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# A Compendium of Gas Phase Basicity and Proton Affinity Measurements

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National Measurement Laboratory
National Bureau of Standards
Department of Commerce
Washington, D.C. 20234

*Ion Energetics Data Center
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Department of Commerce
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**Fein-Marquart Associates
Baltimore, MD 21212

***National Heart Lung and Blood Institute
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U.S. DEPARTMENT OF COMMERCE, Juanita M. Kreps, *Secretary*
Jordan J. Baruch, *Assistant Secretary for Science and Technology*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

# 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 affinites 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

$$M + H^+ \rightarrow MH^+$$

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 kcal = 4.1840 kJ, exactly.

## 1.3 Standard states, conventions, and reference values

The process

$$M + H^+ \rightarrow MH^+$$

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, Cp, 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 $t\text{-}C4H9^+$ 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 $t\text{-}C4H9^+$ (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 $\Delta G$ 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

$$H_2O_2 + h\nu \rightarrow HO_2^+ + H + e$$

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 $HO2^+$, 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 election 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

$$AH^+ + B \rightleftarrows A + BH^+$$

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

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

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 $\Delta S$ 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 $H3^+$ (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 NH3(gas). Lastly, there are a number of empirical correlations of proton affinities with other physical parameters such as core ionization potentials (10).

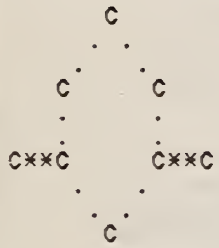
2.5 References

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:

| | |
|---|---|
| C8H10 | CAS REGN : 108-38-3 |
|  | |
| Benzene, 1,3-dimethyl- (9CI)<br>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.,<br>Proton Affinities of Benzene, Toluene, and the Xylenes,<br>J. Am. Chem. Soc. 94, 6630 (1972). | |
| Method used : MS<br>Equilibrium relative to CH3SH and (CH3)2O<br>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<br>Hehre, W. J.,<br>The Proton Affinities of Toluene,<br>J. Am. Chem. Soc. 98, 1990 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium relative to C6H6(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.

M=Q-ZH = HM-Q=Z = H M%%Q%%Z

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 significiant 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.+/-.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<br>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).

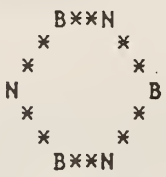
Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

| | |
|---|---|
| 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.,<br>Ion-Molecule Chemistry of BF3 and HBF2 in Hydrogen,<br>Inorg. Chem. 14, 1087 (1975). | |
| Method used : MS<br>Bracketing relative to CH4 and H2. | |

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

| B2H6 | CAS REGN : 19287-45-7 |
|---|---|
| H**B<br>* *<br>* *<br>B**H | |
| Diborane(6) (8CI9CI) | |
| | |
| PA (exp) : 147+/-4 kcal/mol | Temperature : 79-86 K |
| Pierce, R. C., and Porter, R. F.,<br>Low-Temperature Chemical Ionization Mass Spectrometry<br>of Boron Hydrides. The Proton Affinities of Diborane<br>and Tetraborane(10),<br>J. Am. Chem. Soc. 95, 3849 (1973). | |
| Method used : MS<br>Observed reaction C2H9+ + B2H6->2CH4 + B2H7+.<br>Reaction B2H7+ ->B2H5+ + H2 has delta<br>H formation = 3.0+/-.3.<br>Based on delta H formation(B2H5+) = 232. | |

| B3H5N3 | CAS REGN : Not available |
|---|---|

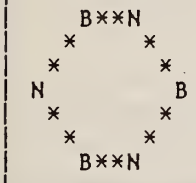


.beta.-Borazinyl radical

| | |
|---|---|
| PA (exp) : 193+/-2 kcal/mol | Temperature : |

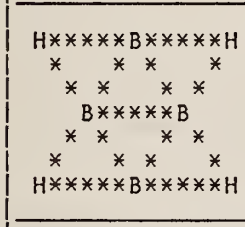
DeStefano, A. J., and Porter, R. F.
Ion-Molecule Reactions of Cyclic Borazine Cations.
Thermodynamic and Kinetic Considerations,
J. Phys. Chem. 80, 2818 (1976).

Method used : MS
Bracketing relative to HCO2C2H5 and (CH3)2CO. The reactant ions are generated by photon impact

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

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

| B4H10 | CAS REGN : 18283-93-7 |
|---|---|



Tetraborane(10) (8CI9CI)

| | |
|---|---|
| PA (exp) : 144+/-5 kcal/mol | Temperature : 140-300 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
Based on delta H formation(B2H5+) and estimating delta S.
Equilibrium of B2H5+ + B2H6 -> B4H11+.

| B5H9 | CAS REGN : 19624-22-7 |
|---|---|

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.,<br>Mass Spectrometric Determination of the Proton<br>Affinities of Various Molecules,<br>J. Phys. Chem. 73, 4328 (1969). | |
| Method used : MS<br>Absolute PA value estimated by assuming that for<br>reaction RH+ + RH -> RH2+ + R; the delta H ~5X TC.<br>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<br>Calculated entropy<br>Equilibrium relative to AsH3, HCO2H and F2CHCH2OH | |

| CC1N | CAS REGN : 506-77-4 |
|---|---|
| N##C**CL | |
| Cyanogen chloride (8CI9CI) | |
| | |
| PA (exp) : 177+/-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<br>Equilibrium relative to F2CH2CH, OH and HCHO | |
| GB (exp) : 169.6+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 177.4+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| | |
|---|---|
| CCl2 | 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.<br>The Proton Affinity of Dichlorocarbene,<br>To be published in J. Am. Chem. Soc. | |
| Method used : ICR<br>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.<br>Reactions of CCl2H+ and CF2H+ with Organic and Inorganic Compounds: Proton Affinities and Heats of Formation of CCl2 and CF2,<br>Intern. J. Mass Spectrom. Ion Phys. 22, 135 (1976). | |
| Method used : ICR<br>Bracketing relative to NH3 and (CH3)2S | |

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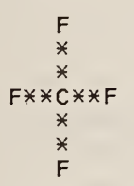
| | |
|---|---|
| GB not calculated for this reference | |
| PA (exp) : 208.3+/-2 kcal/mol | Temperature : 300 K |
| Levi, B. A., Taft, R. W., and Hehre, W. J.<br>Dichlorcarbene,<br>J. Am. Chem. Soc. 99, 8454 (1977). | |
| Method used : ICR<br>Calculated entropy<br>Bracketing relative to CF3CH2CH2NH2 and C6H5NH2;<br>scale based on NH3 | |
| | |
| PA (exp) : 209+/-2 kcal/mol | Temperature : 300 K |
| Levi, B. A., Taft, R. W., and Hehre, W. J.<br>Dichlorocarbene,<br>J. Am. Chem. Soc. 99, 8454 (1977). | |
| Method used : ICR<br>Calculated entropy<br>The deuterium affinity determined by bracketing<br>techniques relative to 2-CF3 Pyridine and<br>CF3(CH2)2NH2; scale based on NH3 | |

| 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.<br>Reactions of CCl2H+ and CF2H+ with Organic and Inorganic Compounds: Proton Affinities and Heats of Formation of CCl2 and CF2,<br>Intern. J. Mass Spectrom. Ion Phys. 22, 135 (1976). | |
| Method used : ICR<br>Bracketing relative to H2S and HCOOH and also observing the following: CD5+ + CF2HCL -> CD4 + DCl + CF2H+ and CD5+ + CF3H -> CD4 + DF + CF2H+. Scale based on PA (H2O) = 170.1 kcal/mol | |

| CF4 | CAS REGN : 75-73-0 |
|---|---|



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<br>*<br>*<br>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<br>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 |
| Freeman, C. G., Harland, P. W., and McEwan, M. J.<br>The Equilibrium H3S+ + HCN = H2CN+ + H2S and the<br>Relative Proton Affinities of HCN and H2S,<br>Intern. J. Mass Spectrom. Ion Phys. 27, 77 (1978). | |
| Method used : FAG<br>Equilibrium relative to H2S; scale based on NH3 | |
| | |
| PA (exp) : 139 kcal/mol | Temperature : |
| Haney, M. A., and Franklin, J. L.,<br>Mass Spectrometric Determination of the Proton Affinities<br>of Various Molecules,<br>J. Phys. Chem. 73, 4328 (1969). | |
| Method used : MS<br>Estimated delta H = 5X translational<br>energy of the product of reaction<br>RH+ + RH -> RH2+ + R | |

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| | |
|---|---|
| GB (exp) : 166.7+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 174.5+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| | |
|---|---|
| CH2F2 | CAS REGN : 75-10-5 |
| F**C**F | |
| Methane, difluoro- (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<br>Bracketing relative to CH3F and CO. Using IP of H and CH2F2, also HA (CH2F2+). | |

| 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.,<br>Gas-Phase Ion Chemistry of Azomethane by Ion Cyclotron Resonance,<br>J. Am. Chem. Soc. 94, 2425 (1972). | |
| Method used : ICR<br>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.,<br>Energetics of Formation of Some Oxygenated Ions and the Proton Affinities of Carbonyl Compounds,<br>Can. J. Chem. 44, 1625 (1966). | |
| Method used : EI<br>Electron impact fragmentation (various molecules). | |

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|---|---|
| | |
| PA (exp) : 169+/-1 kcal/mol | Temperature : 298 K |
| Refaey, K. M. A., and Chupka, W. A.,<br>Photoionization of the Lower Aliphatic Alcohols<br>with Mass Analysis,<br>J. Chem. Phys. 48, 5205 (1968). | |
| Method used : PI<br>Appearance potential by IP fragmentation of CH3OH | |
| | |
| PA (exp) : 170 kcal/mol | Temperature : |
| Lossing, F. P.<br>Heats of Formation of Some Isomeric [CnH2n + 1O]+<br>Ions. Substitutional Effects on Ion Stability,<br>J. Am. Chem. Soc. 99, 7526 (1977). | |
| Method used : EM<br>Electron impact fragmentation (various molecules)<br>using EM. delta Hf(H+) = 365.7 | |
| GB (exp) : 167.2+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 174.6+/-2 kcal/mol | Temperature : 300 K |
| Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M.,<br>McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,<br>Gas Phase Basicities and Relative Proton Affinities of<br>Compounds between Water and Ammonia from Pulsed Ion<br>Cyclotron Resonance Thermal Equilibria Measurements,<br>J. Am. Chem. Soc. 99, 5417 (1977). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| | |
|---|---|
| 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.,<br>Proton Affinities of Some Oxygenated Compounds,<br>J. Am. Chem. Soc. 95, 2427 (1973). | |
| Method used : MS<br>Bracketing relative to CH3OH and H2S. | |
| | |
| PA (exp) : 186.8 kcal/mol | Temperature : |
| Goldenfeld, I. V., Korostyshevsky, I. Z., and<br>Mischanchuk, B. G.,<br>Analysis of Field Ion Energies in a Mass Spectrometer,<br>Int. J. Mass Spectrom. Ion Phys. 13, 297 (1974). | |
| Method used : FI<br>PA derived from field appearance potential. Correction<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| | |
|---|---|
| CH3Br | CAS REGN : 74-83-9 |
| BR*C | |
| 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<br>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.,<br>Proton Affinities of Some Oxygenated Compounds,.<br>J. Am. Chem. Soc. 95, 2427 (1973). | |
| Method used : MS<br>Bracketing relative to H2O. | |
| | |
| PA (exp) : 164+/-3 kcal/mol | Temperature : |
| Haney, M. A., and Franklin, J. L.,<br>Mass Spectrometric Determination of the Proton Affinities<br>of Various Molecules,<br>J. Phys. Chem. 73, 4328 (1969). | |
| Method used : MS<br>Absolute PA value estimated by assuming<br>that for reaction RH+ + RH ->R + RH2+ the<br>delta H ~5X TC.<br>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 CH3CL and HA(CH3CL+). | |

| | |
|---|---|
| CH3F | 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 CH3F and HA of CH3F+. | |

| 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<br>+<br>+<br>O | |
| Methane, nitro- (8CI9CI) | |
| | |
| PA (exp) : ~182 kcal/mol | Temperature : 300 K |
| McAllister, T., and Pitman, P.<br>Ion-Molecule Reactions and Proton Affinities of Methyl Nitrite and Nitromethane,<br>Intern. J. Mass Spectrom. Ion Phys. 19, 241 (1976). | |
| Method used : ICR<br>Bracketing relative to CH3OH and (CH3)2CO | |
| | |
| PA (exp) : 182+/-2 kcal/mol | Temperature : 300 K |
| Kriemler, P., and Buttrill, S. E., Jr.,<br>Ion-Molecule Reactions and the Proton Affinities of the Nitroalkanes. I. Nitro methane and nitroethane,<br>J. Am. Chem. Soc. 95, 1365 (1973). | |
| Method used : ICR<br>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 |
| McAllister, T., and Pitman, P.<br>Ion-Molecule Reactions and Proton Affinities of Methyl Nitrite and Nitromethane,<br>Intern. J. Mass Spectrom. Ion Phys. 19, 241 (1976). | |
| Method used : ICR<br>Bracketing relative to C2H5OH and (CH3)2CO | |

