96, 7162 (1974).</p>	
<p>Method used : ICR Equilibrium; scale based on C6H5CH3(Toluene)</p>	

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GB (exp) : 182.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.6+/-2 kcal/mol	Temperature : 300 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on C6H6(Benzene)	

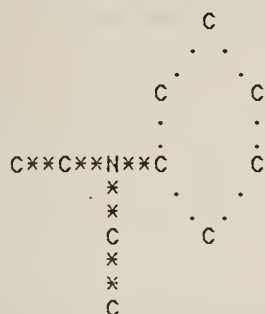
C10H14	CAS REGN : 104-51-8
 <p>The diagram shows a benzene ring with six carbon atoms. The top carbon is labeled 'C'. Moving clockwise, the second carbon is labeled 'C', the third is labeled 'C', the fourth is labeled 'C', the fifth is labeled 'C', and the sixth is labeled 'C'. There are asterisks between the carbon labels: 'C**C**C**C**C**C'. Dotted lines represent the bonds between the carbon atoms in the ring.</p>	
Benzene, butyl- (8CI9CI)	
GB (exp) : 183+/-2 kcal/mol	Temperature : 300 K
<p>Hehre, W. J., McIver, R. T., Jr., Pople, J. A., and Schleyer, P. v. R., Alkyl Substituent Effects on the Stability of Protonated Benzene, J. Am. Chem. Soc. 96, 7162 (1974).</p>	
<p>Method used : ICR Equilibrium; scale based on C6H5CH3(Toluene)</p>	

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GB (exp) : 183+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.8+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 182.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.4+/-2 kcal/mol	Temperature : 300 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on C6H6(Benzene)	

C10H15N

CAS REGN : 91-66-7



Benzenamine, N,N-diethyl- (9CI)
 Aniline, N,N-diethyl- (8CI)

GB (exp) : 212.10+/-2 kcal/mol

Temperature : 600 K

PA (exp) : 229.30+/-2 kcal/mol

Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
 Gas-Phase Basicities of Amines. Hydrogen Bonding
 in Proton-Bound Amine Dimers and Proton-Induced
 Cyclization of alpha,omega-Diamines,
 J. Am. Chem. Soc. 95, 3504 (1973).

Method used : MS
 Equilibrium; scale based on NH3
 Entropy change assumed zero

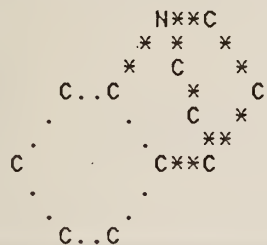
C10H19N	CAS REGN : 31023-92-4
<pre> C**C * * * * * * C *N * *C* * * *C * C*C C * * * * C**C</pre>	
1-Azabicyclo[3.3.3]undecane (9CI)	
PA (exp) : 227.9+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., Photoelectron Spectrum and Gas-Phase Basicity of Manxine. Evidence for a Planar Bridgehead Nitrogen, J. Am. Chem. Soc. 97, 4136 (1975).</p>	
<p>Method used : ICR Equilibrium; scale based on CH3NH2 Van't Hoff plot</p>	

C10H23N	CAS REGN : 2016-57-1
N**C**C**C**C**C**C**C**C**C**C	
1-Decanamine (9CI) Decylamine (8CI)	
GB (exp) : >209.7 kcal/mol	Temperature : 423-473 K
Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).	
Method used : MS Bracketing relative to (CH3)2NH	

C10H24N2	CAS REGN : 111-18-2
C**N**C**C**C**C**C**C**N**C * * * * * * * * * * C * * * * C	
1,6-Hexanediamine, N,N,N',N'-tetramethyl- (8CI9CI)	
GB (exp) : 226.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Equilibrium; scale based on NH3	

C11H13N

CAS REGN : 4363-25-1



2H-1,4-Ethanoquinoline, 3,4-dihydro- (8CI9CI)

GB (exp) : 220.5+/-2 kcal/mol

Temperature : 300 K

PA (exp) : 228.3+/-2 kcal/mol

Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C11H15N

CAS REGN : 4096-20-2



Piperidine, 1-phenyl- (8CI9CI)

GB (exp) : 216.1+/-2 kcal/mol

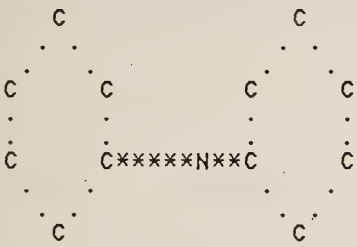
Temperature : 300 K

PA (exp) : 223.9+/-2 kcal/mol

Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C12H11N	CAS REGH : 122-39-4
	
Benzenamine, N-phenyl- (9CI) Diphenylamine (8CI)	
GB (exp) : >193.7 kcal/mol	Temperature : 423-473 K
<p>Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).</p>	
Method used : MS Bracketing relative to NH3	

C12H18	CAS REGN : 87-85-4
<pre> C C * * * * C..C . . C**C C**C . . C..C * * * * C C</pre>	
Benzene, hexamethyl- (8CI9CI)	
GB (exp) : 197.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 205.0+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

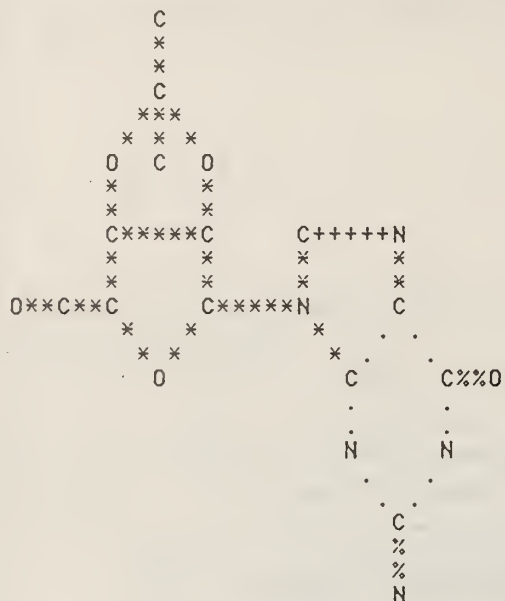
C12H19N	CAS REGN : 22025-87-2
<pre> C C..C * . * . C**N**C . C . . C..C . * . * . * . C**C**C . * . * . C </pre>	
<p>Benzenamine, 2-(1,1-dimethylethyl)-N,N-dimethyl- (9CI) Aniline, o-tert-butyl-N,N-dimethyl- (8CI)</p>	
GB (exp) : 218+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 225.8+/-2 kcal/mol	Temperature : 300 K
<p>Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

C12H27N	CAS REGN : 102-82-9
<p>C**C**C**C**N**C**C**C**C</p> <p style="text-align: center;">* * C * * C * * C * * C</p>	
<p>1-Butanamine, N,N-dibutyl- (9CI) Tributylamine (8CI)</p>	
GB (exp) : 224.1+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 232+/-2 kcal/mol	Temperature : 298 K
<p>Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2</p>	

C13H130P	CAS REGN : 2129-89-7
<pre> C C C C O C C . . + + . . C C C*****P**C C . . x x . . C C C</pre>	
Phosphine oxide, methyldiphenyl- (8CI9CI)	
PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K
<p>Goff, S. D., Jelus, B. L., and Schweizer, E. E. Electron Impact and Chemical Ionization Mass Spectra of Alkyldiphenylphosphine Oxides, Org. Mass Spectrom. 12, 33 (1977).</p>	
<p>Method used : MS Bracketing relative to pyridine and Me3N scale based on NH3</p>	

C13H17N5O5

CAS REGN : 362-76-5



Guanosine, 2',3'-O-(1-methylethylidene)- (9CI)
 Guanosine, 2',3'-O-isopropylidene- (8CI)

PA (exp) : >222 kcal/mol

Temperature :

Wilson, M. S., and McCloskey, J. A.,
 Chemical Ionization Mass Spectrometry of Nucleosides.
 Mechanisms of Ion Formation and Estimations of
 Proton Affinity,
 J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
 Bracketing relative to (CH3)3N.

C13H21N	CAS REGN : 585-48-8
<pre> C . . . C C C C * . . * * . . * C**C**C C**C**C * . . * * . . * C N C </pre>	
Pyridine, 2,6-bis(1,1-dimethylethyl)- (9CI) Pyridine, 2,6-di-tert-butyl- (8CI)	
GB (exp) : 220.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 228.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C14H12	CAS REGN : 530-48-3
<pre> C C C . . C C . . C C . . C*****C**C C C C C </pre>	
Benzene, 1,1'-ethenylidenebis- (9CI) Ethylene, 1,1-diphenyl- (8CI)	
GB (exp) : 201.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 209.2+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C17H210P	CAS REGN : Not available
<pre> C O C . + . . + . C C**P**C C . * . . * . C C C C C . * . . * . C C**C**C C . * . . * . C </pre>	
Phosphine oxide, neopentyldiphenyl-	
PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K
<p>Goff, S. D., Jelus, B. L., and Schweizer, E. E. Electron Impact and Chemical Ionization Mass Spectra of Alkyldiphenylphosphine Oxides, Org. Mass Spectrom. 12, 33 (1977).</p>	
<p>Method used : MS Bracketing relative to pyridine and Me3N scale based on NH3</p>	

C22H310P	CAS REGN : Not available
<pre> C O C . + . . + . C C**P**C C . * . . * . C C C C C . * . . * . C C C . * . . * . . * . C**C**C**C**C**C**C**C </pre>	
Phosphine oxide, decanyldiphenyl-	
PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K
<p>Goff, S. D., Jelus, B. L., and Schweizer, E. E. Electron Impact and Chemical Ionization Mass Spectra of Alkyldiphenylphosphine Oxides, Org. Mass Spectrom. 12, 33 (1977).</p>	
<p>Method used : MS Bracketing relative to pyridine and Me3N scale based on NH3</p>	

Ca	CAS REGN : 7440-70-2
CA	
Calcium (8CI9CI)	
PA (exp) : >211 kcal/mol	Temperature : ~800 K
Eslava, L. A., and Porter, R. F. A Kinetic Study of Proton Transfer Reactions of NH ₄ ⁺ , CH ₃ NH ₃ ⁺ , and PH ₄ ⁺ with Calcium Atoms, Chem. Phys. Letters 52 368 (1977).	
Method used : MS Bracketing relative to NH ₃ , PH ₃ and MeNH ₂	

ClH	CAS REGN : 7647-01-0
CL	
Hydrochloric acid (8CI9CI)	
PA (exp) : 140+/-3 kcal/mol	Temperature :
<p>Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).</p>	
<p>Method used : MS Absolute PA value estimated by assuming that for reaction $RH^+ + RH \rightarrow R + RH_2^+$ the $\Delta H \sim 5X TC$. TC = measured translational energy of the products.</p>	
PA (exp) : >120 kcal/mol	Temperature : 297 K
<p>Fehsenfeld, F. C., and Ferguson, E. E. Rate Constants for the Reactions $Cl^+ + H_2 \rightarrow HCl^+ + H$ and $ClH^+ + H_2 \rightarrow ClH_2^+ + H$, J. Chem. Phys. 60, 5132 (1974).</p>	
<p>Method used : FAG Found reaction $ClH^+ + H_2 \rightarrow ClH_2^+ + H$ react rapidly. Since reaction $Cl^+ + H_2 \rightarrow HCl^+ + H + .22eV$ has a low exothermicity, they assumed HCl^+ to be in ground vibrational state.</p>	

CsHO	CAS REGN : 21351-79-1
CS*O	
Cesium hydroxide (8CI9CI)	
PA (exp) : 270.1 kcal/mol	Temperature : 300 K
Searles, S. K., Dzidic, I., and Kebarle, P., Proton Affinities of the Alkali Hydroxides, J. Am. Chem. Soc. 91, 2810 (1969).	
Method used : MS PA derived from delta H of reaction M+ + H2O -> (MOH2)+.	

D2	CAS REGN : 7782-39-0
H**H	
Deuterium (8CI9CI)	
PA (exp) : 98+/-4 kcal/mol	Temperature :
Harris, H. H., Crowley, M. G., Grossheim, T. R., Woessner, P. J., and Leventhal, J. J., Binding Energy of H3+, J. Chem. Phys. 59, 6181 (1973).	
Method used : MS Threshold measurement of CID of D3+ + HE->D2 + D+ + HE. Correction for collision energies distribution.	

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PA (exp) : 103.8+/-1.1 kcal/mol	Temperature :
<p>Cotter, R. J., Rozett, R. W., and Koski, W. S., Reactions of H2O+ and D2O+ with Molecular Hydrogen. I. Proton Affinity of Hydrogen, J. Chem. Phys. 57, 4100 (1972).</p>	
<p>Method used : MS Threshold measurement of D2O+ + D2 -> D3+ + OD. Correction for Doppler effect.</p>	

D2O	CAS REGN : 7789-20-0
0	
<p>Water-d2 (9CI) Water, heavy (D2O) (8CI)</p>	
PA (exp) : 167+/-3 kcal/mol	Temperature :
<p>Cotter, R. J., and Koski, W. S., Reaction of D3O+ with D2: Proton Affinity of Water, J. Chem. Phys. 59, 784 (1973).</p>	
<p>Method used : MS Correction for Doppler effects. Deuterium affinity. Threshold measurement of D2O+ + D2O -> D3O+ + D0.</p>	

FH	CAS REGN : 7664-39-3
F	
Hydrofluoric acid (8CI9CI)	
PA (exp) : 112+/-2 kcal/mol	Temperature : 300 K
<p>Foster, M. S., and Beauchamp, J. L., Proton Affinity and Gas-Phase Ion Chemistry of Hydrogen Fluoride, Inorg. Chem. 14, 1229 (1975).</p>	
<p>Method used : ICR Calculated entropy. Equilibrium relative to N2.</p>	
PA (exp) : 94.3+/-1.4 kcal/mol	Temperature : 0 K
<p>Ng, C. Y., Trevor, D. J., Tiedemann, P. W., Ceyer, S. T., Kronebusch, P. L., Mahan, B. H., and Lee, Y. T. Photoionization of Dimeric Polyatomic Molecules: Proton Affinities of H2O and HF, J. Chem. Phys. 67, 4235 (1977).</p>	
<p>Method used : PI AP of H2F+ from (HF)2. No temperature correction was applied in this supersonic expansion</p>	

F0	CAS REGN : 12061-70-0
F+0	
Oxygen fluoride	
PA (exp) : 134+/-2 kcal/mol	Temperature : 0 K
Berkowitz, J., Appelman, E. H., and Chupka, W. A. Photoionization of HOF with Mass Analysis, J. Chem. Phys. 58, 1950 (1973).	
Method used : MS Threshold measurement of reaction HOF -> HOF+	

F3N	CAS REGN : 7783-54-2
F**N**F * * F	
Nitrogen fluoride (NF3) (8CI9CI)	
PA (exp) : 151+/-10 kcal/mol	Temperature : 300 K
Holtz, D., Beauchamp, J. L., Henderson, W. G., and Taft, R. W., Basicity of Nitrogen Trifluoride in the Gas Phase by Ion Cyclotron Resonance, Inorg. Chem. 10, 201 (1971).	
Method used : ICR Bracketing relative to C2H4 AND HCL.	