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

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

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

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|---|---|
| | |
| PA (exp) : 182 kcal/mol | Temperature : |
| Haney, M. A., and Franklin, J. L.,<br>Mass Spectrometric Determination of the Proton Affinities<br>of Various Molecules,<br>J. Phys. Chem. 73, 4328 (1969). | |
| Method used : MS<br>Delta H estimated = 5X total translational<br>energy of the products of RH+ + RH -> RH2+ + 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.,<br>Gas-Phase Basicities and Proton Affinities of Compounds<br>between Water and Ammonia and Substituted Benzenes from<br>a Continuous Ladder of Proton Transfer Equilibria<br>Measurements,<br>J. Am. Chem. Soc. 98, 1320 (1976). | |
| Method used : MS<br>Calculated entropy<br>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 |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| | |
|---|---|
| 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 |
| 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<br>Equilibrium; scale based on CH3CHO<br>Entropy change assumed zero | |

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

| | |
|---|---|
| CH5N | CAS REGN : 74-89-5 |
| C**N | |
| Methanamine (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| | |
| PA (exp) : 211 kcal/mol | Temperature : |
| Haney, M. A., and Franklin, J. L.,<br>Mass Spectrometric Determination of the Proton Affinities of Various Molecules,<br>J. Phys. Chem. 73, 4328 (1969). | |
| Method used : MS<br>Estimated delta H = 5X translational energy of the product of reaction RH+ + RH -> RH2+ + 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.<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>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.,<br>Intrinsic Basicities of Ammonia, Methylamines,<br>Anilines, and Pyridine from Gas-Phase Proton-<br>Exchange Equilibria,<br>J. Am. Chem. Soc. 94, 5128 (1972). | |
| Method used : MS<br>Equilibrium; scale based on NH3<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| CO | CAS REGN : 630-08-0 |
|---|---|
| C##O | |
| Carbon monoxide (8CI9CI) | |
| | |
| PA (exp) : 143+/-2 kcal/mol | Temperature : |
| Matthews, C. S., and Warneck, P.,<br>Heats of Formation of CHO+ and C3H3+ by Photoionization,<br>J. Chem. Phys. 51, 854 (1969). | |
| Method used : PI<br>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.,<br>Excess Energies in Mass Spectra of some Oxygen-Containing Organic Compounds,<br>Trans. Faraday Soc. 65, 1794 (1969). | |
| Method used : MS<br>Appearance potential by electron impact from HCOOH, CH3CHO and C2H3CHO. Correction for excess energy. | |

| CO2 | CAS REGN : 124-38-9 |
|---|---|
| O++C++O | |
| Carbon dioxide (8CI9CI) | |
| | |
| PA (exp) : 130.7+/-1 kcal/mol | Temperature : |
| Warneck, P.<br>Heat of Formation of the HCO Radical,<br>Z. Naturforsch. 29, 350 (1974). | |
| Method used : PI<br>Appearance potential by photoionization. delta Hf(H+)<br>= 365.7 | |
| | |
| PA (exp) : 129.1 kcal/mol | Temperature : 298 K |
| Schiff, H. I., and Bohme, D. K.,<br>Flowing Afterglow Studies at York University,<br>Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975). | |
| Method used : FAG<br>Calculated entropy.<br>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.<br>Proton Affinities and Cluster Ion Stabilities in<br>CO2 and CS2. Applications in Martian Ionspheric<br>Chemistry,<br>J. Chem. Phys. 66, 4527 (1977). | |
| Method used : MS<br>Van't Hoff plot<br>Equilibrium; scale based on PA (CH4) = 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.<br>Proton Affinities and Cluster Ion Stabilities in<br>CO2 and CS2. Application in Martian Ionspheric<br>Chemistry,<br>J. Chem. Phys. 66, 4527 (1977). | |
| Method used : MS<br>Calculated entropy<br>The measurements done in the temperature range of<br>400-650K. Using the Hoff plot the delta H and delta S at<br>300K were derived. Using PA (CH4)-126.8 | |

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| | |
|---|---|
| PA (exp) : 123+/-3 kcal/mol | Temperature : 800 K |
| 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). | |
| Method used : FAG<br>Van't Hoff plot<br>Equilibrium relative to N2 and Xe; scale based on PA (N2) = 112.6<br>Van't Hoff plot | |

| | |
|---|---|
| CS2 | 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 |
| Meot-Ner (Mautner), M., and Field, F. H. Proton Affinities and Cluster Ion Stabilities in CO2 and CS2. Applications in Martian Ionspheric Chemistry, J. Chem. Phys. 66, 4527 (1977). | |
| Method used : MS<br>Calculated entropy<br>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 | |

| C2Cl3N | 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 |

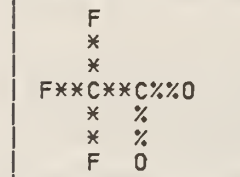
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

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

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

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

| C2HF3O2 | CAS REGN : 76-05-1 |
|---|---|



Acetic acid, trifluoro- (8CI9CI)

| | |
|---|---|
| PA (exp) : 172+/-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 H2S and H2O

| | |
|---|---|
| GB (exp) : 154.7+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 171.9+/-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
Equilibrium; scale based on NH3
Entropy change assumed zero

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| | |
|---|---|
| GB (exp) : 165.1+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 173.3+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| | |
|---|---|
| C2H2ClN | CAS REGN : 107-14-2 |
| CL*C**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 |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

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

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

| C2H2O | CAS REGN : 463-51-4 |
|---|---|
| O++C++C | |
| Ethenone (9CI)<br>Ketene (8CI) | |
| | |
| PA (exp) : 194.1+/-1 kcal/mol | Temperature : 350 K |
| Ausloos, P., and Lias, S. G.<br>The Proton Affinity of Ketene and the Heat of Formation of CH3CO+,<br>Chem. Phys. Letters 51, 53 (1977). | |
| Method used : ICR<br>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.<br>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,<br>J. Am. Chem. Soc. 100, 3478 (1978). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C2H3ClO2 | CAS REGN : 79-11-8 |
|---|---|
| O%%C**C**CL<br>%<br>%<br>O | |
| 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.,<br>Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,<br>J. Am. Chem. Soc. 98, 1320 (1976). | |
| Method used : MS<br>Equilibrium; scale based on NH3<br>Entropy change assumed zero | |

| C2H3Cl3O | 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 |

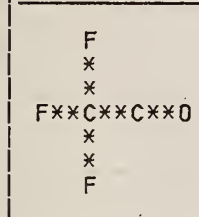
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

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

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

| C2H3FO2 | CAS REGN : 144-49-0 |
|---|---|
| O%%C**C**F<br>%<br>%<br>O | |
| 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.,<br>Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,<br>J. Am. Chem. Soc. 98, 1320 (1976). | |
| Method used : MS<br>Equilibrium; scale based on NH3<br>Entropy change assumed zero | |

| C2H3F3O | CAS REGN : 75-89-8 |
|---|---|



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.,<br>Study of Ion-Molecule Reactions and Reaction Mechanisms in Acetonitrile by Ion Cyclotron Resonance,<br>J. Am. Chem. Soc. 90, 6002 (1968). | |
| Method used : ICR<br>Bracketing relative to CH3CHO and (CH3)2CO | |
| | |
| PA (exp) : 186+/-1 kcal/mol | Temperature : |
| Haney, M. A., and Franklin, J. L.,<br>Mass Spectrometric Determination of the Proton Affinities of Various Molecules,<br>J. Phys. Chem. 73, 4328 (1969). | |
| Method used : MS<br>Translational energy of RH2+ has been measured assuming delta H = 5X translational energy for reaction RH+ + RH -> RH2+ + 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<br>Calculated entropy<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

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

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

| C2H4F2O | CAS REGN : 359-13-7 |
|---|---|
| F**C**C**O<br>*<br>*<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C2H4F3N | CAS REGN : 753-90-2 |
|---|---|
| F<br>*<br>*<br>F**C**C**N<br>*<br>*<br>F | |
| Ethanamine, 2,2,2-trifluoro- (9CI)<br>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.,<br>A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,<br>J. Am. Chem. Soc. 98, 318 (1976). | |
| Method used : ICR<br>Calculated entropy<br>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 |
| 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<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

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

| 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.,<br>Energetics of Formation of Some Oxygenated Ions and<br>the Proton Affinities of Carbonyl Compounds,<br>Can. J. Chem. 44, 1625 (1966). | |
| Method used : EI<br>Electron impact fragmentation | |
| | |
| PA (exp) : 186+/-1 kcal/mol | Temperature : 298 K |
| Refaey, K. M. A., and Chupka, W. A.,<br>Photoionization of the Lower Aliphatic Alcohols<br>with Mass Analysis,<br>J. Chem. Phys. 48, 5205 (1968). | |
| Method used : PI<br>Appearance potential by IP fragmentation of C2H5OH. | |

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| | |
|---|---|
| PA (exp) : 189.4 kcal/mol | Temperature : 298 K |
| Lossing, F. P.<br>Heats of Formation of Some Isomeric [CnH2n + 1O]+ Ions. Substitutional Effects on Ion Stability, J. Am. Chem. Soc. 99, 7526 (1977). | |
| Method used : EM<br>Electron impact fragmentation (various molecules) using EM. delta Hf(H+) = 365.7 | |
| GB (exp) : 177.2+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 185+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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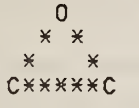
| | |
|---|---|
| GB (exp) : 169.8+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 185.4+/-2 kcal/mol | Temperature : 600 K |

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

| | |
|---|---|
| C2H4O | CAS REGN : 75-21-8 |



Oxirane (9CI)
Ethylene oxide (8CI)

| | |
|---|---|
| | |
| PA (exp) : 185+/-4 kcal/mol | Temperature : |

Beauchamp, J. L., and Dunbar, R. C.,
Identification of C2H5O+ Structural Isomers by Ion Cyclotron Resonance Spectroscopy,
J. Am. Chem. Soc. 92, 1477 (1970).

Method used : ICR
Bracketing relative to CH3OH and (CH3)2O

| C2H4O2 | CAS REGN : 64-19-7 |
|---|---|
| O%%C**C<br>%<br>%<br>O | |
| Acetic acid (8CI9CI) | |
| | |
| PA (exp) : 188+/-3 kcal/mol | Temperature : 323-373 K |
| Long, J., and Munson, B.,<br>Proton Affinities of Some Oxygenated Compounds,<br>J. Am. Chem. Soc. 95, 2427 (1973). | |
| Method used : MS<br>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.,<br>Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,<br>J. Am. Chem. Soc. 98, 1320 (1976). | |
| Method used : MS<br>Calculated entropy<br>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<br>Calculated entropy<br>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<br>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<br>Equilibrium; scale based on CH3CHO<br>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<br>Calculated entropy<br>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 |

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

| | |
|---|---|
| C2H5Br | CAS REGN : 74-96-4 |
| C**C**BR | |
| Ethane, bromo- (8CI9CI) | |
| | |
| PA (exp) : 171+/-2 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 C2H5BR
and assuming HA(CH3BR+)=HA(C2H5BR+).

| | |
|---|---|
| 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+).

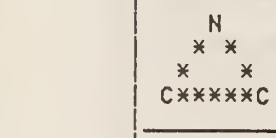
| C2H5F | CAS REGN : 353-36-6 |
|---|---|
| F**C**C | |
| Ethane, fluoro- (8CI9CI) | |
| | |
| PA (exp) : 165+/-5 kcal/mol | Temperature : 300 K |
| Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase 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<br>*<br>*<br>F | |
| Ethanamine, 2,2-difluoro- (9CI)<br>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<br>Calculated entropy<br>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 |
|---|---|
|  | |
| Aziridine (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| GB (exp) : 204.9+/-2 kcal/mol | Temperature : 298 K |
| | |
| Taft, R. W.,<br>Proton-Transfer Reactions,<br>Ed. E. F. Caldin and V. Gold,<br>(John Wiley and Sons, New York, 1975) Ch. 2. | |
| Method used : ICR<br>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%%C**C
%
%
O

Acetamide (8CI9CI)

| | |
|---|---|
| GB (exp) : 188.5+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 205.7+/-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 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

| C2H5NO3 | CAS REGN : 625-58-1 |
|---|---|
| C**C**O**N++O<br>+<br>+<br>O | |
| Nitric acid, ethyl ester (8CI9CI) | |
| | |
| PA (exp) : 181+/-3 kcal/mol | Temperature : 300 K |
| Kriemler, P., and Buttrill, S. E., Jr.,<br>Positive and Negative Ion-Molecule Reactions and<br>the Proton Affinity of Ethyl Nitrate,<br>J. Am. Chem. Soc. 92, 1123 (1970). | |
| Method used : ICR<br>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.,<br>Heats of Formation of Protonated Cyclopropane,<br>Methylcyclopropane, and Ethane,<br>J. Am. Chem. Soc. 94, 6347 (1972). | |
| Method used : MS<br>By applying path degeneracy correction found<br>delta H formation (C2H7+) = 218.8<br>Equilibrium relative to CH4; assume delta S = 0. | |
| | |
| PA (exp) : 139.6 (1) kcal/mol | Temperature : 300 K |
| Hiraoka, K., and Kebarle, P.,<br>Stabilities and Energetics of Pentacoordinated<br>Carbonium Ions. The Isomeric C2H7+ Ions and Some<br>Higher Analogues: C3H9+ and C4H11+,<br>J. Am. Chem. Soc. 98, 6119 (1976). | |
| Method used : MS<br>Based on delta H formation(C2H5+) = 219.<br>Equilibrium of reaction:<br>C2H5+ + H2 -> C2H7+(C-C protonation) (1). | |

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

| | |
|---|---|
| C2H6FN | CAS REGN : 406-34-8 |
| F**C**C**N | |
| Ethanamine, 2-fluoro- (9CI)<br>Ethylamine, 2-fluoro- (8CI) | |
| GB (exp) : 201.8+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 210.2+/-2 kcal/mol | Temperature : 300 K |
| Unpublished work by Wolf, Staley, Koppel, Taagepera,<br>McIver, Beauchamp, and Taft. | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

| | |
|---|---|
| C2H6O | CAS REGN : 64-17-5 |
| O**C**C | |
| Ethanol (9CI)<br>Ethyl alcohol (8CI) | |
| | |
| PA (exp) : 186+/-2 kcal/mol | Temperature : 323-373 K |
| Long, J., and Munson, B.,<br>Proton Affinities of Some Oxygenated Compounds,<br>J. Am. Chem. Soc. 95, 2427 (1973). | |
| Method used : MS<br>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.,<br>Proton Transfer Reactions by Trapped-Ion Mass Spectrometry,<br>Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976). | |
| Method used : MS<br>Equilibrium; scale based on CH3CHO<br>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 |

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) : 178.9+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 186.7+/-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

| C2H6O | CAS REGN : 115-10-6 |
|---|---|
| C**O**C | |
| Methane, oxybis- (9CI)<br>Methyl ether (8CI) | |
| | |
| PA (exp) : 190+/-4 kcal/mol | Temperature : 323-373 K |
| Long, J., and Munson, B.,<br>Proton Affinities of Some Oxygenated Compounds,<br>J. Am. Chem. Soc. 95, 2427 (1973). | |
| Method used : MS<br>Bracketing relative to I-C4H8 and CH3CHO;<br>Scale based on NH3 | |
| | |
| PA (exp) : 189 kcal/mol | Temperature : |
| Haney, M. A., and Franklin, J. L.,<br>Mass Spectrometric Determination of the Proton Affinities<br>of Various Molecules,<br>J. Phys. Chem. 73, 4328 (1969). | |
| Method used : MS<br>Delta H assume = 5X translational energy of<br>the products of reaction RH + RH+ -> RH2+ + 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<br>Equilibrium; scale based on MECHO<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

Continued on next page

| | |
|---|---|
| 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<br>Calculated entropy<br>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<br>Van't Hoff plot<br>Equilibrium relative to H2O. Delta G determined by means of thermodynamic cycles involving mixed clusters. | |

| C2H6OS | CAS REGN : 67-68-5 |
|---|---|
| C**S**C<br>+<br>+<br>O | |
| Methane, sulfinylbis- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| | |
| PA (exp) : 184+/-3 kcal/mol | Temperature : 300 K |
| McAllister, T.<br>Ion Cyclotron Resonance Mass Spectroscopy of Dimethyl Sulfoxide,<br>Intern. J. Mass Spectrom. Ion Phys. 25, 353 (1977). | |
| Method used : ICR<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C2H6S | CAS REGN : 75-18-3 |
|---|---|
| C**S**C | |
| Methane, thiobis- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C2H7N | CAS REGN : 75-04-7 |
|---|---|
| N**C**C | |
| Ethanamine (9CI)<br>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<br>Calculated entropy<br>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.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| | |
|---|---|
| C2H7N | CAS REGN : 124-40-3 |
| C**N**C | |
| Methanamine, N-methyl- (9CI)<br>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<br>Calculated entropy<br>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.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

Continued on next page

| | |
|---|---|
| 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<br>Entropy change assumed zero<br>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<br>Equilibrium; scale based on NH3 | |

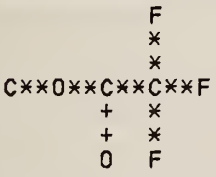
| C2H8N2 | CAS REGN : 57-14-7 |
|---|---|
| C**N**C<br>*<br>*<br>N | |
| Hydrazine, 1,1-dimethyl- (8CI9CI) | |
| GB (exp) : 209.5+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 217.3+/-2 kcal/mol | Temperature : 300 K |
| Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and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

| C2H8N2 | CAS REGN : 107-15-3 |
|---|---|
| N**C**C**N | |
| 1,2-Ethanediamine (9CI)<br>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.,<br>Quantitative Evaluation of Intramolecular Strong<br>Hydrogen Bonding in the Gas Phase,<br>J. Am. Chem. Soc. 95, 2669 (1973). | |
| Method used : ICR<br>Calculated entropy<br>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.,<br>Gas-Phase Basicities of Amines. Hydrogen Bonding<br>in Proton-Bound Amine Dimers and Proton-Induced<br>Cyclization of alpha,omega-Diamines,<br>J. Am. Chem. Soc. 95, 3504 (1973). | |
| Method used : MS<br>Equilibrium; scale based on (CH3)3N<br>Van't Hoff plot | |

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

| C3H2N2 | CAS REGN : 109-77-3 |
|---|---|
| N##C**C**C##N | |
| Propanedinitrile (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C3H3F3O2 | CAS REGN : 431-47-0 |
|---|---|



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 |

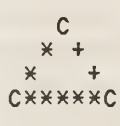
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

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

| C3H3N | CAS REGN : 107-13-1 |
|---|---|
| C++C**C##N | |
| 2-Propenenitrile (9CI)<br>Acrylonitrile (8CI) | |
| GB (exp) : 180.1+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 187.9+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| | |
| PA (exp) : 188.3+/-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<br>Calculated entropy<br>Equilibrium relative to C3H6O2(1,3-Dioxolane) with its PA value = 189.8; relative to Et CHO and MeCN | |

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

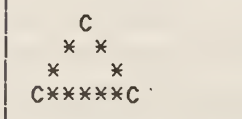
| C3H4 | CAS REGN : 463-49-0 |
|---|---|
| C++C++C | |
| 1,2-Propadiene (9CI)<br>Allene (8CI) | |
| | |
| PA (exp) : 176+/-2 kcal/mol | Temperature : 300 K |
| Aue, D. H., Davidson, W. R., and Bowers, M. T.,<br>Heats of Formation of C3H5+ Ions. Allyl, Vinyl, and<br>Cyclopropyl Cations in Gas-Phase Proton-Transfer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

| C3H4 | CAS REGN : 2781-85-3 |
|---|---|
|  | |
| 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<br>Bracketing relative to (CH3)2O and (C2H5)2O. | |

| C3H4ClN | CAS REGN : 542-76-7 |
|---|---|
| N##C**C**C**CL | |
| Propanenitrile, 3-chloro- (9CI)<br>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<br>Calculated entropy<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C3H5N | CAS REGN : 107-12-0 |
|---|---|
| C**C**C##N | |
| Propanenitrile (9CI)<br>Propionitrile (8CI) | |
| GB (exp) : 182.4+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 190.2+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| | |
| PA (exp) : 190.2+/-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<br>Calculated entropy<br>Equilibrium relative to n-PrCN, HCO2Et, i-PrCHO, Me2O, EtCHO and relative to 1,3-Dioxane using its PA = 189.8 | |

| C3H5N | CAS REGN : 2450-71-7 |
|---|---|
| C##C**C**N | |
| 2-Propyn-1-amine (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C3H6 | CAS REGN : 75-19-4 |
|---|---|
|  | |
| Cyclopropane (8CI9CI) | |
| | |
| PA (exp) : 180.6+/-4 kcal/mol | Temperature : 340 K |
| Chong, S. L., and Franklin, J. L.,<br>Heats of Formation of Protonated Cyclopropane,<br>Methylcyclopropane, and Ethane,<br>J. Am. Chem. Soc. 94, 6347 (1972). | |
| Method used : MS<br>HC(OH)2+ + C-C3H6 -> HCOOH + C-C3H7+.<br>Equilibrium of reactions:<br>CH3OH2+ + C-C3H6 -> CH3OH+C-C3H7+;<br>Apply correction for path degeneracy. Assuming<br>delta S=0. | |

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

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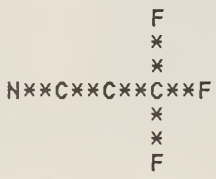
| | |
|---|---|
| GB (exp) : 165.4+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 182.6+/-2 kcal/mol | Temperature : 600 K |

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

| | |
|---|---|
| C3H6F3N | CAS REGN : 460-39-9 |



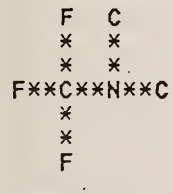
1-Propanamine, 3,3,3-trifluoro- (9CI)
Propylamine, 3,3,3-trifluoro- (8CI)

| | |
|---|---|
| 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

| C3H6F3N | CAS REGN : 677-41-8 |
|---|---|



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 |
|---|---|
|  | |
| Ethanamine, 2,2,2-trifluoro-N-methyl- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C3H6N2 | CAS REGN : 151-18-8 |
|---|---|
| N##C**C**C**N | |
| Propanenitrile, 3-amino- (9CI)<br>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<br>Calculated entropy<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

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| | |
|---|---|
| GB not calculated for this reference | |
| PA (exp) : 188 kcal/mol | Temperature : |
| Haney, M. A., and Franklin, J. L.,<br>Mass Spectrometric Determination of the Proton Affinities<br>of Various Molecules,<br>J. Phys. Chem. 73, 4328 (1969). | |
| Method used : MS<br>Delta H estimated equal 5 times<br>translational energy of the products. | |
| | |
| PA (exp) : 196 kcal/mol | Temperature : 298 K |
| Heats of Formation of Some Isomeric [CnH2n + 1O]+<br>Ions. Substitutional Effects on Ion Stability,<br>J. Am. Chem. Soc. 99, 7526 (1977). | |
| Method used : EM<br>Electron impact fragmentation (various molecules)<br>using EM. delta Hf(H+) = 365.7<br>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 |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| GB (exp) : 186.5+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 193.9+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C3H6O | CAS REGN : 123-38-6 |
|---|---|
| C**C**C++O | |
| Propanal (9CI)<br>Propionaldehyde (8CI) | |
| | |
| PA (exp) : 190+/-3 kcal/mol | Temperature : |
| Harrison, A. G., Ivko, A., and Van Raalte, D.,<br>Energetics of Formation of Some Oxygenated Ions and<br>the Proton Affinities of Carbonyl Compounds,<br>Can. J. Chem. 44, 1625 (1966). | |
| Method used : EI<br>Electron impact fragmentation of various molecules. | |
| | |
| PA (exp) : 187 kcal/mol | Temperature : 298 K |
| Lossing, F. P.<br>Heats of Formation of Some Isomeric [CnH2n + 1O]+<br>Ions. Substitutional Effects on Ion Stability,<br>J. Am. Chem. Soc. 99, 7526 (1977). | |
| Method used : EM<br>Electron impact fragmentation (various molecules)<br>using EM. delta Hf(H+) = 365.7 | |

Continued on next page

| | |
|---|---|
| GB (exp) : 172.3+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 187.9+/-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

| | |
|---|---|
| GB (exp) : 180.2+/-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

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

| C3H6OS | CAS REGN : 1534-08-3 |
|---|---|
| C**C**S**C<br>+<br>+<br>O | |
| Ethanethioic acid, S-methyl ester (9CI)<br>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.<br>The Relative Basicity of Sulfur containing Esters, Tetrahedron 33, 2781 (1977). | |
| Method used : ICR<br>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**C**C<br>%<br>%<br>O | |
| Propanoic acid (9CI)<br>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.,<br>Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,<br>J. Am. Chem. Soc. 98, 1320 (1976). | |
| Method used : MS<br>Equilibrium; scale based on NH3<br>Entropy change assumed zero | |

| C3H6O2 | CAS REGN : 79-20-9 |
|---|---|
| C**C**O**C<br>+<br>+<br>O | |
| Acetic acid, methyl ester (8CI9CI) | |
| | |
| PA (exp) : 194+/-2 kcal/mol | Temperature : 323-373 K |
| Long, J., and Munson, B.,<br>Proton Affinities of Some Oxygenated Compounds,<br>J. Am. Chem. Soc. 95, 2427 (1973). | |
| Method used : MS<br>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.,<br>Proton Transfer Reactions by Trapped-Ion Mass Spectrometry,<br>Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976). | |
| Method used : MS<br>Equilibrium; scale based on (CH3)2CO<br>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 |
| Long, J., and Munson, B.,<br>Proton Affinities of Some Oxygenated Compounds,<br>J. Am. Chem. Soc. 95, 2427 (1973). | |
| Method used : MS<br>Bracketing relative to CH2CO AND I-C4H8;<br>scale based on NH3. | |
| GB (exp) : 183.7+/-2 kcal/mol | Temperature : 298 K |
| PA (exp) : 191.1+/-2 kcal/mol | Temperature : 298 K |
| Harrison, A. G., Lin, P. H., and Tsang, C. W.,<br>Proton Transfer Reactions by Trapped-Ion Mass Spectrometry,<br>Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976). | |
| Method used : MS<br>Equilibrium; scale based on (CH3)2CO<br>Entropy change assumed zero | |

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| | |
|---|---|
| GB (exp) : 175.6+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 191.2+/-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) : 183.4+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 191.2+/-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