F6S	CAS REGN : 2551-62-4
<pre>F F * * ** F**S**F ** * * F F</pre>	
Sulfur fluoride (SF6), (OC-6-11)- (9CI) Sulfur fluoride (SF6) (8CI)	
PA (exp) : <144 kcal/mol	Temperature : 298 K
Gorden, R., Jr., and Sieck, L. W., Ion-Molecule Reactions in Isopropanol: Implications for its Radiolysis, J. Res. NBS 76A, 655 (1972).	
Method used : MS Proton transfer from C2H6+ to SF6 not observed.	

HI	CAS REGN : 10034-85-2
I	
Hydriodic acid (8CI9CI)	
PA (exp) : 145+/-3 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Absolute PA value estimated by assuming that for reaction $RH^+ + RH \rightarrow R + RH_2^+$; the ΔH = 5X TC. TC = measured translational energy of the products.	

HKO	CAS REGN : 1310-58-3
K**O	
Potassium hydroxide (8CI9CI)	
PA (exp) : 263.5 kcal/mol	Temperature : 300 K
Searles, S. K., Dzidic, I., and Kebarle, P., Proton Affinities of the Alkali Hydroxides, J. Am. Chem. Soc. 91, 2810 (1969).	
Method used : MS PA value derived from delta H of reaction: M+ + H2O -> (MOH2)+.	

HLiO	CAS REGN : 1310-65-2
LI*O	
Lithium hydroxide (8CI9CI)	
PA (exp) : 241.6 kcal/mol	Temperature : 300 K
Searles, S. K., Dzidic, I., and Kebarle, P., Proton Affinities of the Alkali Hydroxides, J. Am. Chem. Soc. 91, 2810 (1969).	
Method used : MS PA value derived from delta H of reaction M+ + H2O -> (MOH2)+	

HN _a O	CAS REGN : 1310-73-2
NA*O	
Sodium hydroxide (8CI9CI)	
PA (exp) : 248.5 kcal/mol	Temperature : 300 K
Searles, S. K., Dzidic, I., and Kebarle, P., Proton Affinities of the Alkali Hydroxides, J. Am. Chem. Soc. 91, 2810 (1969).	
Method used : MS PA value derived from delta H of reaction M+ + H2O = (MOH2)+	

H2	CAS REGN : 1333-74-0
H**H	
Hydrogen (8CI9CI)	
PA (exp) : 99.9+/-1 kcal/mol	Temperature :
Duben, A. J., and Lowe, J. P., Correlation Studies on H3+. I. The Wavefunctions, J. Chem. Phys. 55, 4270 (1971).	
Method used : TC SCF-MO-CI calculation.	

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PA (exp) : 97 kcal/mol	Temperature : 298 K
Schwartz, M. E., and Schaad, J. J., Ab Initio Studies of Small Molecules Using 1s Gaussian Basis Function. II. H3+, J. Chem. Physics 47, 5325 (1967).	
Method used : TC SCF-MO-CI calculation.	
PA (exp) : 101.5 kcal/mol	Temperature :
Burt, J. A., Dunn, J. L., McEwan, M. J., Sutton, M. M., Rocke, A. E., and Schiff, H. I., Some Ion-Molecule Reactions of H3+ and the Proton Affinity of H2, J. Chem. Phys. 52, 6062 (1970).	
Method used : FAG Bracketing relative to O2 AND N2.	
PA (exp) : 101+/-2 kcal/mol	Temperature :
Cotter, R. J., Rozett, R. W., and Koski, W. S., Reactions of H2O+ and D2O+ with Molecular Hydrogen. I. Proton Affinity of Hydrogen, J. Chem. Phys. 57, 4100 (1972).	
Method used : MS Correction for Doppler effect. Threshold measurement of H2O+ + H2 -> H3+ + OH.	

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PA (exp) : 96+/-4 kcal/mol	Temperature :
Harris, H. H., Crowley, M. G., Grossheim, T. R., Woessner, P. J., and Leventhal, J. J., Binding Energy of H3+, J. Chem. Phys. 59, 6181 (1973).	
Method used : MS Threshold measurement of CID of H3+ + He -> H2 + H+ +He. Correction for collision energies distribution.	

H2O	CAS REGN : 7732-18-5
0	
Water (8CI9CI)	
PA (exp) : 167+/-7 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to CH2O and C2H4	

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PA (exp) : 182 kcal/mol	Temperature :
<p>Sherman, J., Crystal Energies of Ionic Compounds and Thermochemical Applications, Chem. Rev. 11, 93 (1932).</p>	
<p>Method used : CLE Using thermochemical cycle the value of PA(H₂O) was calculated from PA(NH₃).</p>	
PA (exp) : 171+/-2 kcal/mol	Temperature : 296,355,426 K
<p>Hopkins, J. M., and Bone, L. I., Relative Proton Affinities of Hydrogen Sulfide and Water, J. Chem. Phys. 58, 1473 (1973).</p>	
<p>Method used : MS Van't Hoff plot Equilibrium relative to H₂S. Assume steady state kinetics.</p>	
PA (exp) : 165.8+/-1.8 kcal/mol	Temperature : 0 K
<p>Ng, C. Y., Trevor, D. J., Tiedemann, P. W., Ceyer, S. T., Kronebusch, P. L., Mahan, B. H., and Lee, Y. T. Photoionization of Dimeric Polyatomic Molecules: Proton Affinities of H₂O and HF, J. Chem. Phys. 67, 4235 (1977).</p>	
<p>Method used : PI AP of H₃O⁺ from (H₂O)₂. No temperature correction was applied in this supersonic expansion</p>	

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GB (exp) : 153.3+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 169.3+/-2 kcal/mol	Temperature : 600 K
<p>Yamdaqni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).</p>	
<p>Method used : MS Calculated entropy Equilibrium; scale based on NH3</p>	
GB (exp) : 162.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 170.3+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

H2S	CAS REGN : 7783-06-4
S	
Hydrogen sulfide (H2S) (8CI9CI)	
GB (exp) : 165.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 173.9+/-2 kcal/mol	Temperature : 300 K
<p>Freeman, C. G., Harland, P. W., and McEwan, M. J. The Equilibrium $H_3S^+ + HCN = H_2CN^+ + H_2S$ and the Relative Proton Affinities of HCN and H2S, Intern. J. Mass Spectrom. Ion Phys. 27, 77 (1978).</p>	
<p>Method used : FAG Equilibrium relative to HCN; scale based on NH3</p>	
PA (exp) : 173.3+/-2 kcal/mol	Temperature : 296,355,426 K
<p>Hopkins, J. M., and Bone, L. I., Relative Proton Affinities of Hydrogen Sulfide and Water, J. Chem. Phys. 58, 1473 (1973).</p>	
<p>Method used : MS Equilibrium relative to H2O Van't Hoff plot</p>	

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PA (exp) : 177.1+/-2 kcal/mol	Temperature : 299,329,360 K
<p>Wei, L. Y., and Bone, L. I., Ion-Molecule Reactions in Methanol and Hydrogen Sulfide, J. Phys. Chem. 78, 2527 (1974).</p>	
<p>Method used : MS Equilibrium; scale based on CH3OH Van't Hoff plot</p>	
PA (exp) : 171 kcal/mol	Temperature :
<p>Haney, M. A., and Franklin, J. L., Heats of Formation of H3O+, H3S+, and NH4+ by Electron Impact, J. Chem. Phys. 50, 2028 (1969).</p>	
<p>Method used : EI Appearance potential by electron impact. Correction for excess energy.</p>	
GB (exp) : 165.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 173.9+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

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GB (exp) : 156.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 172.4+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 172.4+/-2.5 kcal/mol	Temperature : 300 K
PA (exp) : 175.3+/-2.5 kcal/mol	Temperature : 300 K
Meot-Ner (Mautner), M., and Field, F. H. Proton Affinities and Cluster Ion Stabilities in CO2 and CS2. Application in Martian Ionospheric Chemistry, J. Chem. Phys. 66, 4527 (1977).	
Method used : MS Calculated entropy The measurements done in the temperature range of 400-650k. Using the Hoff plot the H and S at 300 k were derived. Equilibrium; scale based on NH3	

H ₂ Se	CAS REGN : 7783-07-5
SE	
Hydrogen selenide (H ₂ Se) (8CI9CI)	
GB (exp) : 166.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 174.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH ₃	

H3N	CAS REGN : 7664-41-7
N	
Ammonia (8CI9CI)	
PA (exp) : >197 kcal/mol	Temperature :
Chupka, W. A., and Russell, M. E., Ion-Molecule Reactions of NH3+ by Photoionization, J. Chem. Phys. 48, 1527 (1968).	
Method used : PI NH3+ formed by photoionization and react with H2O.	
PA (exp) : 206.4 kcal/mol	Temperature :
Bleick, W. E., The Lattice Energies of the Ammonium Halides and the Proton Affinity of Ammonia, J. Chem. Phys. PA = 2, 160 (1934).	
Method used : CLE Using thermochemical cycle the PA is derived from crystal lattice energy.	

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PA (exp) : 208 kcal/mol	Temperature :
<p>Haney, M. A., and Franklin, J. L., Heats of Formation of H₃O⁺, H₃S⁺, and NH₄⁺ by Electron Impact, J. Chem. Phys. 50, 2028 (1969).</p>	
<p>Method used : EI Appearance potential by electron impact. Correction for excess energy.</p>	
PA (exp) : 194+/-7 kcal/mol	Temperature :
<p>Vetchinkin, S. I., Pshenichnov, E. A., and Sokolov, N. D., The Effect of the Hydrogen Bond on the Energy of the Ionic Lattice of Ammonium Chloride and Estimation of the Proton Affinity of an Ammonia Molecule, Zh. Fiz. Khim. 33, 1269 (1959).</p>	
<p>Method used : CLE PA from crystal lattice energy, correction for hydrogen bond.</p>	
PA (exp) : 206+/-8 kcal/mol	Temperature :
<p>Sherman, J., Crystal Energies of Ionic Compounds and Thermochemical Applications, Chem. Rev. 11, 93 (1932).</p>	
<p>Method used : CLE Using thermochemical cycle the PA values 209, 208.6 and 202.7 are derived from crystal lattice energy of NH₄Cl, NH₄Br and NH₄I respectively.</p>	

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GB (exp) : 185.1+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 202.3+/-2 kcal/mol	Temperature : 600 K
Yamdaqni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on PA(iso-C4H8)	
GB (exp) : 193.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 202.3+/-2 kcal/mol	Temperature : 300 K
Staley, R. H., Taagepera, M., Henderson, W. G., Koppel, I., Beauchamp, J. L., and Taft, R. W., Effects of Alkyl and Fluoroalkyl Substitution on the Heterolytic and Homolytic Bond Dissociation Energies of Protonated Amines, J. Am. Chem. Soc. 99, 326 (1977).	
Method used : ICR Calculated entropy Equilibrium.	

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PA (exp) : 205.7+/-1 kcal/mol	Temperature : 298.15 K
Meot-Ner (Mautner), M., and Field, F. H. Proton Affinities and Cluster Ion Stabilities in CO ₂ and CS ₂ . Application in Martian Ionspheric Chemistry, J. Chem. Phys. 66, 4527 (1977).	
Method used : CLE Using thermochemical cycle the PA value is derived from crystal lattice energy. Error due to some of the thermochemical data and the similarity of crystal structure.	
PA (exp) : 205.3 kcal/mol	Temperature :
Goodliffe, A. L., Jenkins, H. D. B., Martin, S. V., and Waddington, T. C., The Proton Affinity of Gaseous Ammonia, the Charge Distribution on the NH ₄ ⁺ Ion and the Lattice Energies of NH ₄ Cl, NH ₄ Br, and NH ₄ I, Mol. Phys. 21, 761 (1971).	
Method used : CLE Using thermochemical cycle the PA is derived from crystal lattice energy and the distributed charge on NH ₄ ⁺ .	

H3P	CAS REGN : 7803-51-2
P	
Phosphine (8CI9CI)	
PA (exp) : 200+/-10 kcal/mol	Temperature : 298 K
Wendlendt, W., Proton Affinity of Phosphine in the Phosphonium Halides, Science 122, 831 (1955).	
Method used : CLE Using thermochemical cycle calculate the PA value from crystal lattice energy.	
PA (exp) : 156.2+/-3 kcal/mol	Temperature :
Wada, Y., and Kiser, R. W., A Mass Spectrometric Study of Some Alkyl-Substituted Phosphines, J. Phys. Chem. 68, 2290 (1964).	
Method used : EI Appearance potential by electron impact of (CH3)3P and (C2H5)3P	

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PA (exp) : 194.5+/-5 kcal/mol	Temperature :
Waddington, T. C., Lattice Energies of Phosphonium Bromide and Iodide and the Proton Affinity of Phosphine, Trans. Faraday Soc. 61, 2652 (1965).	
Method used : CLE Using thermochemical cycle they calculated the PA from crystal lattice energy and heats of formation.	
PA (exp) : 186 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Delta H estimated = 5X total translational energy of the products of $RH^+ + RH \rightarrow RH_2^+ + R$.	