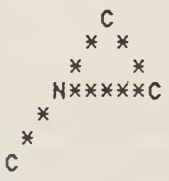
| C3H6O3 | CAS REGN : 616-38-6 |
|---|---|
| C**O**C**O**C<br>+<br>+<br>O | |
| Carbonic acid, dimethyl ester (8CI9CI) | |
| GB (exp) : 189.8+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 197.2+/-2 kcal/mol | Temperature : 300 K |
| Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C3H6S2 | CAS REGN : 2168-84-5 |
|---|---|
| S<br>+<br>+<br>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 Siddigui, J.<br>The Relative Basicity of Sulfur Containing Esters, Tetrahedron 33, 2781 (1977). | |
| Method used : ICR<br>Double resonance technique shows PA (MeCSSMe) > PA (the COSMe) | |

| C3H7N | CAS REGN : 107-11-9 |
|---|---|
| C++C**C**N | |
| 2-Propen-1-amine (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C3H7N | CAS REGN : 503-29-7 |
|---|---|
| C**N<br>* *<br>* *<br>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<br>Calculated entropy<br>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<br>Entropy change assumed zero<br>Equilibrium; scale based on (CH3)3N | |

| C3H7N | CAS REGN : 1072-44-2 |
|---|---|



Aziridine, 1-methyl- (8CI9CI)

| | |
|---|---|
| PA (exp) : 219.4+/-2 kcal/mol | Temperature : 298 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

| C3H7NO | CAS REGN : 68-12-2 |
|---|---|
| C**N**C++O<br>*<br>*<br>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<br>Calculated entropy<br>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 |
| Hiraoka, K., and Kebarle, P.,<br>Information on the Proton Affinity and Protolysis<br>of Propane from Measurement of the Ion Cluster,<br>Equilibrium: C2H5+ + CH4 = C3H9+.<br>Can. J. Chem. 53, 970 (1975). | |
| Method used : MS<br>Equilibrium of reaction<br>C2H5+ + 2CH4 -> C3H9+ + CH4<br>Van't Hoff plot | |
| | |
| PA (exp) : 143 kcal/mol | Temperature : 170 K |
| Field, F. H., and Beggs, D. P.,<br>Reversible Reactions of Gaseous Ions. III. Studies<br>with Methane at 0.1-1.0 Torr and 77-300 K,<br>J. Am. Chem. Soc. 93, 1585 (1971). | |
| Method used : MS<br>Equilibrium of reaction:<br>C2H5+ + CH4 -> C3H9+.<br>Based on delta H formation(C2H5+).<br>Calculated entropy | |

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

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

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

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

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

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

| C3H8S | CAS REGN : 75-33-2 |
|---|---|
| C**C**C<br>*<br>*<br>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<br>Calculated entropy<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C3H8S | CAS REGN : 624-89-5 |
|---|---|
| C**C**S**C | |
| Ethane, (methylthio)- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

| C3H9N | CAS REGN : 75-31-0 |
|---|---|
| C**C**C<br>*<br>*<br>N | |
| 2-Propanamine (9CI)<br>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<br>Calculated entropy<br>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.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| C3H9N | CAS REGN : 75-50-3 |
|---|---|
| C**N**C<br>*<br>*<br>C | |
| Methanamine, N,N-dimethyl- (9CI)<br>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<br>Calculated entropy<br>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.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>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<br>Entropy change assumed zero<br>Equilibrium; scale based on NH3 | |

| C3H9N | CAS REGN : 107-10-8 |
|---|---|
| C**C**C**N | |
| 1-Propanamine (9CI)<br>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<br>Calculated entropy<br>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<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| | |
|---|---|
| C3H9N | CAS REGN : 624-78-2 |
| C**C**N**C | |
| Ethanamine, N-methyl- (9CI)<br>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<br>Calculated entropy<br>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 |

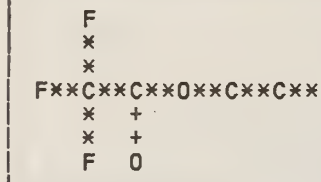
Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Evaluation of Intramolecular Strong
Hydrogen Bonding in the Gas Phase,
J. Am. Chem. Soc. 95, 2669 (1973).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

| C3H9P | CAS REGN : 594-09-2 |
|---|---|
| C**P**C<br>*<br>*<br>C | |
| Phosphine, trimethyl- (8CI9CI) | |
| GB (exp) : 214.9+/-2 kcal/mol | Temperature : 298 K |
| | |
| Taft, R. W.,<br>Proton-Transfer Reactions,<br>Ed. E. F. Caldin and V. Gold,<br>(John Wiley and Sons, New York, 1975) Ch. 2. | |
| Method used : ICR<br>Equilibrium; scale based on NH3 | |
| | |
| PA (exp) : 223.3+/-2 kcal/mol | Temperature : 300 K |
| Staley, P. H., and Beauchamp, J. L.<br>Basicities and Ion-Molecule Reactions of the<br>Methylphosphines in the Gas Phase by Ion Cyclotron<br>Resonance Spectroscopy,<br>J. Am. Chem. Soc. 96, 6252 (1974). | |
| Method used : ICR<br>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 |
| 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<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |
| GB (exp) : 221.10+/-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<br>Equilibrium; scale based on (CH3)3N<br>Van't Hoff plot | |

| C4H4F4O2 | CAS REGN : 1683-88-1 |
|---|---|

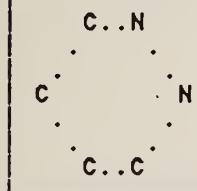


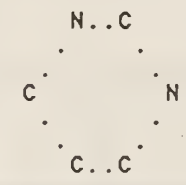
Acetic acid, trifluoro-, 2-fluoroethyl ester (8CI)

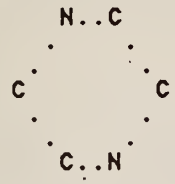
| GB (exp) : 172.3+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 180.1+/-2 kcal/mol | Temperature : 300 K |

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).

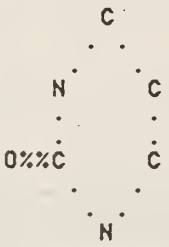
Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H4N2 | CAS REGN : 289-95-2 |
|---|---|
|  | |
| 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<br>Calculated entropy<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H4N2O | CAS REGN : 557-01-7 |
|---|---|



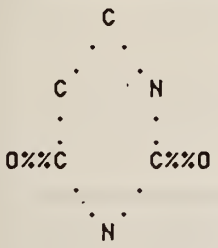
2(1H)-Pyrimidinone (8CI9CI)

| | |
|---|---|
| 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 |
|---|---|



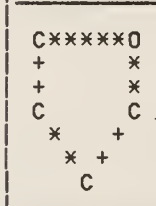
2,4(1H,3H)-Pyrimidinedione (9CI)
Uracil (8CI)

| | |
|---|---|
| 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 |
|---|---|



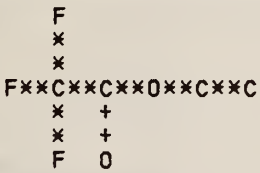
Furan (8CI9CI)

| | |
|---|---|
| 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 |
|---|---|



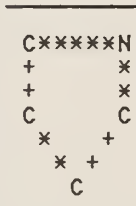
Acetic acid, trifluoro-, ethyl ester (8CI9CI)

| 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 |
|---|---|



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).

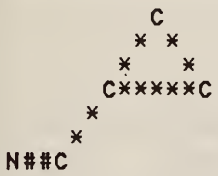
Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

| 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 |
|---|---|



Cyclopropanecarbonitrile (8CI9CI)

| | |
|---|---|
| PA (exp) : 193.2+/-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).

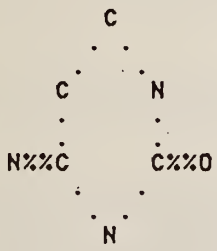
Method used : ICR
Calculated entropy
Equilibrium relative to HCO2-n-C4H9

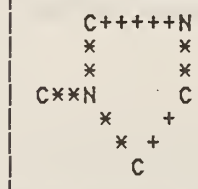
| | |
|---|---|
| GB (exp) : 185.4+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 193.2+/-2 kcal/mol | Temperature : 300 K |

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

| C4H5NO2 | CAS REGN : 623-49-4 |
|---|---|
| N##C**C**O**C**C<br>+<br>+<br>O | |
| Carbonocyanidic acid, ethyl ester (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

| C4H6N2 | CAS REGN : 616-47-7 |
|---|---|
|  | |
| 1H-Imidazole, 1-methyl- (9CI)<br>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<br>Calculated entropy<br>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 |
|---|---|
| C**C**C##N<br>*<br>*<br>C | |
| Propanenitrile, 2-methyl- (9CI)<br>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<br>Calculated entropy<br>Equilibrium relative to HCO2C2H5 | |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H7N | CAS REGN : 109-74-0 |
|---|---|
| N##C**C**C**C | |
| Butanenitrile (9CI)<br>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<br>Calculated entropy<br>Equilibrium relative to HCO2Et, 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<br>Calculated entropy<br>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<br>+<br>+<br>C | |
| 1-Propene, 2-methyl- (9CI)<br>Propene, 2-methyl- (8CI) | |
| | |
| PA (exp) : 192.6+/-2 kcal/mol | Temperature : 363-553 K |
| Goren, A., and Munson, B.<br>Thermochemistry of Alkyl Ions,<br>J. Phys. Chem. 80, 2848 (1976). | |
| Method used : MS<br>Using delta Hf(t-C4H9+) = 169+/-1.8 derived from,<br>delta Hf(t-C4H9) = 9.3 and IP(t-C4H9) = 159.9 | |
| | |
| PA (exp) : 193.7 kcal/mol | Temperature : |
| Lossing F. P., and Semeluk, G. P.<br>Free Radicals by Mass Spectrometry. XLII. Ionization<br>Potentials and Ionic Heats of Formation for C1-C4<br>Alkyl Radicals,<br>Can. J. Chem. 48, 955 (1970). | |
| Method used : EM<br>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

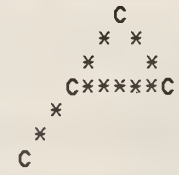
| | |
|---|---|
| GB (exp) : 185.1+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 193.5+/-2 kcal/mol | Temperature : 300 K |

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.<br>Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals,<br>Can. J. Chem. 48, 955 (1970). | |
| Method used : EM<br>Appearance potential of C4H9+ | |

| C4H8 | CAS REGN : 594-11-6 |
|---|---|



Cyclopropane, methyl- (8CI9CI)

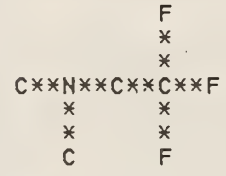
| | |
|---|---|
| PA (exp) : 181+/-2 kcal/mol | Temperature : |

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.<br>Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals,<br>Can. J. Chem. 48, 955 (1970). | |
| Method used : EM<br>Appearance potential of C4H9+ | |

| C4H8F3N | CAS REGN : 819-06-7 |
|---|---|



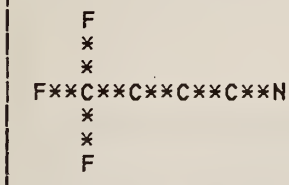
Ethanamine, 2,2,2-trifluoro-N,N-dimethyl- (9CI)
Ethylamine, 2,2,2-trifluoro-N,N-dimethyl- (8CI)

| 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 |
|---|---|



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<br>*<br>*<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H8O | CAS REGN : 78-84-2 |
|---|---|
| C**C**C++O<br>*<br>*<br>C | |
| Propanal, 2-methyl- (9CI)<br>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., 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H8O | CAS REGN : 78-93-3 |
|---|---|
| C**C**C**C<br>+<br>+<br>O | |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| | |
| PA (exp) : 193.7+/-1 kcal/mol | Temperature : 293 K |
| Lossing, F. P.<br>Heats of Formation of Some Isomeric [CnH2n + 1O]+ Ions. Substitutional Effects on Ion Stability,<br>J. Am. Chem. Soc. 99, 7526 (1977). | |
| Method used : EM<br>Electron impact fragmentation (various molecules) using EM. delta Hf(H+) = 365.7 | |

| C4H8O | CAS REGN : 109-99-9 |
|---|---|

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)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

Continued on next page

| | |
|---|---|
| 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).

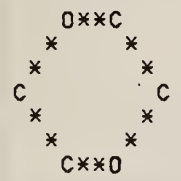
Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

| | |
|---|---|
| GB (exp) : 176.1+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 191.7+/-2 kcal/mol | Temperature : 600 K |

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

| C4H8O2 | CAS REGN : 123-91-1 |
|---|---|



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

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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| GB (exp) : 182.4+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 198+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H8O2 | CAS REGN : 554-12-1 |
|---|---|
| C**O**C**C**C<br>+<br>+<br>O | |
| Propanoic acid, methyl ester (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| | |
| PA (exp) : 197+/-2 kcal/mol | Temperature : 323-373 K |
| Long, J., and Munson, B.,<br>Proton Affinities of Some Oxygenated Compounds,<br>J. Am. Chem. Soc. 95, 2427 (1973). | |
| Method used : MS<br>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 |

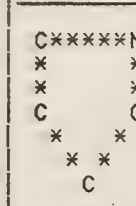
Harrison, A. G., Lin, P. H., and Tsang, C. W.,
Proton Transfer Reactions by Trapped-Ion Mass Spectrometry,
Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).