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GB (exp) : 178.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187.4+/-2 kcal/mol	Temperature : 300 K
<p>Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).</p>	
<p>Method used : ICR Calculated entropy Equilibrium; scale based on NH3</p>	

H4N2	CAS REGN : 302-01-2
N**N	
Hydrazine (8CI9CI)	
PA (exp) : 221 kcal/mol	Temperature :
<p>Jen, J. A., and Thomas, T. D., Core Ionization Potentials in Dimethyl Ether and Methyl Amine, J. Electron Spectrosc. 4, 43 (1974).</p>	
<p>Method used : CIP Assuming that delta H of CH4 + NH2NH3+ -> CH3NH2 + NH4+ is equal to the difference in carbon 1S ionization potentials of CH4 and CH3NH2. CIP = core ionization potential.</p>	

H4Si	CAS REGN : 7803-62-5
SI	
Silane (8CI9CI)	
PA (exp) : 155+/-3 kcal/mol	Temperature :
Cheng, T. M. H., and Lampe, F. W., SiH5+ and the Proton Affinity of Monosilane, Chem. Phys. Letters 19, 532 (1973).	
Method used : MS Bracketing relative to C2H2 AND C3H7.	

He	CAS REGN : 7440-59-7
HE	
Helium (8CI9CI)	
PA (exp) : 41.5 kcal/mol	Temperature :
Bel'skii, V. E., and Izmailov, R. I., Proton Affinity of Atoms and Ions, Zh. Obshch. Khim. 44, 2297 (1974).	
Method used : TC Using thermochemical cycles.	

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PA (exp) : 42 kcal/mol	Temperature :
Beauchamp, J. L., Interactions between Ions and Molecules, Ed. P. Ausloos, (Plenum Press, New York and London, 1975) p. 413.	
Method used : HE Literature Survey.	

Kr	CAS REGN : 7439-90-9
KR	
Krypton (8CI9CI)	
PA (exp) : 115+/-15 kcal/mol	Temperature :
Munson, M. S. B., and Field, F. H., Reactions of Gaseous Ions. XVI. Effects of Additives on Ionic Reactions in Methane, J. Am. Chem. Soc. 87, 4243 (1965).	
Method used : MS Bracketing relative to H2 and CH4.	

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PA (exp) : 100.3+/-0.5 kcal/mol	Temperature :
<p>Payzant, J. D., Schiff, H. I., and Bohme, D. K., Determination of the Proton Affinity from the Kinetics of Proton Transfer Reactions. V. The Equilibrium $H_3^+ + Kr = KrH^+ + H_2$ and the Relative Proton Affinity of Kr and H_2, J. Chem. Phys. 63, 149 (1975).</p>	
<p>Method used : FAG Equilibrium relative to H_2. Delta S estimated from the entropies of the particles.</p>	

Mg	CAS REGN : 7439-95-4
MG	
Magnesium (8CI9CI)	
PA (exp) : ~198 kcal/mol	Temperature : 350 K
<p>Po, P. L., and Porter, R. F. High-Temperature Ion-Molecule Chemistry. A Kinetic Study of Gas-Phase Reactions of Magnesium Atoms with D_3^+, Methanium, Ammonium, and tert-C₄H₉⁺ Ions, J. Am. Chem. Soc. 99, 4922 (1977).</p>	
<p>Method used : MS Bracketing relative to (CH₃)₂C=CH₂ and NH₃</p>	

Mg ₂	CAS REGN : 29904-79-8
Mg+Mg	
Magnesium molecule	
PA (exp) : 219+/-7 kcal/mol	Temperature : 700 K
Po, P. L., and Porter, R. F. A Thermodynamic Study of the Reactions of Mg+(g) and MgH+(g) with Magnesium, J. Phys. Chem. 81, 2233 (1977).	
Method used : MS Calculated entropy From the K equilibrium of reaction MgH+ + Mg(s) = Mg ₂ H+ and using PA (Mg) = 196 and delta Hf(H+) = 365.7	

NO	CAS REGN : 10102-43-9
N++0	
Nitrogen oxide (NO) (8CI9CI)	
PA (exp) : <127 kcal/mol	Temperature :
<p>Munson, M. S. B., and Field, F. H., Reactions of Gaseous Ions. XVI. Effects of Additives on Ionic Reactions in Methane, J. Am. Chem. Soc. 87, 4243 (1965).</p>	
<p>Method used : MS Bracketing relative to CH₄.</p>	
PA (exp) : 126.9+/-1.1 kcal/mol	Temperature : 300 K
<p>Hemsworth, R S., Payzant, J. D., Schiff, H. I., and Bohme, D. K., Rate Constants at 297 K for Proton Transfer Reactions with NH₃ Comparisons with Classical Theories and Exothermicity, Chem. Phys. Letters 26, 417 (1974).</p>	
<p>Method used : FAG Equilibrium relative to H₂. Use PA (H₂) from J. Chem. Phys. 55, 4270 (1971).</p>	

N2	CAS REGN : 7727-37-9
N##N	
Nitrogen (8CI9CI)	
PA (exp) : 112.6+/-1 kcal/mol	Temperature : 298 K
Schiff, H. I., and Bohme, D. K., Flowing Afterglow Studies at York University, Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975).	
Method used : FAG Equilibrium scale based on H2. Delta S derived from theoretical entropies and entropies of iso-electronic particles.	
PA (exp) : 130+/-2 kcal/mol	Temperature :
Willis, C., Lossing, F. P., and Back, R. A. The Heat of Formation of N2H2 and the Proton Affinity of N2, Can. J. Chem. 54, 1 (1976).	
Method used : EM The PA is derived from the appearance potentials of N2+ and N2H+	

N2O	CAS REGN : 10024-97-2
O++N++N	
Nitrogen oxide (N2O) (8CI9CI)	
PA (exp) : 138.4 kcal/mol	Temperature : 298 K
Schiff, H. I., and Bohme, D. K., Flowing Afterglow Studies at York University, Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975).	
Method used : FAG Calculated entropy Equilibrium; scale based on CO.	

O2	CAS REGN : 7782-44-7
O++O	
Oxygen (8CI9CI)	
PA (exp) : 100.9+/- .5 kcal/mol	Temperature : 298 K
McCulloh, K. E., To be published.	
Method used : PI Photoionization of H2O2.	

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PA (exp) : 100.4+/-1.5 kcal/mol	Temperature : 298 K
Kim, J. K., Theard, L. P., and Huntress, W. T., Jr., Proton Transfer Reactions from H3+ Ions to N2, O2, and CO Molecules, Chem. Phys. Letters 32, 610 (1975).	
Method used : ICR Equilibrium relative to H2. Entropy change estimated from the known theoretical iso-electronic counterpart entropies of the species.	
PA (exp) : 100+/-1 kcal/mol	Temperature : 298 K
Fennelly, P. F., Hemsworth, R. S., Schiff, H. I., and Bohme, D. K., Determination of the Proton Affinity from the Kinetics of Proton Transfer Reactions. IV. The Equilibrium O2H+ + H2 = H3+ + O2 and the Relative Proton Affinity of O2 and H2, J. Chem. Phys. 59, 6405 (1973).	
Method used : FAG Equilibrium relative to H2. Entropy change estimated from the known theoretical iso-electronic counterpart entropies of the species.	

03S	CAS REGN : 7446-11-9
0++S++0 + + 0	
Sulfur trioxide (8CI9CI)	
PA (exp) : 142+/-2 kcal/mol	Temperature :
Munson, B., Smith, D., and Polley, C. The Mass Spectrum, Proton Affinity and Ion-Molecule Reactions of SO ₃ , Intern. J. Mass Spectrom. Ion Phys. 25, 323 (1977).	
Method used : MS Bracketing relative to HBr and CO. Use $\Delta H_f(H^+) = 366$.	

U	CAS REGN : 7440-61-1
U	
Uranium (8CI9CI)	
PA (exp) : 238+/-4 kcal/mol	Temperature : 400 K
Armentrout, P., Hodges, R., and Beauchamp, J. L. Metal Atoms as Superbases: the Gas Phase Proton Affinity of Uranium, J. Am. Chem. Soc. 99, 3162 (1977).	
Method used : MS Threshold measurement of UD+. Correction for D(UD+) - D(UH+) assuming $\Delta H_{400} = \Delta H_{298}$ Entropy change assumed zero	

Xe	CAS REGN : 7440-63-3
XE	
Xenon (8CI9CI)	
PA (exp) : 118+/-11 kcal/mol	Temperature :
<p>Munson, M. S. B., and Field, F. H., Reactions of Gaseous Ions. XVI. Effects of Additives on Ionic Reactions in Methane, J. Am. Chem. Soc. 87, 4243 (1965).</p>	
<p>Method used : MS Bracketing relative to CH₄ and reaction XE+(2P^{1/2}) + CH₄.</p>	
PA (exp) : 113.2+/-1.5 kcal/mol	Temperature : 800 K
<p>Fehsenfeld, F. C., Lindinger, W., Schiff, H. I., Hemsworth, R. S., and Bohme, D. K. Determination of the Proton Affinity from the Kinetics of Proton Transfer Reactions. VI. The Relative Proton Affinities of N₂, Xe, and CO₂, J. Chem. Phys. 64, 4887 (1976).</p>	
<p>Method used : FAG Van't Hoff plot Equilibrium relative to N₂; scale based on PA (N₂) = 112.6</p>	

123.0	41
153.3	453
154.7	46
156.4	456
162.3	453
162.5	24
164.4	55
165.1	47
165.4	108,253
165.7	42,454
165.9	256,455
166.5	33
166.7	20,457
166.8	51,265
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2730-67-8	110
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B3H5N3	6
B3H6N3	7
B4H8	8
B4H10	9
B5H9	10
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CF4	17
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CHN	19-20
CH2F2	20
CH2N2	21
CH2O	21-22
CH2O2	23-25
CH3Br	25
CH3Cl	26-27
CH3F	27
CH3I	28
CH3NO2	29-30
CH4	30-31
CH4O	32-34
CH4S	34-35
CH5N	36-37
CH5P	38
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C2D6O	44
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C2H3F	53
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C2H5NO	75-76
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C3H4	100-102
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C3H5N	104-105
C3H6	106-108
C3H6F3N	108-110
C3H6N2	111
C3H6O	112-117
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C3H6O2	119-123
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C3H6S2	125
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C3H7NO	129
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C4H6N2	156
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C4H8F3N	166-167
C4H8N2	168
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C5H6N2O2	216
C5H7F3O2	217
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C5H8O	219
C5H8O2	220-221
C5H9N	222
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C5H10O	225-229
C5H10O2	230-232
C5H11N	233-235
C5H11NO2	235
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C5H13N	238-243
C5H14N2	244-245
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C6HF5	247
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C6H3F3	251-253
C6H4F2	254-257
C6H4F3N	258-260
C6H4N2	261-263
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C6H5F	266-267
C6H5NO2	268
C6H6	269-270
C6H6ClN	271-272
C6H6FN	273-274
C6H6N4	275
C6H6O	276-277
C6H7N	278-284
C6H7NO	285-289
C6H7N5O	290
C6H8N2	291-293
C6H9F3O2	294
C6H10	295-297
C6H10F3NO	298
C6H10O	299-300

C6H11N	300
C6H11NO	301-302
C6H12	303-306
C6H12N2	307-308
C6H12O	308
C6H12O2	309
C6H13N	310-312
C6H14O	312-314
C6H14S	315-316
C6H15N	317-321
C6H16N2	322-323
C6H17NSi	324
C7H5ClO	325
C7H5D3	326
C7H5FO	327-328
C7H5N	329
C7H6O	330
C7H7NO	331-332
C7H8	333-336
C7H8O	337
C7H9N	338-346
C7H9NO	347-349
C7H10	350
C7H10N2	351
C7H12	352-353
C7H13N	354-355
C7H17N	355-357
C7H18N2	358
C8H4D6	359
C8H5F3O	360
C8H5NO	361
C8H8	362
C8H3O	363-364
C8H8O2	365-366
C8H10	367-373
C8H11N	374-376
C8H13S	377
C8H19N	378-382
C8H20N2	383
C9H9Cl	384
C9H9F	385
C9H9N	386
C9H10	387
C9H12	388-392
C9H12N2O6	393
C9H13N	394-395
C9H13N3O5	396
C9H14N2O6	397
C9H15N	398
C9H21N	399-400
C10H8	401
C10H9F3	402
C10H10Fe	403
C10H12	404
C10H12N4O4	405
C10H12O	406
C10H13N	407

C10H13N5	408
C10H13N5O4	409
C10H14	410-413
C10H14N2O5	414
C10H15N	415
C10H19N	416
C10H23N	417
C10H24N2	418
C11H13N	419
C11H15N	420
C12H11N	421
C12H16N2O6	422
C12H18	423
C12H19N	424
C12H27N	425
C13H100	426
C13H130P	427
C13H17N5O5	428
C13H21N	429
C14H12	430
C14H150P	431
C15H170P	432-433
C16H190P	434-435
C17H210P	436
C18H15N	437
C22H310P	438
Ca	439
ClH	440
CsHO	441
D2	441-442
D2O	442
FH	443
FO	444
F3N	445
F6S	446
HI	447
HKO	448
HLiO	448
HNaO	449
H2	449-451
H2O	451-453
H2S	454-456
H2Se	457
H3N	458-461
H3P	462-464
H4N2	464
H4Si	465
He	465-466
Kr	466-467
Mg	467
Mg2	468
NO	469
N2	470
N2O	471
O2	471-472
O3S	473
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Xe