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<br>+<br>+<br>O | |
| Carbonothioic 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H8O3 | CAS REGN : 623-53-0 |
|---|---|
| C**O**C**O**C**C<br>+<br>+<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H9N | CAS REGN : 123-75-1 |
|---|---|



Pyrrolidine (8CI9CI)

| GB (exp) : 213.70+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 221.90+/-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

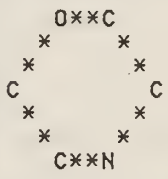
| GB (exp) : 213.30+/-2 kcal/mol | Temperature : 298 K |
|---|---|
| PA (exp) : 221.50+/-2 kcal/mol | Temperature : 298 K |

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

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

| C4H9NO | CAS REGN : 110-91-8 |
|---|---|



Morpholine (8CI9CI)

| GB (exp) : 208.6+/-2 kcal/mol | Temperature : 298 K |
|---|---|
| PA (exp) : 216.8+/-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

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

| C4H9NO | CAS REGN : 563-83-7 |
|---|---|
| C**C**C%%N<br>* %<br>* %<br>C O | |
| Propanamide, 2-methyl- (9CI)<br>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<br>Calculated entropy<br>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 |
| Hiraoka, K., and Kebarle, P.,<br>Stabilities and Energetics of Pentacoordinated<br>Carbonium Ions. The Isomeric C2H7+ Ions and Some<br>Higher Analogues: C3H9+ and C4H11+,<br>J. Am. Chem. Soc. 98, 6119 (1976). | |
| Method used : MS<br>Van't Hoff plot<br>C-H protonation (2)<br>Equilibrium of reaction t-C4H9+ + H2 -> C4H11+ (2) | |
| | |
| PA (exp) : 164 (1) kcal/mol | Temperature : 291 K |
| Hiraoka, K., and Kebarle, P.,<br>Stabilities and Energetics of Pentacoordinated<br>Carbonium Ions. The Isomeric C2H7+ Ions and Some<br>Higher Analogues: C3H9+ and C4H11+,<br>J. Am. Chem. Soc. 98, 6119 (1976). | |
| Method used : MS<br>Van't Hoff plot<br>C-C protonation (1)<br>Equilibrium of reaction C3H7+ + CH4 -> C4H11+ (1) | |

| C4H10N2 | CAS REGN : 110-85-0 |
|---|---|

| Piperazine (8CI9CI) | |
|---|---|
| GB (exp) : 210.9+/-2 kcal/mol | Temperature : 298 K |
| PA (exp) : 218.9+/-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

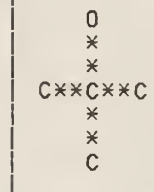
| C4H10O | CAS REGN : 60-29-7 |
|---|---|
| C**C**O**C**C | |
| Ethane, 1,1'-oxybis- (9CI)<br>Ethyl ether (8CI) | |
| | |
| PA (exp) : 198+/-4 kcal/mol | Temperature : 323-373 K |
| Long, J., and Munson, B.,<br>Proton Affinities of Some Oxygenated Compounds,<br>J. Am. Chem. Soc. 95, 2427 (1973). | |
| Method used : MS<br>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.,<br>Proton Transfer Reactions by Trapped-Ion Mass Spectrometry,<br>Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976). | |
| Method used : MS<br>Equilibrium; scale based on (CH3)2CO<br>Entropy change assumed zero | |

Continued on next page

| | |
|---|---|
| GB (exp) : 182.5+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 197.3+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| GB (exp) : 190+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 197.4+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H10O | CAS REGN : 71-36-3 |
|---|---|
| O**C**C**C**C | |
| 1-Butanol (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H10O | CAS REGN : 75-65-0 |
|---|---|



2-Propanol, 2-methyl- (9CI)
tert-Butyl alcohol (8CI)

| | |
|---|---|
| PA (exp) : 194+/-1 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 CH2CO and I-C5H10

| | |
|---|---|
| PA (exp) : 192 kcal/mol | Temperature : |

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).

Method used : MS
Equilibrium relative to known standard acids

| 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)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C4H11N | CAS REGN : 75-64-9 |
|---|---|

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<br>*<br>*<br>C | |
| 1-Propanamine, 2-methyl- (9CI)<br>Isobutylamine (8CI) | |
| GB (exp) : 207.7+/-2 kcal/mol | Temperature : 298 K |
| | |
| Taft, R. W.,<br>Proton-Transfer Reactions,<br>Ed, E. F. Caldin and V. Gold,<br>(John Wiley and Sons, New York, 1975) Ch. 2. | |
| Method used : ICR<br>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.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| C4H11N | CAS REGN : 109-73-9 |
|---|---|
| N**C**C**C**C | |
| 1-Butanamine (9CI)<br>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<br>Calculated entropy<br>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.,<br>A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,<br>J. Am. Chem. Soc. 98, 318 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| | |
|---|---|
| C4H11N | CAS REGN : 109-89-7 |
| C**C**N**C**C | |
| Ethanamine, N-ethyl- (9CI)<br>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<br>Calculated entropy<br>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.,<br>Quantitative Proton Affinities, Ionization Potontials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| C4H11N | CAS REGN : 598-56-1 |
|---|---|
| C**N**C**C<br>*<br>*<br>C | |
| Ethanamine, N,N-dimethyl- (9CI)<br>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<br>Calculated entropy<br>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.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>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

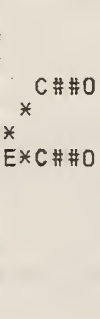
| GB (exp) : 209.3+/-2 kcal/mol | Temperature : 298 K |
|---|---|
| PA (exp) : 217.7+/-2 kcal/mol | Temperature : 298 K |

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<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| C5Fe05 | CAS REGN : 13463-40-6 |
|---|---|



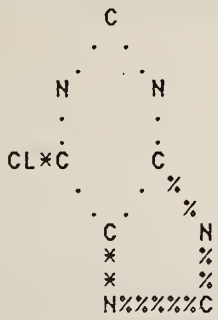
Iron carbonyl (Fe(CO)5), (TB-5-11)- (9CI)
Iron carbonyl (Fe(CO)5) (8CI)

| | |
|---|---|
| PA (exp) : 200+/-3 kcal/mol | Temperature : 300 K |

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).

Method used : ICR
Bracketing relative to (CH3O)2CO and NH3.

| C5H3ClN4 | CAS REGN : 87-42-3 |
|---|---|

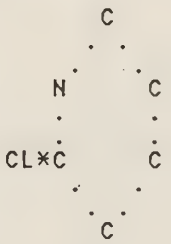


1H-Purine, 6-chloro- (9CI)
Purine, 6-chloro- (8CI)

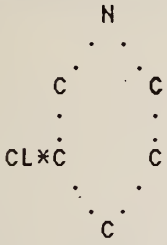
| | |
|---|---|
| PA (exp) : 207+/-5 kcal/mol | Temperature : |

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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H4ClN | CAS REGN : 626-60-8 |
|---|---|

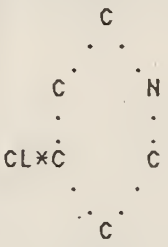



Pyridine, 3-chloro- (8CI9CI)

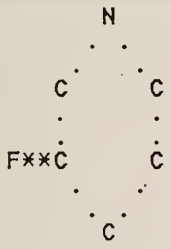
| GB (exp) : 204.5+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 212.3+/-2 kcal/mol | Temperature : 300 K |

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 |
| Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft. | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H4FN | CAS REGN : 372-47-4 |
|---|---|

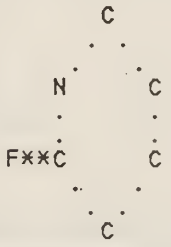


Pyridine, 3-fluoro- (8CI9CI)

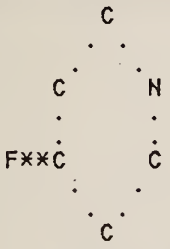
| GB (exp) : 203.7+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 211.5+/-2 kcal/mol | Temperature : 300 K |

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 |
| Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft. | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H4FN | CAS REGN : 694-52-0 |
|---|---|



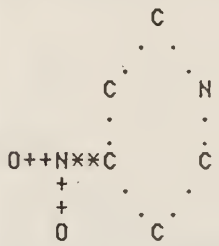
Pyridine, 4-fluoro- (8CI9CI)

| 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 |
|---|---|



Pyridine, 4-nitro- (8CI9CI)

| GB (exp) : 198.4+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 206.2+/-2 kcal/mol | Temperature : 300 K |

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

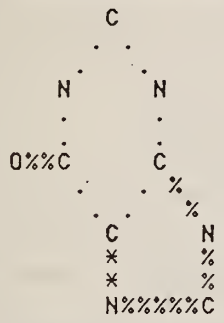
Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

| | |
|---|---|
| PA (exp) : 201+/-2 kcal/mol | Temperature : 300 K |

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).

Method used : ICR
Equilibrium; scale based on Pyridine

| C5H4N4O | CAS REGN : 68-94-0 |
|---|---|

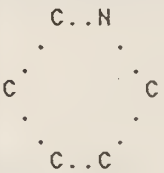


6H-Purin-6-one, 1,7-dihydro- (9CI)
Hypoxanthine (8CI)

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

Continued on next page

| | |
|---|---|
| GB (exp) : 209.8+/-2 kcal/mol | Temperature : 298 K |
| PA (exp) : 217.6+/-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) : 203.7+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 220.9+/-2 kcal/mol | Temperature : 600 K |

Briggs, J. P., Yamdagni, R., and Kebarle, P.,
Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phas Proton-Exchange Equilibria,
J. Am. Chem. Soc. 94, 5128 (1972).

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

| C5H5N5 | CAS REGN : 73-24-5 |
|---|---|

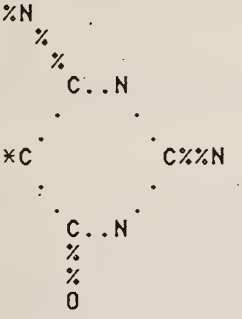
1H-Purin-6-amine (9CI)
Adenine (8CI)

| | |
|---|---|
| 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

| C5H5N5O | CAS REGN : 73-40-5 |
|---|---|



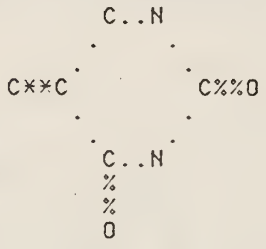
6H-Purin-6-one, 2-amino-1,7-dihydro- (9CI)
Guanine (8CI)

| | |
|---|---|
| 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 |
|---|---|



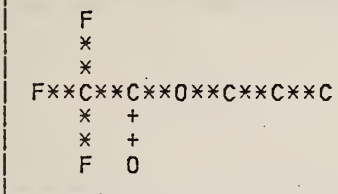
2,4(1H,3H)-Pyrimidinedione, 5-methyl- (9CI)
Thymine (8CI)

| | |
|---|---|
| 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 |
|---|---|



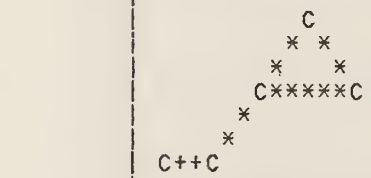
Acetic acid, trifluoro-, propyl ester (8CI9CI)

| 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., 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

| C5H8 | CAS REGN : 693-86-7 |
|---|---|



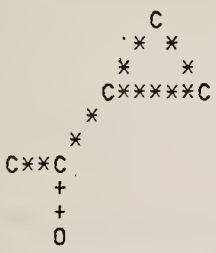
Cyclopropane, ethenyl- (9CI)
Cyclopropane, vinyl- (8CI)

| GB (exp) : 187.4+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 195.2+/-2 kcal/mol | Temperature : 300 K |

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

| C5H8O | CAS REGN : 765-43-5 |
|---|---|



Ethanone, 1-cyclopropyl- (9CI)
Ketone, cyclopropyl methyl (8CI)

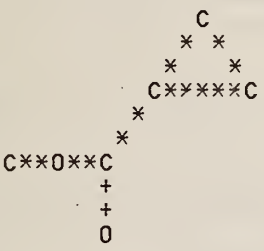
| GB (exp) : 194.4+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 202.2+/-2 kcal/mol | Temperature : 300 K |

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<br>+ +<br>+ +<br>O O | |
| 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<br>Calculated entropy<br>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##N | |
| Pentanenitrile (9CI)<br>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<br>Calculated entropy<br>Equilibrium relative to HCO2C2H5 | |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

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

Continued on next page

| | |
|---|---|
| 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 |

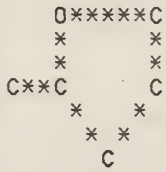
```
C**C**C**C**C
      +
      +
      O
```

3-Pentanone (8CI9CI)

| | |
|---|---|
| GB (exp) : 191.1+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 198.5+/-2 kcal/mol | Temperature : 300 K |

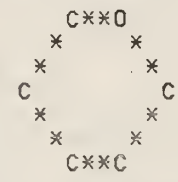
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

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

| C5H10O | CAS REGN : 96-47-9 |
|---|---|
|  | |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H10O | CAS REGN : 110-62-3 |
|---|---|
| C**C**C**C**C++O | |
| Pentanal (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H10O | CAS REGN : 142-68-7 |
|---|---|



2H-Pyran, tetrahydro- (8CI9CI)

| GB (exp) : 189.7+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 197.1+/-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

| C5H10O | CAS REGN : 563-80-4 |
|---|---|
| C**C**C**C<br>  *  +<br>  *  +<br>  C  O | |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H1002 | CAS REGN : 109-60-4 |
|---|---|
| C**C**O**C**C**C<br>+<br>+<br>O | |
| Acetic acid, propyl ester (8CI9CI) | |
| | |
| PA (exp) : 200+/-3 kcal/mol | Temperature : |
| Long, J., and Munson, B.,<br>Proton Affinities of Some Oxygenated Compounds,<br>J. Am. Chem. Soc. 95, 2427 (1973). | |
| Method used : MS<br>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.,<br>Gas-Phase Basicities and Proton Affinities of Compounds<br>Between Water and Ammonia and Substituted Benzenes from<br>A Continuous Ladder of Proton Transfer Equilibria<br>Measurements,<br>J. Am. Chem. Soc. 98, 1320 (1976). | |
| Method used : MS<br>Equilibrium; scale based on NH3<br>Entropy change assumed zero | |

| C5H10O2 | CAS REGN : 547-63-7 |
|---|---|

```
C**O**C**C**C
      +  *
      +  *
      O  C
```

Propanoic acid, 2-methyl-, methyl ester (9CI)
Isobutyric acid, methyl ester (8CI)

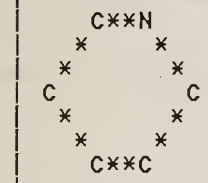
| GB (exp) : 191.1+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 198.9+/-2 kcal/mol | Temperature : 300 K |

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**C**C**C**C | |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H11N | CAS REGN : 110-89-4 |
|---|---|



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

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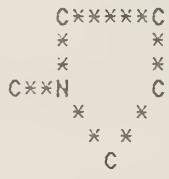
| | |
|---|---|
| GB (exp) : 209.60+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 226.80+/-2 kcal/mol | Temperature : 600 K |
| Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am.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

| | |
|---|---|
| C5H11N | CAS REGN : 120-94-5 |



Pyrrolidine, 1-methyl- (8CI9CI)

| | |
|---|---|
| GB (exp) : 217.80+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 225.60+/-2 kcal/mol | Temperature : 300 K |
| Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft. | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

Continued on next page

| | |
|---|---|
| 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<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| | |
|---|---|
| C5H11NO2 | CAS REGN : 687-48-9 |
| C**N**C**O**C**C<br>* +<br>* +<br>C O | |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H12O | CAS REGN : 625-54-7 |
|---|---|
| C**C**O**C**C<br>*<br>*<br>C | |
| Propane, 2-ethoxy- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H12O | 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)<br>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.,<br>Quantitative Evaluation of Intramolecular Strong<br>Hydrogen Bonding in the Gas Phase,<br>J. Am. Chem. Soc. 95, 2669 (1973). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| C5H13N | CAS REGN : 594-39-8 |
|---|---|

```
   N
   *
   *
C**C**C**C
   *
   *
   C
```

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<br>*<br>*<br>C | |
| Ethanamine, N-ethyl-N-methyl- (9CI)<br>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<br>Calculated entropy<br>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.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| C5H13N | CAS REGN : 996-35-0 |
|---|---|
| C**C**N**C<br>* *<br>* *<br>C C | |
| 2-Propanamine, N,N-dimethyl- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H13N | CAS REGN : 5813-64-9 |
|---|---|

```
    C
    *
    *
C**C**C**N
    *
    *
    C
```

1-Propanamine, 2,2-dimethyl- (9CI)
Neopentylamine (8CI)

| GB (exp) : 208.8+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 217.2+/-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

| GB (exp) : 209.0+/-2 kcal/mol | Temperature : 298 K |
|---|---|
| PA (exp) : 217.4+/-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).

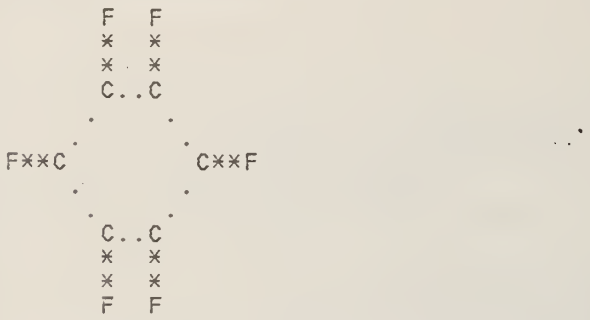
Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

| C5H13N | CAS REGN : 19961-27-4 |
|---|---|
| C**C**N**C**C<br>*<br>*<br>C | |
| 2-Propanamine, N-ethyl- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C5H14N2 | CAS REGN : 109-55-7 |
|---|---|
| C**N**C**C**C**N<br>*<br>*<br>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<br>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<br>Calculated entropy<br>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<br>Equilibrium; scale based on (CH3)3N<br>Van't Hoff plot | |

| C6F6 | CAS REGN : 392-56-3 |
|---|---|



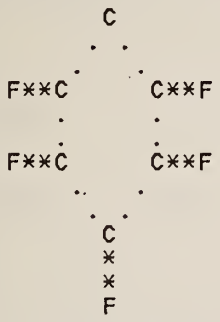
Benzene, hexafluoro- (8CI9CI)

| GB (exp) : 171.2 kcal/mol | Temperature : 373 K |
|---|---|
| PA (exp) : 178.5+/-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

| C6HF5 | CAS REGN : 363-72-4 |
|---|---|



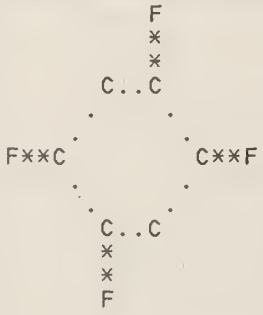
Benzene, pentafluoro- (8CI9CI)

| 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 |
|---|---|



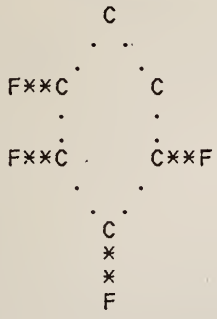
Benzene, 1,2,4,5-tetrafluoro- (8CI9CI)

| GB (exp) : 173.1+/-2 kcal/mol | Temperature : 373 K |
|---|---|
| PA (exp) : 180.3+/-2 kcal/mol | Temperature : 373 K |

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 : 551-62-2 |
|---|---|



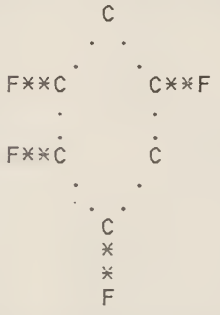
Benzene, 1,2,3,4-tetrafluoro- (8CI9CI)

| 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 |
|---|---|



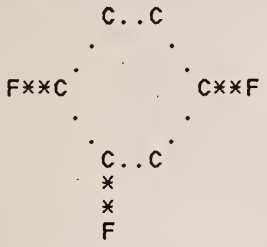
Benzene, 1,2,3,5-tetrafluoro- (8CI9CI)

| GB (exp) : 173.4+/-2 kcal/mol | Temperature : 373 K |
|---|---|
| PA (exp) : 180.5+/-2 kcal/mol | Temperature : 373 K |

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 : 367-23-7 |
|---|---|



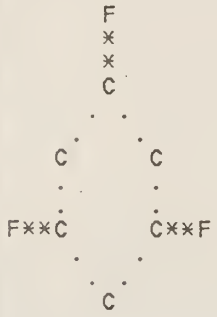
Benzene, 1,2,4-trifluoro- (8CI9CI)

| 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 |
|---|---|



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 |

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

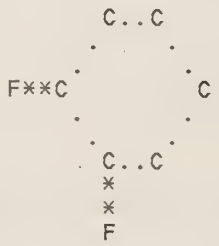
Continued on next page

| | |
|---|---|
| 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 |
|---|---|



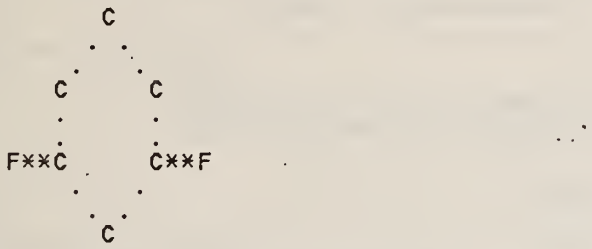
Benzene, 1,2-difluoro- (9CI)
Benzene, o-difluoro- (8CI)

| 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

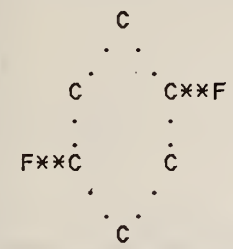
Continued on next page

| | |
|---|---|
| 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 |
|---|---|



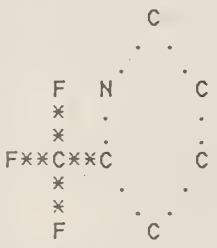
Benzene, 1,4-difluoro- (9CI)
Benzene, p-difluoro- (8CI)

| 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 |
|---|---|

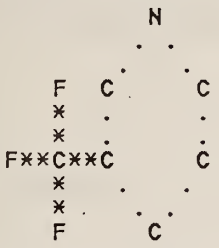


Pyridine, 2-(trifluoromethyl)- (8CI9CI)

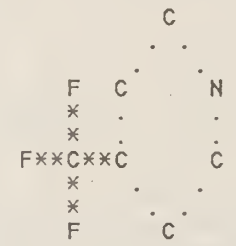
| GB (exp) : 201.2+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 209.0+/-2 kcal/mol | Temperature : 300 K |

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

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

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

| C6H4F3N | CAS REGN : 3796-24-5 |
|---|---|



Pyridine, 4-(trifluoromethyl)- (8CI9CI)

| GB (exp) : 202.5+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 210.3+/-2 kcal/mol | Temperature : 300 K |

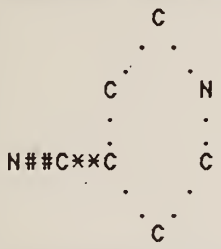
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

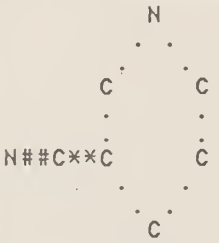
Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

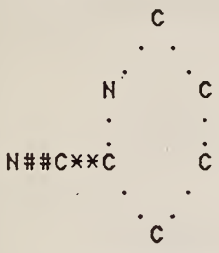
| | |
|---|---|
| PA (exp) : 207.1+/-2 kcal/mol | Temperature : 298 K |

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).

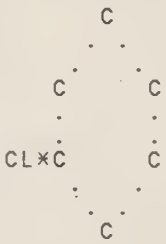
Method used : ICR
Equilibrium; scale based on C5H5N(Pyridine)

| C6H4N2 | CAS REGN : 100-48-1 |
|---|---|
|  | |
| 4-Pyridinecarbonitrile (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H4N2 | CAS REGN : 100-54-9 |
|---|---|
|  | |
| 3-Pyridinecarbonitrile (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H4N2 | CAS REGN : 100-70-9 |
|---|---|
|  | |
| 2-Pyridinecarbonitrile (9CI)<br>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<br>Calculated entropy<br>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

Continued on next page

| | |
|---|---|
| GB (exp) : 166.8+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 182.3+/-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).

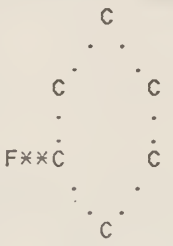
Method used : MS
Calculated entropy
Equilbrium relative to C6H6. Using GB and PA values respectively 167.8+/-2 and 181.2+/-2 kcal/mol

| | |
|---|---|
| GB (exp) : 166.8+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 182.5+/-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
Calculated entropy
Equilibrium; scale based on NH3

| 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

Continued on next page

| | |
|---|---|
| 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).

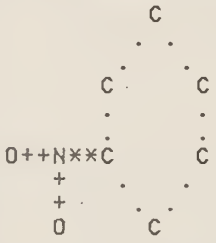
Method used : MS
Calculated entropy
Equilibrium relative to C6H6. Using GB and PA values respectively 167.8+/-2 and 181.2+/-2 kcal/mol

| | |
|---|---|
| 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 |
|---|---|



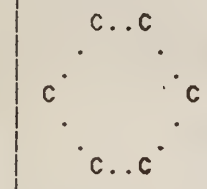
Benzene, nitro- (8CI9CI)

| GB (exp) : 176.7+/-2 kcal/mol | Temperature : 600 K |
|---|---|
| PA (exp) : 192.2+/-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+/-2

| 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 |

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 HCOOH
Entropy change assumed zero

| GB (exp) : 174.7+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 181.4+/-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).