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Acetic acid, trifluoro- (8CI9CI)	46-47	
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Acetic acid, trifluoro-, ethyl ester (8CI9CI)		151
Acetic acid, trifluoro-, methyl ester (8CI9CI)		97
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Acetonitrile, (methylamino)- (8CI9CI)		111
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3-Amino-1-(dimethylamino)propane	244
3-Amino-1-propene	126
6-Amino-1H-purine	214
4-Amino-2(1H)-pyrimidinone	155
4-Amino-2-hydroxypyrimidine	155
1-Amino-2-methoxybenzene	347
2-Amino-2-methylbutane	239
1-Amino-2-methylpropane	196
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1-Amino-3-(dimethylamino)propane	244
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1-Aminoethane	90
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Aminohexahydrobenzene	310-311
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Aminopropionitrile	111	
3-Aminopropionitrile	111	
3-Aminopropylene	126	
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Benzenamine, 3-methoxy- (9CI)		349
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Benzene, 1-methoxy-4-(1-methylethenyl)- (9CI)		406
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Benzene, 1,2-difluoro- (9CI)	254	
Benzene, 1,2-dimethyl- (9CI)	367-368	
Benzene, 1,2,3,4-tetrafluoro- (8CI9CI)		249
Benzene, 1,2,3,5-tetrafluoro- (8CI9CI)		250
Benzene, 1,2,4-trifluoro- (8CI9CI)	251	
Benzene, 1,2,4,5-tetrafluoro- (8CI9CI)		248
Benzene, 1,3-difluoro- (9CI)	255-256	
Benzene, 1,3-dimethyl- (9CI)	373	
Benzene, 1,3,5-trifluoro- (8CI9CI)		252-253
Benzene, 1,3,5-trimethyl- (9CI)	392	
Benzene, 1,4-(dimethyl-d3)-	359	
Benzene, 1,4-difluoro- (9CI)	257	
Benzene, 1,4-dimethyl- (9CI)	372	
Benzenecarbonal	330	
Benzenecarboxaldehyde	330	
m-Benzenediamine	293	
o-Benzenediamine	291	
p-Benzenediamine	292	
1,2-Benzenediamine (9CI)	291	
1,3-Benzenediamine (9CI)	293	
1,4-Benzenediamine (9CI)	292	
Benzenemethanamine (9CI)	338	
Benzenol	276	
Benzofur D	292	
Benzoic acid nitrile	329	
Benzoic acid, methyl ester (8CI9CI)		365
Benzoic aldehyde	330	
Benzol	269-270	
Benzole	269-270	
Benzonitrile (8CI9CI)	329	
Benzonitrile, p-formyl-	361	
Benzonitrile, 4-formyl- (9CI)		361
Benzophenone (8CI)	426	
Benzoquinuclidine	419	
Benzoyl methide	363	
Benzoylbenzene	426	
Benzylamine (8CI)	338	
Bicarburretted hydrogen	59	
Bicyclo[2.2.1]hept-2-ene (9CI)		350
Bicyclo[2.2.1]heptene	350	
Bicyclo[2.2.2]-1,4-diazaoctane		307-308
Bicyclo[5.3.0]decapentaene	401	
Bilorin	23-25	
Bimethyl	79-80	
Bis(.eta.-cyclopentadienyl)iron		403
Bis(cyclopentadienyl)iron	403	
1,4-Bis(dimethylamino)butane	383	
1,2-Bis(dimethylamino)ethane	322	
1,6-Bis(dimethylamino)hexane	418	
1,3-Bis(dimethylamino)propane		358
Bis(methyl-d3) ether	44	
Bis(1-methylpropyl)amine	380	

N,N-Bis(2-methylpropyl)amine	378	
Bis[(dimethylamino)methyl]methane		358
Blausauere	19-20	
Blood-coagulation factor IV	439	
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Boniton	409	
Borane, difluoro- (8CI9CI)	3	
Borane, trifluoro- (9CI)	4	
Borazine (8CI9CI)	7	
.beta.-Borazinyl radical	6	
Borazole	7	
Borazyne, cyclic trimer	7	
Boron fluoride	4	
Boron fluoride (BF ₃) (8CI)	4	
Boron fluoride hydride (BHF ₂)		3
Boron hydride (B ₂ H ₆)	5	
Boron hydride (B ₄ H ₁₀)	9	
Boron trifluoride	4	
Bromic ether	69	
Bromine cyanide	12	
Bromine cyanide (BrCN)	12	
Bromocyan	12	
Bromocyanide	12	
Bromocyanide (BrCN)	12	
Bromocyanogen	12	
Bromoethane	69	
Bromomethane	25	
Butafume	200	
Butal	172	
Butaldehyde	172	
n-Butan-1-ol	191	
n-Butanal	172	
Butanal (9CI)	172	
Butanaldehyde	172	
1-Butanamine (9CI)	197	
2-Butanamine (9CI)	200	
2-Butanamine, N-(1-methylpropyl)- (9CI)		380
1-Butanamine, N-butyl- (9CI)	379	
1-Butanamine, N,N-dibutyl- (9CI)	425	
2-Butanamine, 2-methyl- (9CI)	239	
1-Butanamine, 4,4,4-trifluoro- (9CI)		167
n-Butane	187	
Butane .alpha.,.delta.-oxide	171	
Butane (8CI9CI)	187	
Butane, 1-cyano-	222	
Butane, 1,4-epoxy-	171	
1,4-Butanediamine (8CI9CI)	201	
1,4-Butanediamine, N,N,N',N'-tetramethyl- (8CI9CI)		383
Butanenitrile (9CI)	159	
tert-Butanethiol	193	
n-Butanol	191	
t-Butanol	192	
tert-Butanol	192	
Butanol	191	
1-Butanol (9CI)	191	
Butanone	170	
2-Butanone (8CI9CI)	170	

2-Butanone, 3-methyl- (8CI9CI)	229	
2-Butanone, 3,3-dimethyl- (8CI9CI)		308
.alpha.-Butene	160	
(E)-2-Butene	165	
(Z)-2-Butene	163	
cis-Butene	163	
cis-2-Butene	163	
iso-Butene	161-162	
trans-Butene	165	
trans-2-Butene	165	
2-trans-Butene	165	
1-Butene (8CI9CI)		160
Butene-1	160	
2-Butene, (E)- (8CI9CI)		165
2-Butene, (Z)- (8CI9CI)		163
1-Butene, 2-ethyl-	303	
1-Butene, 2-methyl- (8CI9CI)		224-225
2-Butene, 2-methyl- (8CI9CI)		223
n-Butyl alcohol	191	
tert-Butyl alcohol (8CI)		192
Butyl alcohol (8CI)		191
n-Butyl aldehyde	172	
Butyl aldehyde	172	
Butyl cyanide	222	
tert-Butyl ethyl ether		314
n-Butyl formate	232	
Butyl formate	232	
Butyl hydroxide	191	
tert-Butyl mercaptan		193
tert-Butyl methyl ether		237
tert-Butyl methyl ketone		308
tert-Butyl sulfide (8CI)		377
Butyl trifluoroacetate		294
i-Butylamine	196	
iso-Butylamine		196
n-Butylamine	197	
t-Butylamine	195	
2-Butylamine	200	
sec-Butylamine (8CI)		200
tert-Butylamine (8CI)		195
Butylamine (8CI)	197	
Butylamine, 4,4,4-trifluoro- (8CI)		167
n-Butylbenzene	412-413	
t-Butylbenzene	410-411	
tert-Butylbenzene		410-411
Butylbenzene	412-413	
tert-Butyldimethylamine		321
.alpha.-Butylene	160	
.gamma.-Butylene	161-162	
cis-Butylene	163	
1-Butylene	160	
Butylenediamine	201	
1,4-Butylenediamine		201
Butylenimine	182	
t-Butylmercaptan	193	
tert-Butylthiol	193	
N-Butyltrifluoroacetamide		298

Butyral	172	
iso-Butyraldehyde		169
n-Butyraldehyde	172	
Butyraldehyde (8CI)		172
Butyric aldehyde	172	
n-Butyronitrile	159	
Butyronitrile (8CI)		159
Butyrylaldehyde	172	
Butyrylonitrile	159	
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C.I. Azoic Coupling Component	107	340
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C.I. 76060	292	
Cadaverine	245	
Calcium (8CI9CI)	439	
Campilit	12	
Carbacryl	99	
Carbamic acid, dimethyl-, ethyl ester (8CI9CI)		235
Carbinamine	36-37	
Carbinol	32-34	
Carbolic acid	276	
Carbomethene	50	
Carbon bisulfide	42	
Carbon bisulphide	42	
Carbon chloride (CCl ₂)		14-15
Carbon difluoride	16	
Carbon dioxide (8CI9CI)		40-42
Carbon disulfide (8CI9CI)		42
Carbon disulphide	42	
Carbon fluoride (CF ₂)	16	
Carbon fluoride (CF ₄)	17	
Carbon fluoride hydride (CF ₂ H ₂)		20
Carbon hydride nitride (CHN)		19-20
Carbon monoxide (8CI9CI)	39	
Carbon oxide (CO)	39	
Carbon oxide (CO ₂)	40-42	
Carbon sulfide (CS ₂)	42	
Carbon tetrafluoride (8CI)		17
Carbon trifluoride	18	
Carbonic acid gas	40-42	
Carbonic acid, dimethyl ester (8CI9CI)		124
Carbonic acid, ethyl methyl ester (8CI9CI)		181
Carbonic anhydride	40-42	
Carbonocyanidic acid, ethyl ester (9CI)		154
Carbonothioic acid, S-ethyl O-methyl ester (9CI)		180
Carboxyethane	119	

Caustic potash	448	
Caustic soda	449	
Cesium hydroxide (8CI9CI)		441
Chelen	70	
Chloroacetic acid	51	
Chloroacetonitrile		47
Chlorene	70	
Chlorethyl	70	
Chloridum	70	
Chlorine cyanide	13	
Chlorine cyanide (ClCN)		13
p-Chloro-.alpha.-methylstyrene		384
4-Chloro-.alpha.-methylstyrene		384
4-Chloro-1-aminobenzene	271	
1-Chloro-2-cyanoethane	103	
1-Chloro-4-isoproprenylbenzene		384
6-Chloro-9H-purine	203	
.alpha.-Chloroacetic acid		51
Chloroacetic acid	51	
.alpha.-Chloroacetonitrile		47
Chloroacetonitrile		47
2-Chloroacetonitrile	47	
m-Chloroaniline	272	
p-Chloroaniline	271	
3-Chloroaniline	272	
4-Chloroaniline	271	
p-Chlorobenzaldehyde	325	
4-Chlorobenzaldehyde	325	
3-Chlorobenzenamine	272	
4-Chlorobenzenamine	271	
Chlorobenzene	264-265	
Chlorocyan	13	
Chlorocyanide	13	
Chlorocyanide (ClCN)		13
Chlorocyanogen	13	
Chloroethane	70	
Chloroethanoic acid	51	
Chlorohydric acid	440	
Chloromethane	26-27	
Chloromethyl cyanide	47	
2-(p-Chlorophenyl)propene		384
2-(4-Chlorophenyl)propene		384
m-Chlorophenylamine	272	
p-Chlorophenylamine	271	
3-Chloropropanenitrile		103
3-Chloropropanonitrile		103
.beta.-Chloropropionitrile		103
3-Chloropropionitrile		103
6-Chloropurine	203	
.alpha.-Chloropyridine		204
.gamma.-Chloropyridine		206
m-Chloropyridine	205	
o-Chloropyridine	204	
2-Chloropyridine	204	
3-Chloropyridine	205	
4-Chloropyridine	206	
Chleryl	70	

Chloryl Anesthetic	70	
Cinnamene	362	
Cloretilo	70	
Clorius	365	
Coal naphtha	269-270	
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Cratagine	366	
Cumene (8CI)	388-389	
Cumol	388-389	
Curafume	25	
1-Cyano-1-methylethane		158
Cyanoacetonitrile	96	
p-Cyanobenzaldehyde	361	
4-Cyanobenzaldehyde	361	
Cyanobenzene	329	
Cyanobromide	12	
1-Cyanobutane	222	
Cyanocyclopropane		153
Cyanoethane	104	
.beta.-Cyanoethylamine		111
2-Cyanoethylamine	111	
Cyanoethylene	99	
Cyanogen bromide (BrCN)	12	
Cyanogen bromide (8CI9CI)		12
Cyanogen chloride (ClCN)	13	
Cyanogen chloride (8CI9CI)		13
Cyanogen monobromide	12	
Cyanomethane	56-57	
N-(Cyanomethyl)dimethylamine		168
Cyanomethylamine	62	
1-Cyanopropane	159	
2-Cyanopropane	158	
.gamma.-Cyanopyridine		261
2-Cyanopyridine	263	
3-Cyanopyridine	262	
4-Cyanopyridine	261	
Cyanotrichloromethane	43	
Cyclohexanamine (9CI)	310-311	
Cyclohexanone (8CI9CI)	299	
Cyclohexatriene	269-270	
Cyclohexene, 1-methyl- (8CI9CI)		352
Cyclohexylamine (8CI)	310-311	
Cyclooxabutane	117	
Cyclopentacycloheptene	401	
Cyclopentane, methylene- (8CI9CI)		296
Cyclopentene, 1-methyl- (8CI9CI)	295	
Cyclopentene, 1,2-dimethyl- (8CI9CI)		353
Cyclopentimine	233-234	
9-Cyclopentyladenine	408	
Cyclopropane (8CI9CI)	106	
Cyclopropane, (1-methylethenyl)- (9CI)		297
Cyclopropane, ethenyl- (9CI)	218	
Cyclopropane, methyl- (8CI9CI)		164

Cyclopropane, vinyl- (8CI)	218	
Cyclopropanecarbonitrile (8CI9CI)	153	
Cyclopropanecarboxylic acid, methyl ester (8CI9CI)		221
Cyclopropanenitrile	153	
Cyclopropene (8CI9CI)	102	
Cyclopropyl cyanide	153	
Cyclopropyl methyl ketone		219
2-Cyclopropyl-1-propene	297	
Cyclopropylethylene	218	
Cyclopropylnitrile	153	
2-Cyclopropylpropene	297	
Cyclotetramethylene oxide		171
Cyd	396	
Cymonic acid	54	
Cypentil	233-234	
Cyt	155	
Cytidine (9CI)	396	
Cytosine (8CI)	155	
Cytosine riboside		396
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Decahydrotetraborane		9
Decanamine	417	
1-Decanamine (9CI)		417
n-Decylamine	417	
1-Decylamine	417	
Decylamine (8CI)	417	
Dehydro-p-cymene	404	
Demsodrox	87	
Denatured ethanol		82-83
Deoxythymidine	414	
2'-Deoxythymidine		414
Deuterium (8CI9CI)		441-442
Deuterium oxide	442	
Deuterium oxide (D20)		442
Developer C	293	
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Devoton	120-121	
Dew Pearl	215	
Di-.pi.-cyclopentadienyl iron		403
Di-n-butylamine	379	
Di-n-propyl ether		313
Di-n-propylamine	320	
Di-sec-butylamine (8CI)		380
Di-t-Butylamine	382	
Di-tert-butyl sulfide		377
Di-tert-butylamine (8CI)		382
2,6-Di-tert-butylpyridine		429
Di-2-propenylamine	300	