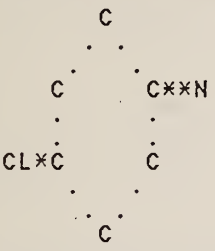
Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

Continued on next page

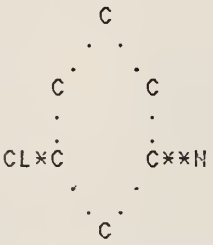
| | |
|---|---|
| GB (exp) : 167.8+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 181.2+/-2 kcal/mol | Temperature : 600 K |

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 |
|---|---|
|  | |
| Benzenamine, 4-chloro- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H6ClN | CAS REGN : 108-42-9 |
|---|---|



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 |
|---|---|

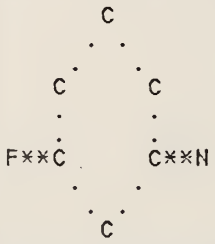
Benzenamine, 4-fluoro- (9CI)
Aniline, p-fluoro- (8CI)

| 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 |
|---|---|



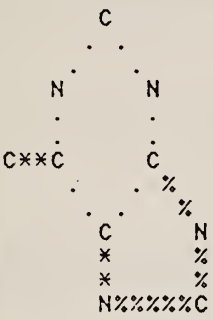
Benzenamine, 3-fluoro- (9CI)
Aniline, m-fluoro- (8CI)

| 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 |
|---|---|



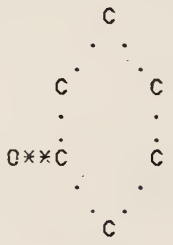
1H-Purine, 6-methyl- (9CI)
Purine, 6-methyl- (8CI)

| | |
|---|---|
| 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 : |

DeFrees, D. J. McIver, R. T., and Hehre, W. J.
The Proton Affinities of Phenol,
J. Am. Chem. Soc. 99, 3853 (1977).

Method used : ICR
Bracketing relative to various molecules. Oxygen protonation

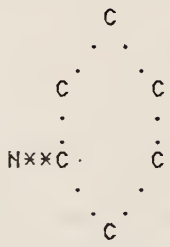
| GB (exp) : 179.1+/-2 kcal/mol | Temperature : 600 K |
|---|---|
| PA (exp) : 194.6+/-2 kcal/mol | Temperature : 600 K |

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 : ICR
Calculated entropy
Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2

| C6H6O | CAS REGN : 6921-27-3 |
|---|---|
| C##C**C**C**O**C**C##C | |
| 1-Propyne, 3,3'-oxybis- (9CI)<br>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<br>Calculated entropy<br>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

Continued on next page

| | |
|---|---|
| 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).

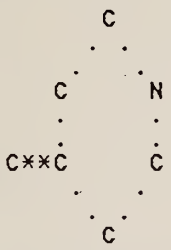
Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

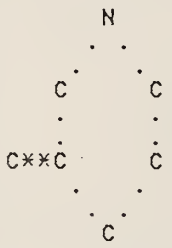
Continued on next page

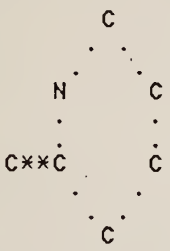
| | |
|---|---|
| GB (exp) : 199.9+/-2 kcal/mol | Temperature : 298 K |
| PA (exp) : 203.9+/-2 kcal/mol | Temperature : 298 K |

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

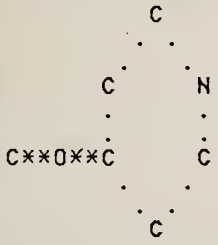
| C6H7N | CAS REGN : 108-89-4 |
|---|---|
|  | |
| Pyridine, 4-methyl- (9CI)<br>4-Picoline (8CI) | |
| GB (exp) : 214.30+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 222.10+/-2 kcal/mol | Temperature : 300 K |
| Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft. |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

| C6H7N | CAS REGN : 108-99-6 |
|---|---|
|  | |
| Pyridine, 3-methyl- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H7N | CAS REGN : 109-06-8 |
|---|---|
|  | |
| Pyridine, 2-methyl- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H7N | CAS REGN : 6921-28-4 |
|---|---|
| C#CC**C**N**C**C#C | |
| 2-Propyn-1-amine, N-2-propynyl- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H7NO | CAS REGN : 620-08-6 |
|---|---|



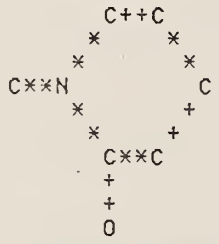
Pyridine, 4-methoxy- (8CI9CI)

| 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 |
|---|---|

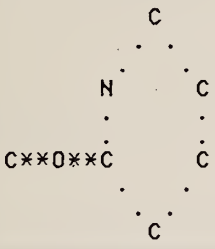


2(1H)-Pyridinone, 1-methyl- (9CI)
2(1H)-Pyridone, 1-methyl- (8CI)

| | |
|---|---|
| PA (exp) : 217.2+/-2 kcal/mol | Temperature : |

Cook, M. J., Katritzky, A. R., Taagepera, M., 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).

Method used : ICR
Equilibrium relative to pyridine. Use value of PA (pyridine) = 210.1
Entropy change assumed zero

| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

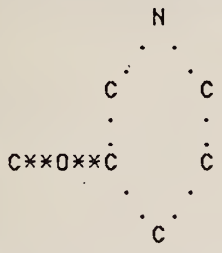
Continued on next page

| | |
|---|---|
| PA (exp) : 219.8+/-2 kcal/mol | Temperature : |

Cook, M. J., Katritzky, A. R., Taagepera, M., 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).

Method used : ICR
Equilibrium relative to t-Butylamine. Use value of PA (t-C4H9NH2) = 218.8
Entropy change assumed zero

| C6H7NO | CAS REGN : 7295-76-3 |
|---|---|



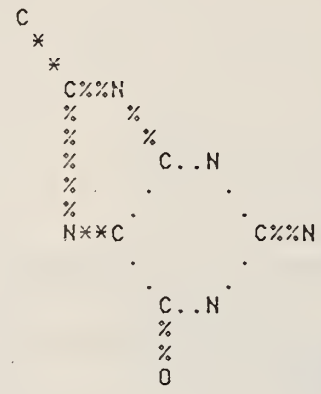

Pyridine, 3-methoxy- (8CI9CI)

| 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 |
|---|---|



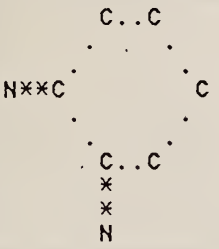
6H-Purin-6-one, 2-amino-1,7-dihydro-8-methyl- (9CI)
Guanine, 8-methyl- (8CI)

| | |
|---|---|
| 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 |
|---|---|



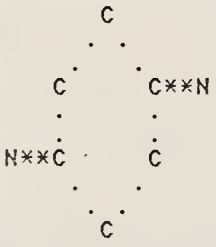
1,2-Benzenediamine (9CI)
o-Phenylenediamine (8CI)

| 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 |
|---|---|



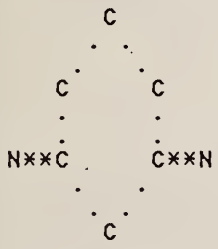
1,4-Benzenediamine (9CI)
p-Phenylenediamine (8CI)

| 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 |
|---|---|



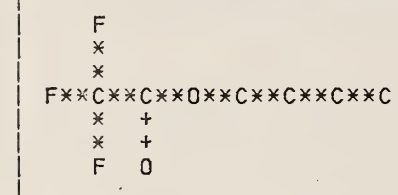
1,3-Benzenediamine (9CI)
m-Phenylenediamine (8CI)

| GB (exp) : >202.9 kcal/mol | Temperature : 424-473 K |
|---|---|
| | |

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 CH3NH2

| C6H9F3O2 | CAS REGN : 367-64-6 |
|---|---|



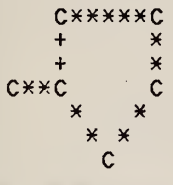
Acetic acid, trifluoro-, butyl ester (8CI9CI)

| GB (exp) : 176.6+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 184.4+/-2 kcal/mol | Temperature : 300 K |

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

| C6H10 | CAS REGN : 693-89-0 |
|---|---|



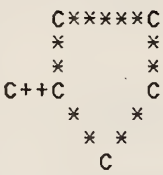
Cyclopentene, 1-methyl- (8CI9CI)

| 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 |
|---|---|



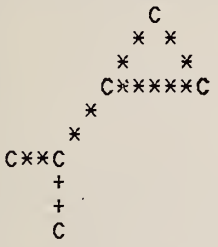
Cyclopentane, methylene- (8CI9CI)

| 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 |
|---|---|



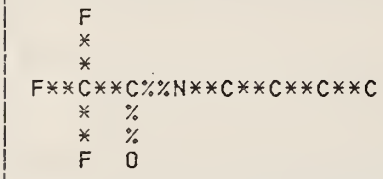
Cyclopropane, (1-methylethenyl)- (9CI)
Propene, 2-cyclopropyl- (8CI)

| 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 |
|---|---|



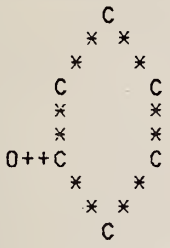
Acetamide, N-butyl-2,2,2-trifluoro- (8CI9CI)

| GB (exp) : 193.9+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 201.7+/-2 kcal/mol | Temperature : 300 K |

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

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

| C6H10O | CAS REGN : 108-94-1 |
|---|---|



Cyclohexanone (3CI9CI)

| | |
|---|---|
| PA (exp) : 204 kcal/mol | Temperature : |

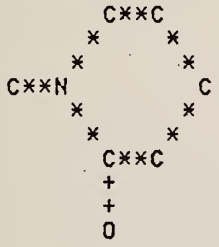
Jelus, B. L., Murray, R. K., Jr., Munson, B.,
Studies in Chemical Ionization Mass Spectrometry.
Secondary Alcohols with Isobutane,
J. Am. Chem. Soc. 97, 2362 (1975).

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

| C6H10O | CAS REGN : 557-40-4 |
|---|---|
| C++C**C**O**C**C++C | |
| 1-Propene, 3,3'-oxybis- (9CI)<br>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<br>Calculated entropy<br>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)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H11NO | CAS REGN : 931-20-4 |
|---|---|



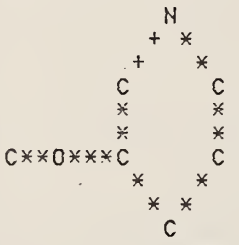
2-Piperidinone, 1-methyl- (9CI)
2-Piperidone, 1-methyl- (8CI)

| | |
|---|---|
| PA (exp) : 216.8+/-2 kcal/mol | Temperature : |

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).

Method used : ICR
Equilibrium relative to i-C3H7NH2. Use value of PA (i-C3H7NH2) = 216.5
Entropy change assumed zero

| C6H11NO | CAS REGN : 53687-79-9 |
|---|---|



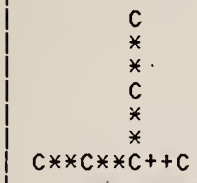
Piperidine, 2-methoxy-

| | |
|---|---|
| PA (exp) : 226.3+/-2 kcal/mol | Temperature : |

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).

Method used : ICR
Equilibrium relative to (i-C3H7)2NH. Use value of PA(i-C3H7)2NH = 266.6
Entropy change assumed zero

| C6H12 | CAS REGN : Not available |
|---|---|



| 1-Butene, 2-ethyl- | |
|---|---|
| | |
| PA (exp) : 197.7+/-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 : 616-12-6 |
|---|---|
| C**C++C**C**C<br>*<br>*<br>C | |
| 2-Pentene, 3-methyl-, (E)- (8CI9CI) | |
| | |
| PA (exp) : 196.1+/-2 kcal/mol | Temperature : 363-553 K |
| Goren, A., and Munson, B.<br>Thermochemistry of Alkyl Ions,<br>J. Phys. Chem. 80, 2848 (1976). | |
| Method used : MS<br>Equilibrium of hydride transfer reaction between<br>(t-C4H9+) + Et2CHMe and between (t-C5H11+) + Et2CHMe.<br>This delta H of the reaction was determined from van't<br>Hoff plot. PA (M) derived from the obtained delta Hf(MH+);<br>scale based on delta Hf(t-C4H9+) = 169 | |

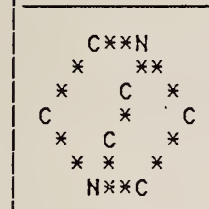
| C6H12 | CAS REGN : 625-27-4 |
|---|---|
| C**C**C++C**C<br>*<br>*<br>C | |
| 2-Pentene, 2-methyl- (8CI9CI) | |
| | |
| PA (exp) : 196.4+/-2 kcal/mol | Temperature : 363-553 K |

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

| C6H12N2 | CAS REGN : 280-57-9 |
|---|---|



1,4-Diazabicyclo[2.2.2]octane (8CI9CI)

| GB (exp) : 217.20+/-2 kcal/mol | Temperature : |
|---|---|
| | |

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) : 217.90+/-2 kcal/mol | Temperature : 298 K |
|---|---|
| PA (exp) : 225.90+/-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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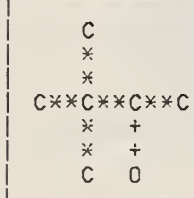
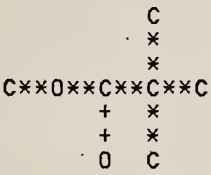
| | |
|---|---|
| PA (exp) : 225.50+/-2 kcal/mol | Temperature : |
| Staley, R., and Beauchamp, J. L.,<br>Relationship of Nitrogen Lone Pair Interactions<br>to Thermodynamic Parameters Associated with Amine<br>Basicities,<br>J. Am. Chem. Soc. 96, 1604 (1974). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| | |
|---|---|
| C6H12O | CAS REGN : 75-97-8 |
|  | |
| 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 |
| Unpublished work by Wolf, Staley, Koppel, Taagepera,<br>McIver, Beauchamp, and Taft. | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H12O2 | CAS REGN : 598-98-1 |
|---|---|