Di-2-propynylamine (8CI)	284	
Di-2,4-cyclopentadien-1-yliron		403
Diacetylmethane	220	
Diallyl ether	300	
Diallylamine (8CI)	300	
1,6-Diamino-n-hexane	323	
m-Diaminobenzene	293	
o-Diaminobenzene	291	
p-Diaminobenzene	292	
1,2-Diaminobenzene	291	
1,3-Diaminobenzene	293	
1,4-Diaminobenzene	292	
1,4-Diaminobutane	201	
1,2-Diaminoethane	94	
1,6-Diaminohexane	323	
1,5-Diaminopentane	245	
1,3-Diaminopropane	143	
1,2-Diazabenzene	145	
1,3-Diazabenzene	146	
1,4-Diazabenzene	147	
1,4-Diazabicyclo[2.2.2]octane (8CI9CI)		307-308
1,4-Diazacyclohexane	188	
Diazene, dimethyl-, (E)- (9CI)	81	
m-Diazine	146	
p-Diazine	147	
1,2-Diazine	145	
1,3-Diazine	146	
1,4-Diazine	147	
Diazirine	21	
Diazomethane	21	
Diborane	5	
Diborane (B ₂ H ₆)	5	
Diborane(6) (8CI9CI)	5	
Diboron hexahydride	5	
Dibutylamine (8CI)	379	
Dichlorocarbene	14-15	
Dichloromethylene	14-15	
Dicyanomethane	96	
Dicyclopentadienyliron		403
Dideuterium oxide	442	
Dietary calcium	439	
Diethyl	187	
Diethyl ether	189-190	
Diethyl ketone	225	
Diethyl oxide	189-190	
Diethyl sulfide	194	
N,N-Diethylamine	198	
Diethylamine (8CI)	198	
Diethylamine, N-methyl- (8CI)		240
Diethylamine, 1-methyl- (8CI)		243
N,N-Diethylaminobenzene	415	
Diethylaniline	415	
N,N-Diethylaniline	415	
Diethylene dioxide	175	
1,4-Diethylene dioxide	175	
Diethylene ether	175	
Diethylene imidoxide	184	

Diethylene oxide	175	
Diethylene oximide	184	
Diethylenediamine	188	
Diethyleneimine	188	
Diethylenimide oxide	184	
Diethylmethanamine	240	
N,N-Diethylmethanamine	240	
Diethylphenylamine	415	
Diethylpropylamine	356	
Diethylthioether	194	
m-Difluorobenzene	255-256	
o-Difluorobenzene	254	
p-Difluorobenzene	257	
1,2-Difluorobenzene	254	
1,3-Difluorobenzene	255-256	
1,4-Difluorobenzene	257	
Difluoroborane	3	
Difluorocarbene	16	
2,2-Difluoroethanol	60	
cis-1,2-Difluoroethene	49	
trans-1,2-Difluoroethene	49	
1,1-Difluoroethene	48	
2,2-Difluoroethylamine	72	
(E)-1,2-Difluoroethylene	49	
cis-Difluoroethylene	49	
cis-1,2-Difluoroethylene	49	
trans-Difluoroethylene	49	
trans-1,2-Difluoroethylene	49	
1,1-Difluoroethylene	48	
Difluoromethane	20	
Difluoromethylene	16	
Difluoromethylene radical	16	
Difluorocarbene	16	
3,4-Dihydro-2H-1,4-ethanoquinoline	419	
1,6-Dihydro-6-iminopurine	214	
3,6-Dihydro-6-iminopurine	214	
Dihydrogen monosulfide	454-456	
Dihydrogen selenide	457	
Dihydrogen sulfide	454-456	
Dihydrooxirene	65	
Dihydrouridine	397	
5,6-Dihydrouridine	397	
2,4-Dihydroxy-5-methylpyrimidine	216	
2,4-Dihydroxypyrimidine	149	
Diisobutylamine (8CI)	378	
Diisopropyl ether	312	
Diisopropyl oxide	312	
Diisopropyl sulfide	316	
Diisopropylamine (8CI)	317	
Diisopropylethylamine	381	
N,N-Diisopropylethylamine	381	
Dilute hydrochloric acid	440	
Dimazin	93	
Dimazine	93	
Dimethyl	79-80	
Dimethyl carbonate	124	
Dimethyl ether	84-86	

Dimethyl ketone	112-114	
Dimethyl monosulfide	89	
Dimethyl oxide	84-86	
Dimethyl sulfide	89	
Dimethyl sulfoxide	87	
Dimethyl sulphoxide	87	
Dimethyl thioether	89	
N,N-Dimethyl-m-methylaniline	394	
Dimethyl-m-toluidine	394	
N,N-Dimethyl-m-toluidine	394	
Dimethyl-tert-butylamine	321	
N,N-Dimethyl-tert-butylamine	321	
N,N-Dimethyl-N-(3-aminopropyl)amine		244
1,2-Dimethyl-1-cyclopentene	353	
N,N-Dimethyl-1,3-diaminopropane		244
N,N-Dimethyl-1,3-propanediamine		244
N,N-Dimethyl-1,3-propylenediamine		244
3,3-Dimethyl-2-butanone	308	
2,2-Dimethyl-3-butanone	308	
N,N-Dimethyl-3-methylaniline	394	
2,4-Dimethyl-3-thiapentane	316	
N,N-Dimethyl-4-aminopyridine	351	
N,N-Dimethyl-4-pyridinamine	351	
Dimethylacetamide	185	
N,N-Dimethylacetamide	185	
Dimethylacetone	225	
Dimethylamide acetate	185	
Dimethylamine (8CI)	91-92	
4-Dimethylaminepyridine	351	
3-(Dimethylamino)-1-propanamine		244
3-(Dimethylamino)-1-propylamine		244
(Dimethylamino)acetonitrile	168	
(Dimethylamino)benzene	375-376	
[(Dimethylamino)methyl]trimethylsilane		324
3-(Dimethylamino)propylamine	244	
.gamma.-(Dimethylamino)pyridine		351
4-(Dimethylamino)pyridine	351	
1-Dimethylamino-3-aminopropane		244
2-Dimethylaminopropane	241	
.gamma.-Dimethylaminopropylamine		244
Dimethylaniline	375-376	
N,N-Dimethylaniline	375-376	
m-Dimethylbenzene	373	
o-Dimethylbenzene	367-368	
p-Dimethylbenzene	372	
1,2-Dimethylbenzene	367-368	
1,3-Dimethylbenzene	373	
1,4-Dimethylbenzene	372	
2,2-Dimethylbutanone	308	
3,3-Dimethylbutanone	308	
Dimethylcarbinol	131-132	
1,2-Dimethylcyclopentene	353	
(E)-Dimethyldiazene	81	
Dimethylene oxide	65	
Dimethylenediamine	94	
Dimethylenemethane	101	
Dimethylenimine	74-75	

1,1-Dimethylethanethiol	193	
1,1-Dimethylethanol	192	
Dimethylethoxyformamide	235	
N,N-Dimethylethylamine	199	
1,1-Dimethylethylamine	195	
Dimethylethylbenzene	410-411	
cis-1,2-Dimethylethylene	163	
trans-1,2-Dimethylethylene	165	
1,1-Dimethylethylene	161-162	
Dimethylformaldehyde	112-114	
Dimethylformamide	129	
N,N-Dimethylformamide	129	
u-Dimethylhydrazine	93	
unsym-Dimethylhydrazine	93	
N,N-Dimethylhydrazine	93	
1,1-Dimethylhydrazine	93	
Dimethylisopropylamine	241	
N,N-Dimethylisopropylamine	241	
Dimethylmethane	130-131	
N,N-Dimethylneopentylamine	357	
Dimethylphenylamine	375-376	
Dimethylphosphine	92	
.alpha.,.alpha.-Dimethylpropylamine	239	239
1,1-Dimethylpropylamine	239	
2,2-Dimethylpropylamine	242	
N,N-Dimethylpropylenediamine	244	
.alpha.,.alpha.'-Dimethylpyridine	344	344
.alpha.,.gamma.-Dimethylpyridine	343	343
2,4-Dimethylpyridine	343	
2,5-Dimethylpyridine	345	
2,6-Dimethylpyridine	344	
3,5-Dimethylpyridine	346	
.alpha.,p-Dimethylstyrene	404	
.alpha.,4-Dimethylstyrene	404	
p,.alpha.-Dimethylstyrene	404	
1,1'-Dimethyltriethylamine	381	
N,N-Dimethyltrimethylenediamine	244	
Dimethyl[2-(dimethylamino)ethyl]amine	322	322
Dimexide	87	
Dinitrogen monoxide	471	
Dinitrogen oxide	471	
1,4-Dioxacyclohexane	175	
p-Dioxan	175	
Dioxan	175	
1,4-Dioxan	175	
Dioxane	175	
p-Dioxane (8CI)	175	
1,4-Dioxane (9CI)	175	
1,4-Dioxin, tetrahydro-	175	
2,4-Dioxopentane	220	
2,4-Dioxopyrimidine	149	
Dioxyethylene ether	175	
Diphenyl ketone	426	
Diphenyl(ethyl)phosphine oxide	431	431
Diphenylamine (8CI)	421	
N,N-Diphenylaniline	437	
1,1-Diphenylethene	430	

.alpha.,.alpha.-Diphenylethylene	430
unsym.-Diphenylethylene	430
Diphenylethylene	430
1,1-Diphenylethylene	430
Diphenylmethanone	426
Diphenylmethylphosphine oxide	427
Dipirartril-tropico	87
Diplogen	441-442
Dipropargyl ether	277
Dipropargyl oxide	277
Dipropargylamine	284
Dipropyl ether	313
Dipropyl oxide	313
Dipropyl sulfide	315
Dipropyl thioether	315
n-Dipropylamine	320
Dipropylamine (8CI)	320
Direct Brown BR	293
Direct Brown GG	293
Dispermine	188
Distilled water	451-453
Dithiocarbonic anhydride	42
Divinylene oxide	150
Divinyleneimine	152
Dolicur	87
Dromisol	87
Dry ice	40-42
Dublofix	70
Durafur Black R	292
Durasorb	87
DDNU	430
DEK	225
DFA	421
DMA	185
DMF	129
DMF (amide)	129
DMFA	129
DMS	89
DMS 70	87
DMS 90	87
DMSO	87
DPA	421
DT	414
DThyd	414
Elayl	59
Elegas	446
Embafume	25
3,6-Endomethylenecyclohexene	350
Epoxyethane	65
1,2-Epoxyethane	65
1,3-Epoxypropane	117
Eraverm	188
Essence of Mirbane	268
Essence of Myrbane	268
ps-Estragole	406
Ethanal	63-65
Ethanamide	75

Ethanamine (9CI)	90		
Ethanamine, N-ethyl- (9CI)	198		
Ethanamine, N-ethyl-N-methyl- (9CI)		240	
Ethanamine, N-ethyl-N-propyl-	356		
Ethanamine, N-ethylidene- (9CI)	183		
Ethanamine, N-methyl- (9CI)	140-141		
Ethanamine, N,N-diethyl- (9CI)	319		
Ethanamine, N,N-dimethyl- (9CI)	199		
Ethanamine, 2-fluoro- (9CI)	80		
Ethanamine, 2-methoxy- (9CI)	141		
Ethanamine, 2,2-difluoro- (9CI)	72		
Ethanamine, 2,2,2-trifluoro- (9CI)		61-62	
Ethanamine, 2,2,2-trifluoro-N-methyl- (9CI)			110
Ethanamine, 2,2,2-trifluoro-N,N-dimethyl- (9CI)			166
Ethane (8CI9CI)	79-80		
Ethane(dithioic)acid, methyl ester		125	
Ethane, (methylthio)- (9CI)	135		
Ethane, bromo- (8CI9CI)	69		
Ethane, chloro- (8CI9CI)	70		
Ethane, fluoro- (8CI9CI)	71		
Ethane, iodo- (8CI9CI)	73		
Ethane, methoxy- (9CI)	133		
Ethane, nitro- (8CI9CI)	77		
Ethane, 1,1'-oxybis- (9CI)		189-190	
Ethane, 1,1'-thiobis- (9CI)		194	
Ethane, 2-ethoxy-1,1,1-trifluoro- (9CI)			157
Ethancarboxylic acid	119		
1,2-Ethanediamine (9CI)	94		
1,2-Ethanediamine, N,N,N',N'-tetramethyl- (9CI)			322
Ethanenitrile	56-57		
Ethanethioic acid, S-methyl ester (9CI)			118
Ethanethiol (8CI9CI)	88		
Ethanoic acid	66-67		
Ethanol (9CI)	82-83		
Ethanol, 2,2-difluoro- (8CI9CI)	60		
Ethanol, 2,2,2-trichloro- (8CI9CI)		52	
Ethanol, 2,2,2-trifluoro- (8CI9CI)		55	
Ethanol, 2,2,2-trifluoro-, formate (9CI)			98
Ethanone, 1-(3-pyridinyl)- (9CI)	331		
Ethanone, 1-(4-pyridinyl)- (9CI)	332		
Ethanone, 1-cyclopropyl- (9CI)	219		
Ethanone, 1-phenyl- (9CI)	363		
2H-1,4-Ethanoquinoline, 3,4-dihydro- (8CI9CI)			419
Ethene (9CI)	59		
Ethene oxide	65		
Ethene, cyclopropyl-	218		
Ethene, fluoro- (9CI)	53		
Ethene, trifluoro- (9CI)	45		
Ethene, 1,1-difluoro- (9CI)		48	
Ethene, 1,2-difluoro-, (E)- (9CI)			49
Ethene, 1,2-difluoro-, (Z)- (9CI)			49
Ethenone (9CI)	50		
Ether	189-190		
Ether chloratus	70		
Ether cyanatus	104		
Ether hydrochloric		70	
Ether muriatic	70		

Ether, ethyl isopropyl (8CI)	236	
Ether, ethyl methyl (8CI)	133	
Ether, ethyl 2,2,2-trifluoroethyl (8CI)		157
Ether, tert-butyl ethyl (8CI)	314	
Ether, tert-butyl methyl (8CI)	237	
Ethiridine	74-75	
Ethoxyethane	189-190	
Ethyl acetate	176-177	
Ethyl acetic ester	176-177	
Ethyl alcohol (8CI)	82-83	
Ethyl aldehyde	63-65	
Ethyl bromide	69	
Ethyl carbinol	132-133	
Ethyl chloride	70	
Ethyl cyanide	104	
Ethyl cyanoformate	154	
Ethyl dimethylcarbamate	235	
Ethyl ethanoate	176-177	
Ethyl ether (8CI)	189-190	
Ethyl fluoride	71	
Ethyl formate	122-123	
Ethyl hydrate	82-83	
Ethyl hydride	79-80	
Ethyl hydrosulfide	88	
Ethyl hydroxide	82-83	
Ethyl iodide	73	
Ethyl isopropyl ether	236	
Ethyl ketone	225	
Ethyl mercaptan	88	
Ethyl methanoate	122-123	
Ethyl methyl carbonate	181	
Ethyl methyl ether	133	
Ethyl methyl ketone	170	
Ethyl methyl sulfide	135	
Ethyl monosulfide	194	
Ethyl nitrate	78	
Ethyl nitrile	56-57	
Ethyl sulfhydrate	88	
Ethyl sulfide (8CI)	194	
Ethyl tert-butyl ether	314	
Ethyl tert-butyl oxide	314	
Ethyl thioalcohol	88	
Ethyl thioether	194	
Ethyl trifluoroacetate	151	
Ethyl N,N-dimethylcarbamate	235	
S-Ethyl O-methyl thiocarbonate		180
N-Ethyl-N-methylaniline	395	
N-Ethyl-N-phenylamine	374	
N-Ethyl-N,N-diisopropylamine	381	
Ethylamine (8CI)	90	
Ethylamine, N-ethylidene- (8CI)	183	
Ethylamine, N-methyl- (8CI)	140-141	
Ethylamine, N,N-dimethyl- (8CI)	199	
Ethylamine, N,N,1-trimethyl- (8CI)		241
Ethylamine, N,N,1,1-tetramethyl- (8CI)		321
Ethylamine, 2-fluoro- (8CI)	80	
Ethylamine, 2-methoxy- (8CI)	141	

Ethylamine, 2,2-difluoro- (8CI)	72	
Ethylamine, 2,2,2-trifluoro- (8CI)		61-62
Ethylamine, 2,2,2-trifluoro-N-methyl- (8CI)		110
Ethylamine, 2,2,2-trifluoro-N,N-dimethyl- (8CI)		166
N-Ethylaminobenzene	374	
Ethylaniline	374	
N-Ethylaniline	374	
N-Ethylbenzenamine	374	
Ethylbenzene	369-371	
Ethylbenzol	369-371	
Ethyl-diisopropylamine	381	
N-Ethyl-diisopropylamine	381	
Ethyl-diphenylphosphine oxide	431	
Ethylene (8CI)	59	
Ethylene oxide (8CI)	65	
Ethylene trifluoride	45	
Ethylene, cyclopropyl-	218	
Ethylene, fluoro- (8CI)	53	
Ethylene, trifluoro- (8CI)	45	
Ethylene, 1,1-difluoro- (8CI)	48	
Ethylene, 1,1-diphenyl- (8CI)	430	
Ethylene, 1,2-difluoro-, (E)- (8CI)	49	
Ethylene, 1,2-difluoro-, (Z)- (8CI)	49	
1,2-Ethylenediamine	94	
Ethylenediamine (8CI)	94	
Ethylenediamine, N,N,N',N'-tetramethyl- (8CI)		322
Ethyleneimine	74-75	
N,N'-endo-Ethylenepiperazine	307-308	
1,4-Ethylenepiperazine	307-308	
1,4-Ethylenepiperidine	354-355	
Ethylenimine (8CI)	74-75	
Ethylethylene	160	
Ethylformic acid	119	
Ethyllic acid	66-67	
Ethylideneethylamine	183	
N-Ethylideneethylamine	183	
Ethylisopropylamine	243	
N-Ethylisopropylamine	243	
Ethylmethylaniline	140-141	
Ethylphenylamine	374	
Ethylthioethane	194	
Exhaust gas	39	
EB	369-371	
EI	74-75	
ETO	65	
Fannoform	21-22	
Fast Orange GC Base	272	
Ferrocene (8CI9CI)	403	
Ferrotsen	403	
Flue gas	39	
Fluorhydric acid	443	
p-Fluoro-.alpha.-methylstyrene	385	
4-Fluoro-.alpha.-methylstyrene	385	
1-Fluoro-4-isopropenylbenzene	385	
Fluoroacetic acid	54	
m-Fluoroaniline	274	
p-Fluoroaniline	273	

3-Fluoroaniline	274	
4-Fluoroaniline	273	
m-Fluorobenzaldehyde	327	
p-Fluorobenzaldehyde	328	
3-Fluorobenzaldehyde	327	
4-Fluorobenzaldehyde	328	
Fluorobenzene	266-267	
Fluoroethane	71	
Fluoroethanoic acid	54	
Fluoroethene	53	
.beta.-Fluoroethylamine		80
2-Fluoroethylamine		80
Fluoroethylene	53	
Fluoroform	18	
Fluoromethane	27	
2-(4-Fluorophenyl)propene		385
p-Fluorophenylamine	273	
p-Fluoropyridine	209	
2-Fluoropyridine	208	
3-Fluoropyridine	207	
4-Fluoropyridine	209	
Fluoryl	18	
Formaldehyde (8CI9CI)		21-22
Formaldehyde solution		21-22
Formaldehyde, gas		21-22
Formalin	21-22	
Formalith	21-22	
Formamide, N-methyl- (8CI9CI)		76
Formamide, N,N-dimethyl- (8CI9CI)		129
Formic acid (8CI9CI)	23-25	
Formic acid, butyl ester (8CI9CI)		232
Formic acid, cyano-, ethyl ester (8CI)		154
Formic acid, ethyl ester (8CI9CI)		122-123
Formic acid, isopropyl ester (8CI)		179
Formic acid, methyl ester (8CI9CI)		67-69
Formic acid, propyl ester (8CI9CI)		173-174
Formic acid, 1-methylethyl ester (9CI)		179
Formic aldehyde	21-22	
Formic anammonide		19-20
Formisoton	23-25	
Formol	21-22	
Formonitrile	19-20	
p-Formylanisole	366	
p-Formylbenzotrile	361	
4-Formylbenzotrile	361	
N-Formyldimethylamine		129
Formylic acid	23-25	
p-Formyltoluene	364	
Fouramine D	292	
Fourrine D	292	
Fourrine 1	292	
Freon F-23	18	
Freon 14	17	
Freon 23	18	
Freon 290		130-131
Freon 32	20	
Freon 40	26-27	

Freon 41	27		
Freon 600	187		
Fuers Rohr	449		
Fumigrain	99		
Fur Black 41867	292		
Fur Brown 41866	292		
Fur Yellow	292		
Furan (8CI9CI)	150		
Furan, tetrahydro- (8CI9CI)	171		
Furan, tetrahydro-2-methyl- (8CI9CI)	226		
Furanidine	171		
Furfuran	150		
Furro D	292		
Futramine D	292		
Fyde	21-22		
FC 14	17		
T-Gas	65		
Genetron 1132a	48		
Genetron 23	18		
Genetron 32	20		
Gifblaar poison	54		
Glacial acetic acid	66-67		
Glycinenitrile	62		
Glycinenitrile	62		
Glycinonitrile, N-methyl-	111		
Guanin	215		
Guanine (8CI)	215		
Guanine enol	215		
Guanine, 8-methyl- (8CI)	290		
Guanosine, 2',3'-O-(1-methylethylidene)- (9CI)	428		
Guanosine, 2',3'-O-isopropylidene- (8CI)	428		
Halon 1001	25		
Haltox	25		
Hartosol	131-132		
Heavy water	442		
Heavy water-d2	442		
o-Helium	465-466		
p-Helium	465-466		
Helium (8CI9CI)	465-466		
Helium-4	465-466		
Hemostyp	191		
1-Heptanamine (9CI)	355		
n-Heptylamine	355		
Heptylamine (8CI)	355		
Hexafluorobenzene	246		
Hexahydro-s-triazaborine	7		
Hexahydroaniline	310-311		
Hexahydropyrazine	188		
Hexahydropyridine	233-234		
Hexamethylbenzene	423		
Hexamethylenebis(dimethylamine)	418		
Hexamethylenediamine	323		
1-Hexanamine (9CI)	318		
1,6-Hexanediamine (8CI9CI)	323		
1,6-Hexanediamine, N,N,N',N'-tetramethyl- (8CI9CI)	418		
Hexanon	299		
Hexazane	233-234		

n-Hexylamine	318		
1-Hexylamine	318		
Hexylamine (8CI)	318		
1,6-Hexylenediamine		323	
Hyadur	87		
Hydrazine (8CI9CI)		464	
Hydrazine, 1,1-dimethyl- (8CI9CI)			93
Hydriodic acid (8CI9CI)		447	
Hydriodic ether	73		
Hydrobromic acid (8CI9CI)			11
Hydrobromic ether	69		
Hydrochloric acid (8CI9CI)			440
Hydrochloric acid gas		440	
Hydrochloric ether	70		
Hydrochloride	440		
Hydrocyanic acid (8CI9CI)			19-20
Hydrocyanic ether	104		
Hydrofluoric acid (8CI9CI)			443
Hydrofluoric acid gas		443	
Hydrogen (8CI9CI)		449-451	
Hydrogen arsenide		2	
Hydrogen bromide	11		
Hydrogen bromide (HBr)		11	
Hydrogen carboxylic acid		23-25	
Hydrogen chloride	440		
Hydrogen chloride (HCl)		440	
Hydrogen cyanide	19-20		
Hydrogen fluoride	443		
Hydrogen fluoride (HF)		443	
Hydrogen iodide	447		
Hydrogen iodide (HI)		447	
Hydrogen phosphide		462-464	
Hydrogen selenide		457	
Hydrogen selenide (H ₂ Se) (8CI9CI)			457
Hydrogen sulfide	454-456		
Hydrogen sulfide (H ₂ S) (8CI9CI)			454-456
Hydrogen sulphide	454-456		
Hydrogen-2	441-442		
Hydrosulfuric acid	454-456		
Hydrouracil, 1-.beta.-D-ribofuranosyl- (8CI)			397
6-Hydroxy-1H-purine	211		
Hydroxybenzene	276		
(Hydroxymethyl)trichloromethane			52
6-Hydroxypurine	211		
2-Hydroxypyrimidine	148		
Hypnon	363		
Hypnone	363		
Hypoxanthine (8CI)		211	
Hypoxanthine enol		211	
Hypoxanthine, 2-amino-		215	
Hytrol O	299		
HFA	54		
HMDA	323		
Ice	451-453		
Imidazole, 1-methyl- (8CI)		156	
1H-Imidazole, 1-methyl- (9CI)			156
Imidole	152		

Imsol A	131-132		
Infiltrina	87		
Iodoethane	73		
Iodomethane	28		
Iron bis(cyclopentadienide)		403	
Iron carbonyl (Fe(CO) ₅) (8CI)		202	
Iron carbonyl (Fe(CO) ₅), (TB-5-11)- (9CI)			202
Iron dicyclopentadienyl	403		
Iron pentacarbonyl	202		
Iron, bis(.eta.5-2,4-cyclopentadien-1-yl)-			403
Isobrome	25		
.beta.-Isoamylene		223	
.gamma.-Isoamylene		224-225	
1-Isoamylene	224-225		
Isobutanal	169		
2-Isobutanethiol	193		
Isobutene	161-162		
Isobutylamine (8CI)		196	
Isobutylene	161-162		
Isobutyraldehyde (8CI)		169	
Isobutyramide (8CI)		186	
Isobutyric acid, methyl ester (8CI)			231
Isobutyrimidic acid	186		
Isobutyronitrile (8CI)		158	
Isocumene	390-391		
Isohol	131-132		
Isonicotinic acid nitrile		261	
Isonicotinonitrile (8CI)		261	
Isopropanethiol	134		
Isopropanol	131-132		
p-Isopropenylanisole	406		
Isopropenylbenzene	387		
Isopropenylcyclopropane		297	
p-Isopropenyltoluene	404		
4-Isopropenyltoluene	404		
2-Isopropoxypropane	312		
Isopropyl alcohol (8CI)		131-132	
Isopropyl aldehyde	169		
Isopropyl cyanide	158		
Isopropyl ether (8CI)		312	
Isopropyl formate	179		
Isopropyl mercaptan	134		
Isopropyl methyl ketone		229	
Isopropyl nitrile	158		
Isopropyl sulfide (8CI)		316	
Isopropylamine (8CI)	137		
Isopropylamine, N-ethyl-		243	
Isopropylbenzene	388-389		
Isopropyl dimethylamine		241	
Isopropyl diphenylphosphine oxide		432	
Isopropyl formaldehyde	169		
Isopropylformamide	186		
Isopropylidene guanosine	428		
2',3'-Isopropylidene guanosine		428	
2',3'-O-Isopropylidene guanosine		428	
Isopropylidene methylene	161-162		
2',3'-Isopropylidene uridine		422	

2',3'-O-Isopropylideneuridine	422	
Isopropylthiol	134	
Isopurine, ribosyl-	405	
Isothiocyanatomethane	58	
Isothiocyanic acid, methyl ester (8CI)		58
p-Isoxazine, tetrahydro-	184	
Ivalon	21-22	
Izal	276	
Jaysol	82-83	
Jaysol S	82-83	
Kelene	70	
Ketene (8CI)	50	
Ketone, cyclopropyl methyl (8CI)		219
Ketone, methyl 3-pyridyl (8CI)		331
Ketone, methyl 4-pyridyl (8CI)		332
.beta.-Ketopropane	112-114	
Krypton (8CI9CI)	466-467	
Laughing gas	471	
Leuco-4	214	
Levoxine	464	
Liquefied petroleum gas	130-131	
Liquefied petroleum gas	187	
Lithium hydroxide (8CI9CI)		448
Lithium Hydrate	448	
Lumbrical	188	
Luprosil	119	
.alpha.,.alpha.'-Lutidine		344
2,4-Lutidine (8CI)	343	
2,5-Lutidine (8CI)	345	
2,6-Lutidine (8CI)	344	
3,5-Lutidine (8CI)	346	
Lutosol	131-132	
Lysoform	21-22	
LPG	130-131	
LPG	187	
Magnesium (8CI9CI)	467	
Magnesium molecule	468	
Malonic acid dinitrile		96
Malonodinitrile	96	
Malononitrile (8CI)		96
Manxin	416	
Manxine	416	
Marsh gas	30-31	
Mearlmaid	215	
Mellitene	423	
Mercaptoethane	88	
Mercaptomethane	34-35	
2-Mercaptopropane		134
Mesitylene (8CI)	392	
Metacetone	225	
Metacetic acid	119	
Metadiazine	146	
Methacetone	225	
Methacide	333-336	
Methan-d3-amine, N,N-di(methyl-d3)- (9CI)		95
Methanal	21-22	
Methanamine (9CI)	36-37	

Methanamine, N-ethyl-N-methyl-	199	
Methanamine, N-methyl- (9CI)	91-92	
Methanamine, N,N-dimethyl- (9CI)	138-139	
Methanamine, N,N-dimethyl-1-(trimethylsilyl)- (9CI)		324
Methanamine, 1,1,1-trifluoro-N,N-dimethyl-	109	
Methane (8CI9CI)	30-31	
Methane-d3, oxybis- (9CI)	44	
Methane, bromo- (8CI9CI)	25	
Methane, chloro- (8CI9CI)		26-27
Methane, cyano-	56-57	
Methane, diazo- (8CI9CI)	21	
Methane, dicyano-	96	
Methane, difluoro- (8CI9CI)	20	
Methane, ethoxy-	133	
Methane, fluoro- (8CI9CI)	27	
Methane, iodo- (8CI9CI)	28	
Methane, isothiocyanato- (9CI)		58
Methane, nitro- (8CI9CI)	29	
Methane, oxybis- (9CI)	84-86	
Methane, sulfinylbis- (9CI)	87	
Methane, tetrafluoro- (9CI)	17	
Methane, thiobis- (9CI)	89	
Methane, trifluoro- (8CI9CI)	18	
Methanecarbonitrile	56-57	
Methanecarboxamide	75	
Methanecarboxylic acid	66-67	
Methanethiol (8CI9CI)	34-35	
Methanoic acid	23-25	
Methanol (8CI9CI)	32-34	
Methanone, diphenyl- (9CI)	426	
p-Methoxy-.alpha.-methylstyrene		406
4-Methoxy-.alpha.-methylstyrene		406
2-Methoxy-1-aminobenzene	347	
1-Methoxy-2-aminoethane	141	
2-Methoxy-2-methylpropane		237
m-Methoxyaniline	349	
o-Methoxyaniline	347	
p-Methoxyaniline	348	
2-Methoxyaniline	347	
3-Methoxyaniline	349	
4-Methoxyaniline	348	
p-Methoxybenzaldehyde	366	
4-Methoxybenzaldehyde	366	
4-Methoxybenzenamine	348	
Methoxybenzene	337	
4-Methoxybenzeneamine	348	
2-Methoxyethanamine	141	
.beta.-Methoxyethylamine	141	
Methoxyethylamine	141	
2-Methoxyethylamine	141	
Methoxymethane	84-86	
2-(p-Methoxyphenyl)propene	406	
2-(p-Methoxyphenyl)propylene	406	
p-Methoxyphenylamine	348	
.beta.-Methoxypyridine	289	
.gamma.-Methoxypyridine	285	
2-Methoxypyridine	287-288	

3-Methoxypyridine	289	
4-Methoxypyridine	285	
Methyl .beta.-pyridyl ketone		331
Methyl acetate	120-121	
Methyl alcohol	32-34	
Methyl aldehyde	21-22	
Methyl benzenecarboxylate		365
Methyl benzoate	365	
Methyl bromide	25	
Methyl carbonate	124	
Methyl carbonate ((MeO)2CO)		124
Methyl chloride	26-27	
Methyl cyanide	56-57	
Methyl cyclopropanecarboxylate		221
Methyl cyclopropyl ketone		219
Methyl cyclopropylcarboxylate		221
Methyl ether (8CI)	84-86	
(Methyl ether)-d6 (8CI)	44	
Methyl ethyl ether	133	
Methyl ethyl ketone	170	
Methyl ethyl sulfide	135	
Methyl fluoride	27	
Methyl formate	67-69	
Methyl hydride	30-31	
Methyl hydroxide	32-34	
Methyl iodide	28	
Methyl isobutyrate	231	
Methyl isopropyl ketone		229
Methyl isothiocyanate		58
Methyl ketone	112-114	
Methyl mercaptan	34-35	
Methyl methanoate	67-69	
Methyl monosulfide	89	
Methyl mustard oil	58	
Methyl nitrite	30	
Methyl phenyl ether	337	
Methyl phenyl ketone	363	
Methyl pivalate	309	
Methyl propanoate	178	
Methyl propionate	178	
Methyl propylate	178	
Methyl sulfide (8CI)	89	
Methyl sulfocyanate	58	
Methyl sulfoxide (8CI)		87
Methyl tert-butyl ether		237
Methyl tert-butyl ketone		308
S-Methyl thioacetate	118	
Methyl thiocyanate	58	
Methyl thioisocyanate		58
Methyl trifluoride	18	
Methyl trifluoroacetate		97
Methyl trimethylacetate		309
Methyl 2-methylpropanoate		231
Methyl 2-methylpropionate		231
Methyl 3-pyridyl ketone		331
Methyl 4-pyridyl ketone		332
p-Methyl-.alpha.-methylstyrene		404

4-Methyl-.alpha.-methylstyrene	404
N-Methyl-.delta.-valerolactam	301
Methyl-d3 ether	44
N-Methyl-N-ethylamine	140-141
N-Methyl-N-ethylaniline	395
m-Methyl-N,N-dimethylaniline	394
2-Methyl-1-butene	224-225
1-Methyl-1-cyclopentene	295
2-Methyl-1-pentene	306
1-Methyl-1-phenylethylene	387
2-Methyl-1-propene	161-162
1-Methyl-1,2-dihydro-2-pyridinone	286
1-Methyl-2(1H)-pyridinone	286
1-Methyl-2(1H)-pyridone	286
2-Methyl-2-aminopropane	195
3-Methyl-2-butanone	229
2-Methyl-2-butene	223
3-Methyl-2-butene	223
2-Methyl-2-methoxypropane	237
(E)-3-Methyl-2-pentene	304
trans-3-Methyl-2-pentene	304
2-Methyl-2-pentene	305
2-Methyl-2-phenylpropane	410-411
N-Methyl-2-piperidinone	301
1-Methyl-2-piperidinone	301
N-Methyl-2-piperidone	301
1-Methyl-2-piperidone	301
2-Methyl-2-propanethiol	193
2-Methyl-2-propanol	192
3-Methyl-2-propylamine	196
1-Methyl-2-pyridinone	286
N-Methyl-2-pyridone	286
1-Methyl-2-pyridone	286
4-Methyl-3-pentene	305
1-Methyl-4-isopropenylbenzene	404
4-Methyl-4-pentene	306
Methylacetaldehyde	115-116
Methylacetylene	100
Methylamine (8CI)	36-37
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(Methylamino)benzene	339
N-Methylaminoacetonitrile	111
Methylaminoethane	140-141
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p-Methylaniline	340
N-Methylaniline	339
3-Methylaniline	341-342
4-Methylaniline	340
N-Methylaziridine	128
1-Methylaziridine	128
p-Methylbenzaldehyde	364
4-Methylbenzaldehyde	364
m-Methylbenzenamine	341-342
p-Methylbenzenamine	340
N-Methylbenzenamine	339
3-Methylbenzenamine	341-342
4-Methylbenzenamine	340

Methylbenzene	333-336	
Methylbenzol	333-336	
Methylbutanone	229	
Methylcarbinol	82-83	
.alpha.-Methylcyclohexene		352
1-Methylcyclohexene	352	
1-Methylcyclopentene	295	
Methylcyclopropane	164	
5-Methyldeoxyuridine	414	
Methyldiethylamine	240	
N-Methyldiethylamine	240	
Methyldiphenylphosphine oxide		427
Methylene cyanide	96	
Methylene difluoride	20	
Methylene oxide	21-22	
.alpha.-Methylene-diphenylmethane		430
Methylene, dichloro- (8CI9CI)		14-15
Methylene, difluoro- (8CI9CI)		16
Methylenecyclopentane	296	
Methylenedinitrile	96	
1-Methylethanethiol	134	
Methylethylamine	140-141	
N-Methylethylamine	140-141	
1-Methylethylamine	137	
Methylethylene	107-108	
N-Methylethylenimine	128	
1-Methylethylenimine	128	
Methylformamide	76	
N-Methylformamide	76	
8-Methylguanine	290	
N-Methylimidazole	156	
1-Methylimidazole	156	
Methylmethane	79-80	
Methylol	32-34	
Methylolpropane	191	
2-(p-Methylphenyl)propene		404
Methylphenylamine	339	
N-Methylphenylamine	339	
Methylphosphine	38	
N-Methylpiperidine	311-312	
1-Methylpiperidine	311-312	
2-Methylpropanal	169	
2-Methylpropanamide	186	
1-Methylpropanamine	200	
2-Methylpropane nitrile		158
2-Methylpropene	161-162	
.alpha.-Methylpropionaldehyde		169
2-Methylpropionaldehyde		169
2-Methylpropionitrile		158
1-Methylpropylamine	200	
2-Methylpropylamine	196	
6-Methylpurine	275	
.alpha.-Methylpyridine		283
.beta.-Methylpyridine		282
.gamma.-Methylpyridine		281
p-Methylpyridine	281	
2-Methylpyridine	283	

3-Methylpyridine	282	
4-Methylpyridine	281	
N-Methylpyrrolidine	234-235	
1-Methylpyrrolidine	234-235	
.alpha.-Methylstyrene	387	
.alpha.-Methylstyrol	387	
2-Methyltetrahydrofuran	226	
N-Methyltetrahydropyrrole		234-235
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o-Methyltoluene	367-368	
5-Methyluracil	216	
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Molecular hydrogen		449-451
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Mono-n-butylamine	197	
Mono-n-hexylamine	318	
Mono-n-propylamine	139-140	
Monoallylamine	126	
Monoamylamine	238	
Monobenzylamine	338	
Monobromoethane	69	
Monobromomethane	25	
Monobutylamine	197	
Monocarbon difluoride		16
Monochlorethane	70	
Monochloroacetonitrile		47
Monochlorobenzene	264-265	
Monochloroethane	70	
Monochloroethanoic acid		51
Monochloromethane	26-27	
Monochloromethyl cyanide		47
Monoethylamine	90	
Monofluoroacetic acid		54
Monofluorobenzene	266-267	
Monofluoroethane	71	
Monofluoroethylene		53
Monohydroxybenzene		276
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Monoisobutylamine		196
Monoisopropylamine		137
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Monophenol	276	
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Monopyrrole	152	
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Niobe oil	365		
Nitric acid, ethyl ester (8CI9CI)			78
Nitric oxide	469		
Nitric oxide (NO)		469	
Nitro-Sil	458-461		
Nitrobenzene	268		
Nitrobenzol	268		
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Nitroethane	77		
Nitrogen (8CI9CI)		470	
Nitrogen fluoride		445	
Nitrogen fluoride (NF3) (8CI9CI)			445
Nitrogen gas	470		
Nitrogen monoxide		469	
Nitrogen oxide (NO) (8CI9CI)			469
Nitrogen oxide (N2O) (8CI9CI)			471
Nitrogen trifluoride		445	
Nitrogen-14	470		
Nitromethane	29		
4-Nitropyridine		210	
Nitrosyl radical		469	
Nitrous acid, methyl ester (8CI9CI)			30
Nitrous oxide		471	
Norbornene	350		
2-Norbornene (8CI)		350	
Norbornylene	350		
2-Norbornylene		350	
Norcamphene	350		
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Oxacyclohexane	228		
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Oxacyclopentane	171		
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Oxane	65		
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2H-1,4-Oxazine, tetrahydro-			184
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Oxirene, dihydro-	65		
.alpha.-Oxodiphenylmethane			426
.alpha.-Oxoditane	426		
Oxolane	171		
Oxole	150		
Oxomethane	21-22		
6-Oxopurine	211		
2-Oxopyrimidine	148		
Oxybenzene	276		
1,1'-Oxybispropane		313	
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Pentaborane (B5H9)	10		
Pentaborane(9) (8CI9CI)		10	
Pentacarbonyl iron	202		
2,4-Pentadione	220		
Pentafluorobenzene	247		
1,2,3,4,5-Pentafluorobenzene			247
Pentamethylene oxide	228		
Pentamethylenediamine		245	
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Pentanal (9CI)	227		
1-Pentanamine (9CI)	238		
1,5-Pentanediamine (8CI9CI)		245	
2,4-Pentanedione (8CI9CI)		220	
Pentanenitrile (9CI)	222		
3-Pentanone (8CI9CI)	225		
1-Pentene, 2-methyl- (8CI9CI)			306
2-Pentene, 2-methyl- (8CI9CI)			305
2-Pentene, 3-methyl-, (E)- (8CI9CI)			304
n-Pentylamine	238		

1-Pentylamine	238	
tert-Pentylamine (8CI)		239
Pentylamine (8CI)	238	
Perfluoroacetic acid	46-47	
Perfluoroammonia	445	
Perfluorobenzene	246	
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Phenic acid	276	
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Phenyl alcohol	276	
Phenyl chloride	264-265	
Phenyl cyanide	329	
Phenyl fluoride	266-267	
Phenyl hydrate	276	
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Phenyl hydroxide	276	
Phenyl ketone	426	
Phenyl methyl ether	337	
Phenyl methyl ketone	363	
1-Phenyl-1-methylethylene		387
2-Phenyl-1-propene	387	
Phenylamine	278-280	
N-Phenylaniline	421	
1-Phenylbutane	412-413	
1,2-Phenylenediamine	291	
1,3-Phenylenediamine	293	
1,4-Phenylenediamine	292	
m-Phenylenediamine (8CI)	293	
o-Phenylenediamine (8CI)	291	
p-Phenylenediamine (8CI)	292	
Phenylethane	369-371	
1-Phenylethanone	363	
Phenylethene	362	
Phenylethylene	362	
Phenylic acid	276	
Phenylic alcohol	276	
Phenylmethanal	330	
Phenylmethane	333-336	
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N-Phenylmethylamine	339	
N-Phenylpiperidine	420	
1-Phenylpiperidine	420	
1-Phenylpropane	390-391	
2-Phenylpropane	388-389	
2-Phenylpropene	387	
.beta.-Phenylpropylene		387
N-Phenylpyrrolidine	407	
1-Phenylpyrrolidine	407	
.alpha.-Phenylstyrene		430
Phenyltrimethylmethane	410-411	
Phosphine (PH3)	462-464	
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Phosphine oxide, butyldiphenyl-	435	

Phosphine oxide, decanyldiphenyl-	438	
Phosphine oxide, diphenylpropyl-	433	
Phosphine oxide, ethyldiphenyl- (8CI9CI)	431	431
Phosphine oxide, isobutyldiphenyl-	434	
Phosphine oxide, isopropyldiphenyl- (8CI)		432
Phosphine oxide, methyldiphenyl- (8CI9CI)		427
Phosphine oxide, neopentyldiphenyl-	436	
Phosphine, dimethyl- (8CI9CI)	92	
Phosphine, methyl- (8CI9CI)	38	
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Phosphorus trihydride	462-464	
Piazine	147	
.alpha.-Picoline	283	
.beta.-Picoline	282	
.gamma.-Picoline	281	
m-Picoline	282	
o-Picoline	283	
p-Picoline	281	
2-Picoline (8CI)	283	
3-Picoline (8CI)	282	
4-Picoline (8CI)	281	
Picolinic acid nitrile	263	
Picolinonitrile (8CI)	263	
Pimelic ketone	299	
Pimelin ketone	299	
Pinacolin	308	
Pinacoline	308	
Pinacolone	308	
Piperazidine	188	
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Piperazine (8CI9CI)	188	
Piperidine (8CI9CI)	233-234	
Piperidine, 1-methyl- (8CI9CI)	311-312	
Piperidine, 1-phenyl- (8CI9CI)	420	
Piperidine, 2-methoxy-	302	
2-Piperidinone, 1-methyl- (9CI)	301	
2-Piperidone, 1-methyl- (8CI)	301	
Pipersol	188	
Pirod	149	
Pivalic acid, methyl ester (8CI)	309	
Potassa	448	
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Prolamine	182	
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Propadiene	101	
1,2-Propadiene (9CI)	101	
Propaldehyde	115-116	
n-Propan-1-ol	132-133	
n-Propan-2-ol	131-132	
Propanal (9CI)	115-116	
Propanal, 2-methyl- (9CI)	169	
Propanamide, 2-methyl- (9CI)	186	
1-Propanamine (9CI)	139-140	
2-Propanamine (9CI)	137	
2-Propanamine, N-(1-methylethyl)- (9CI)	317	

2-Propanamine, N-(1,1-dimethylethyl)-2-methyl- (9CI)	382
2-Propanamine, N-ethyl- (9CI)	243
2-Propanamine, N-ethyl-N-(1-methylethyl)- (9CI)	381
1-Propanamine, N-propyl- (9CI)	320
1-Propanamine, N,N-diethyl- (9CI)	356
2-Propanamine, N,N-dimethyl- (9CI)	241
1-Propanamine, N,N-dipropyl- (9CI)	399
2-Propanamine, N,N,2-trimethyl- (9CI)	321
1-Propanamine, N,N,2,2-tetramethyl- (9CI)	357
1-Propanamine, 2-methyl- (9CI)	196
2-Propanamine, 2-methyl- (9CI)	195
1-Propanamine, 2-methyl-N-(2-methylpropyl)- (9CI)	378
1-Propanamine, 2,2-dimethyl- (9CI)	242
1-Propanamine, 3,3,3-trifluoro- (9CI)	108
n-Propane	130-131
Propane (8CI9CI)	130-131
.alpha.,.gamma.-Propane oxide	117
Propane, 1,1'-oxybis- (9CI)	313
Propane, 1,1'-thiobis- (9CI)	315
Propane, 1,3-epoxy-	117
Propane, 2-ethoxy- (9CI)	236
Propane, 2-ethoxy-2-methyl- (9CI)	314
Propane, 2-methoxy-2-methyl- (9CI)	237
Propane, 2,2'-oxybis- (9CI)	312
Propane, 2,2'-thiobis- (9CI)	316
Propane, 2,2'-thiobis[2-methyl- (9CI)]	377
1,3-Propanediamine (8CI9CI)	143
1,3-Propanediamine, N,N-dimethyl- (8CI9CI)	244
1,3-Propanediamine, N,N,N',N'-tetramethyl- (8CI9CI)	358
Propanedinitrile (9CI)	96
Propanenitrile (9CI)	104
Propanenitrile, 2-methyl- (9CI)	158
Propanenitrile, 3-amino- (9CI)	111
Propanenitrile, 3-chloro- (9CI)	103
Propanethiol	134
1-Propanethiol (8CI9CI)	134
2-Propanethiol (8CI9CI)	134
2-Propanethiol, 2-methyl- (8CI9CI)	193
Propanoic acid (9CI)	119
Propanoic acid, methyl ester (9CI)	178
Propanoic acid, 2-methyl-, methyl ester (9CI)	231
Propanoic acid, 2,2-dimethyl-, methyl ester (9CI)	309
n-Propanol	132-133
1-Propanol (9CI)	132-133
2-Propanol (9CI)	131-132
2-Propanol, 2-methyl- (9CI)	192
Propanone	112-114
2-Propanone (9CI)	112-114
2-Propanone, acetyl-	220
Propargyl ether	277
Propargylamine	105
2-Propen-1-amine (9CI)	126
2-Propen-1-amine, N-2-propenyl- (9CI)	300
2-Propen-1-amine, N,N-di-2-propenyl- (9CI)	398
Propene (8CI)	107-108
1-Propene (9CI)	107-108
Propene, 2-cyclopropyl- (8CI)	297

Propene, 2-methyl- (8CI)	161-162	
1-Propene, 2-methyl- (9CI)	161-162	
1-Propene, 2-phenyl-	387	
1-Propene, 3,3'-oxybis- (9CI)		300
Propenenitrile	99	
2-Propenenitrile (9CI)	99	
Propine	100	
Propional	115-116	
Propionaldehyde (8CI)	115-116	
Propione	225	
Propionic acid (8CI)	119	
Propionic acid, methyl ester (8CI)		178
Propionic aldehyde	115-116	
Propionic nitrile	104	
Propionitrile (8CI)	104	
Propionitrile, 3-amino- (8CI)		111
Propionitrile, 3-chloro- (8CI)		103
Propionitrile	104	
Propol	131-132	
n-Propyl acetate	230	
Propyl acetate	230	
1-Propyl acetate	230	
n-Propyl alcohol	132-133	
sec-Propyl alcohol	131-132	
Propyl alcohol (8CI)	132-133	
Propyl carbinol	191	
Propyl cyanide	159	
Propyl ether (8CI)	313	
n-Propyl formate	173-174	
Propyl formate	173-174	
Propyl hydride	130-131	
n-Propyl mercaptan	134	
Propyl mercaptan	134	
Propyl methanoate	173-174	
Propyl monosulfide	315	
Propyl sulfide (8CI)	315	
Propyl trifluoroacetate		217
Propylaldehyde	115-116	
n-Propylamine	139-140	
sec-Propylamine	137	
1-Propylamine	139-140	
2-Propylamine	137	
Propylamine (8CI)	139-140	
Propylamine, N-tert-butyl-1,1-dimethyl- (8CI)		400
Propylamine, N,N-diethyl- (8CI)	356	
Propylamine, N,N,2,2-tetramethyl- (8CI)		357
Propylamine, 3,3,3-trifluoro- (8CI)	108	
n-Propylbenzene	390-391	
Propylbenzene	390-391	
1-Propylbenzene	390-391	
Propylene	107-108	
1-Propylene	107-108	
1,3-Propylene oxide	117	
1,3-Propylenediamine	143	
1,3-Propylenimine	127	
Propylic alcohol	132-133	
Propylic aldehyde	115-116	

1-Propylmercaptan	134		
2-Propylmercaptan	134		
Propyl nitrile	104		
2-Propyn-1-amine (9CI)	105		
2-Propyn-1-amine, N-2-propynyl- (9CI)		284	
2-Propyn-1-amine, N,N-di-2-propynyl- (9CI)			386
Propyne (8CI)	100		
1-Propyne (9CI)	100		
1-Propyne, 3,3'-oxybis- (9CI)		277	
2-Propynyl ether (8CI)	277		
2-Propynylamine (8CI)	105		
Prozoin	119		
Prussic acid	19-20		
Pseudoacetic acid	119		
Pseudobutylbenzene	410-411		
Pseudoestragole	406		
Pure oxygen	471-472		
9H-Purin-1-amine, 9-cyclopentyl- (9CI)		408	
Purin-6(1H)-one	211		
9H-Purin-6(1H)-one	211		
Purin-6(3H)-one	211		
1H-Purin-6-amine (9CI)	214		
9H-Purin-6-amine, 9-.beta.-D-ribofuranosyl-			409
Purin-6-ol	211		
3H-Purin-6-ol	211		
9H-Purin-6-ol	211		
6H-Purin-6-one, 1,7-dihydro- (9CI)	211		
6H-Purin-6-one, 2-amino-1,7-dihydro- (9CI)		215	
6H-Purin-6-one, 2-amino-1,7-dihydro-8-methyl- (9CI)			290
Purine ribonucleoside	405		
Purine riboside	405		
Purine, 6-chloro- (8CI)	203		
1H-Purine, 6-chloro- (9CI)	203		
Purine, 6-methyl- (8CI)	275		
1H-Purine, 6-methyl- (9CI)	275		
9H-Purine, 9-.beta.-D-ribofuranosyl- (8CI9CI)			405
Purinosine	405		
Putrescin	201		
Putrescine	201		
2H-Pyran, tetrahydro- (8CI9CI)	228		
Pyrazine (8CI9CI)	147		
Pyrazine hexahydride	188		
Pyrazine, hexahydro-	188		
Pyridazine (8CI9CI)	145		
4-Pyridinamine, N,N-dimethyl- (9CI)	351		
Pyridine (8CI9CI)	212-213		
Pyridine, hexahydro-	233-234		
Pyridine, 2-(trifluoromethyl)- (8CI9CI)		258	
Pyridine, 2-chloro- (8CI9CI)	204		
Pyridine, 2-fluoro- (8CI9CI)	208		
Pyridine, 2-methoxy- (8CI9CI)		287-288	
Pyridine, 2-methyl- (9CI)	283		
Pyridine, 2,4-dimethyl- (9CI)	343		
Pyridine, 2,5-dimethyl- (9CI)	345		
Pyridine, 2,6-bis(1,1-dimethylethyl)- (9CI)			429
Pyridine, 2,6-di-tert-butyl- (8CI)	429		
Pyridine, 2,6-dimethyl- (9CI)	344		

Pyridine, 3-(trifluoromethyl)- (8CI)	259	
Pyridine, 3-chloro- (8CI9CI)	205	
Pyridine, 3-fluoro- (8CI9CI)	207	
Pyridine, 3-methoxy- (8CI9CI)	289	
Pyridine, 3-methyl- (9CI)	282	
Pyridine, 3,5-dimethyl- (9CI)	346	
Pyridine, 4-(dimethylamino)- (8CI)	351	
Pyridine, 4-(trifluoromethyl)- (8CI9CI)	260	
Pyridine, 4-chloro- (8CI9CI)	206	
Pyridine, 4-fluoro- (8CI9CI)	209	
Pyridine, 4-methoxy- (8CI9CI)	285	
Pyridine, 4-methyl- (9CI)	281	
Pyridine, 4-nitro- (8CI9CI)	210	
2-Pyridinecarbonitrile (9CI)	263	
3-Pyridinecarbonitrile (9CI)	262	
4-Pyridinecarbonitrile (9CI)	261	
2(1H)-Pyridinone, 1-methyl- (9CI)	286	
2(1H)-Pyridone, 1-methyl- (8CI)	286	
3-Pyridyl methyl ketone	331	
4-Pyridyl methyl ketone	332	
2-Pyridyl nitrile	263	
3-Pyridylcarbonitrile	262	
Pyrimidine (8CI9CI)	146	
2,4-Pyrimidinediol	149	
2,4-Pyrimidinedione	149	
2,4(1H,3H)-Pyrimidinedione (9CI)	149	
2,4(1H,3H)-Pyrimidinedione, dihydro-1-.beta.-D-ribofuranosyl-	397	
2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-.beta.-D-erythro-pentofuranosyl	414	
2,4(1H,3H)-Pyrimidinedione, 5-methyl- (9CI)	216	
2-Pyrimidinol	148	
2-Pyrimidinone	148	
2(1H)-Pyrimidinone (8CI9CI)	148	
2(1H)-Pyrimidinone, 4-amino- (9CI)	155	
2(1H)-Pyrimidinone, 4-amino-1-.beta.-D-ribofuranosyl-	396	
2(1H)-Pyrimidone	148	
2-Pyrimidone	148	
Pyroacetic ether	112-114	
Pyrobenzol	269-270	
Pyrobenzole	269-270	
Pyrod	149	
Pyrrol	152	
Pyrrole (8CI)	152	
1H-Pyrrole (9CI)	152	
Pyrrole, tetrahydro-	182	
Pyrrolidine (8CI9CI)	182	
Pyrrolidine ring	182	
Pyrrolidine, 1-methyl- (8CI9CI)	234-235	
Pyrrolidine, 1-phenyl- (8CI9CI)	407	
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Quinuclidine (8CI)	354-355	
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Renal PF	292	
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.beta.-D-Ribofuranoside, adenine-9	409	
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