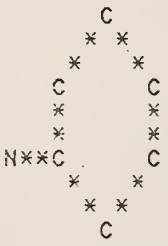
Propanoic acid, 2,2-dimethyl-, methyl ester (9CI)
Pivalic acid, methyl ester (8CI)

| 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 |
|---|---|



| Cyclohexanamine (9CI)<br>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<br>Calculated entropy<br>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 Bowers, M. T.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

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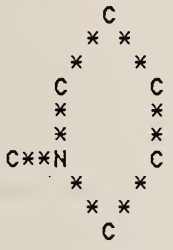
| | |
|---|---|
| GB (exp) : 204.8+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 222+/-2 kcal/mol | Temperature : 600 K |
| Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem.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

| | |
|---|---|
| C6H13N | CAS REGN : 626-67-5 |



| | |
|---|---|
| Piperidine, 1-methyl- (8CI9CI) | |
| GB (exp) : 218.8+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 226.6+/-2 kcal/mol | Temperature : 300 K |
| Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft. | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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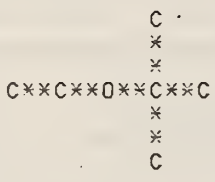
| | |
|---|---|
| GB (exp) : 218.3+/-2 kcal/mol | Temperature : 298 K |
| PA (exp) : 226.1+/-2 kcal/mol | Temperature : 298 K |
| Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).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

| | |
|---|---|
| C6H14O | CAS REGN : 108-20-3 |
| C**C**O**C**C<br>* *<br>* *<br>C C | |
| Propane, 2,2'-oxybis- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H14O | CAS REGN : 111-43-3 |
|---|---|
| C**C**C**O**C**C**C | |
| Propane, 1,1'-oxybis- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H14O | CAS REGN : 637-92-3 |
|---|---|
|  | |
| Propane, 2-ethoxy-2-methyl- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H14S | CAS REGN : 111-47-7 |
|---|---|
| C**C**C**S**C**C**C | |
| Propane, 1,1'-thiobis- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H14S | CAS REGN : 625-80-9 |
|---|---|
| C**C**S**C**C<br>*  *<br>*  *<br>C  C | |
| Propane, 2,2'-thiobis- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H15N | CAS REGN : 108-18-9 |
|---|---|

```
C**C**N**C**C
   *     *
   *     *
   C     C
```

2-Propanamine, N-(1-methylethyl)- (9CI)
Diisopropylamine (8CI)

| GB (exp) : 218.40+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 226.60+/-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) : 217.90+/-2 kcal/mol | Temperature : 298 K |
|---|---|
| PA (exp) : 226.1+/-2 kcal/mol | Temperature : 298 K |

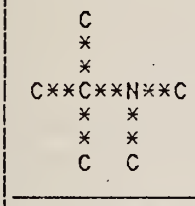
Aue, D. H., Webb, H. M., and Bowers, M. T.,
A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,
J. Am. Chem. Soc. 98, 318 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

| C6H15N | CAS REGN : 111-26-2 |
|---|---|
| N**C**C**C**C**C**C | |
| 1-Hexanamine (9CI)<br>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.,<br>Quantitative Evaluation of Intramolecular Strong<br>Hydrogen Bonding in the Gas Phase,<br>J. Am. Chem. Soc. 95, 2669 (1973). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

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

| | |
|---|---|
| C6H15N | CAS REGN : 142-84-7 |
| C**C**C**N**C**C**C | |
| 1-Propanamine, N-propyl- (9CI)<br>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<br>Calculated entropy<br>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.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| C6H15N | CAS REGN : 918-02-5 |
|---|---|
|  | |
| 2-Propanamine, N,N,2-trimethyl- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C6H16N2 | CAS REGN : 110-18-9 |
|---|---|
| C**N**C**C**N**C<br>*  *<br>*  *<br>C  C | |
| 1,2-Ethanediamine, N,N,N',N'-tetramethyl- (9CI)<br>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, Taagepera, McIver, Beauchamp, and Taft. | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |
| GB (exp) : 224+/-2 kcal/mol | Temperature : 298 K |
| | |
| Taft, R. W.,<br>Proton-Transfer Reactions,<br>Ed. E. F. Caldin and V. Gold,<br>(John Wiley and Sons, New York, 1975) Ch. 2. | |
| Method used : ICR<br>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<br>Calculated entropy<br>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<br>Equilibrium; scale based on (CH3)3N<br>Van't Hoff plot | |

| C6H17NSi | CAS REGN : 18182-40-6 |
|---|---|

```
          C
          *
          *
C**N**C**SI*C
   *      *
   *      *
   C      C
```

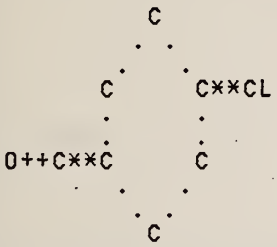
Methanamine, N,N-dimethyl-1-(trimethylsilyl)- (9CI)
Trimethylamine, (trimethylsilyl)- (8CI)

| 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 |
|---|---|



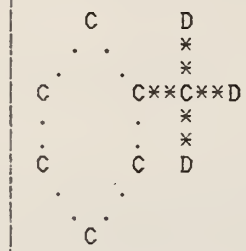

Benzaldehyde, 4-chloro- (9CI)
Benzaldehyde, p-chloro- (8CI)

| 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 |
|---|---|



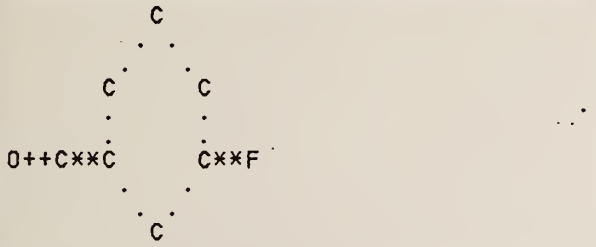
Benzene, methyl-d3-

| GB (exp) : 180.9+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 188.7+/-2 kcal/mol | Temperature : 300 K |

Ausloos, P., and Lias, S. G.
Equilibrium Isotope Effects on the Proton Transfer Reactions of Methylbenzenes,
J. Am. Chem. Soc. 99, 4198 (1977).

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

| C7H5FO | CAS REGN : 456-48-4 |
|---|---|

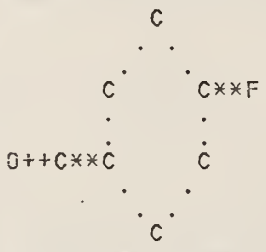


Benzaldehyde, 3-fluoro- (9CI)
Benzaldehyde, m-fluoro- (8CI)

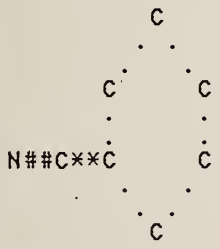
| GB (exp) : 186.3+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 194.1+/-2 kcal/mol | Temperature : 300 K |

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)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C7H5N | CAS REGN : 100-47-0 |
|---|---|



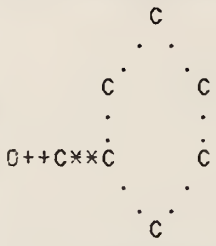
Benzonitrile (8CI9CI)

| GB (exp) : 179.2+/-2 kcal/mol | Temperature : 600 K |
|---|---|
| PA (exp) : 194.7+/-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+/-2

| C7H6O | CAS REGN : 100-52-7 |
|---|---|



| Benzaldehyde (8CI9CI) | |
|---|---|
| GB (exp) : 190.4 kcal/mol | Temperature : 300 K |
| PA (exp) : 198.2 kcal/mol | Temperature : 300 K |

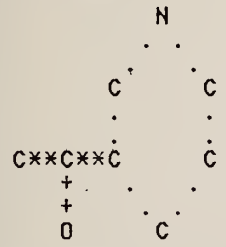
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

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

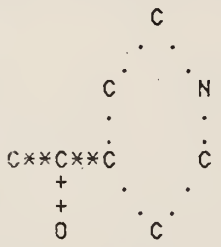
| | |
|---|---|
| GB (exp) : 183.2+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 198.7+/-2 kcal/mol | Temperature : 600 K |

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+/-2

| C7H7NO | CAS REGN : 350-03-8 |
|---|---|
|  | |
| Ethanone, 1-(3-pyridinyl)- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C7H7NO | CAS REGN : 1122-54-9 |
|---|---|



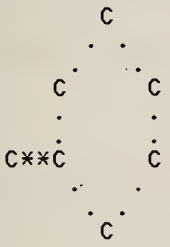
Ethanone, 1-(4-pyridinyl)- (9CI)
Ketone, methyl 4-pyridyl (8CI)

| 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

Continued on next page

| | |
|---|---|
| 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<br>Equilibrium relative to C6H6(Benzene)<br>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<br>Equilibrium relative to C6H6(Benzene)<br>Protonation position 1 | |
| GB (exp) : 174.1+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 189.6+/-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<br>Calculated entropy<br>Equilibrium relative to C6H6. Using GB and PA values respectively 167.8+/-2 and 181.2+/-2 kcal/mol | |

Continued on next page

| | |
|---|---|
| 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

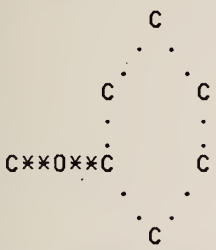
Continued on next page

| | |
|---|---|
| GB (exp) : 180.1+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 187.9+/-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)

| C7H8O | CAS REGN : 100-66-3 |
|---|---|

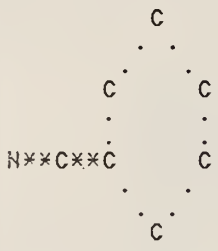


Benzene, methoxy- (9CI)
Anisole (8CI)

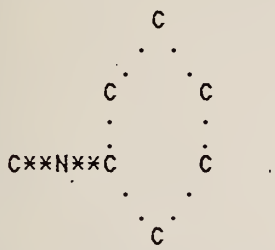
| GB (exp) : 183.5+/-2 kcal/mol | Temperature : 600 K |
|---|---|
| PA (exp) : 199+/-2 kcal/mol | Temperature : 600 K |

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+/-2

| C7H9N | CAS REGN : 100-46-9 |
|---|---|
|  | |
| Benzenemethanamine (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C7H9N | CAS REGN : 100-61-8 |
|---|---|



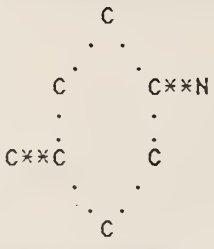
Benzenamine, N-methyl- (9CI)
Aniline, N-methyl- (8CI)

| GB (exp) : 200.2+/-2 kcal/mol | Temperature : 600 K |
|---|---|
| PA (exp) : 217.4+/-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

| C7H9N | CAS REGN : 106-49-0 |
|---|---|



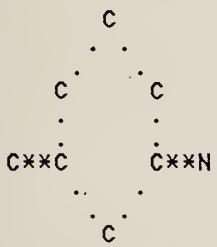
Benzenamine, 4-methyl- (9CI)
p-Toluidine (8CI)

| 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 |

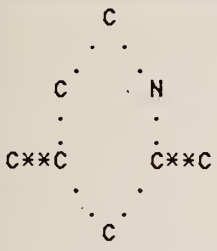
Pollack, S. K., Devlin, J. L., III, Summerhays, K. D., Taft, R. W., and Hehre, W J.
The Site of Protonation in Aniline,
J. Am. Chem. Soc. 99, 4583 (1977).

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

Continued on next page

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

| C7H9N | CAS REGN : 108-47-4 |
|---|---|



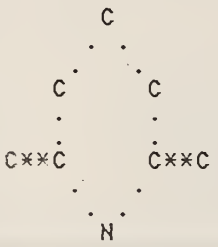
Pyridine, 2,4-dimethyl- (9CI)
2,4-Lutidine (8CI)

| | |
|---|---|
| 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 |
|---|---|



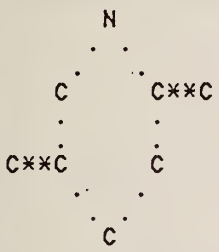
Pyridine, 2,6-dimethyl- (9CI)
2,6-Lutidine (8CI)

| | |
|---|---|
| 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 |
|---|---|

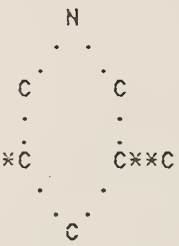



Pyridine, 2,5-dimethyl- (9CI)
2,5-Lutidine (8CI)

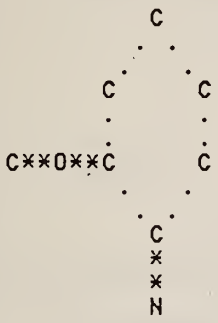
| | |
|---|---|
| PA (exp) : 224.5+/-2 kcal/mol | Temperature : 298 K |

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 |
|---|---|
|  | |
| Pyridine, 3,5-dimethyl- (9CI)<br>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.<br>A Quantitative Comparison of Gas- and Solution-Phase Basicities of Substituted Pyridines,<br>J. Am. Chem. Soc. 98, 854 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C7H9NO | CAS REGN : 90-04-0 |
|---|---|



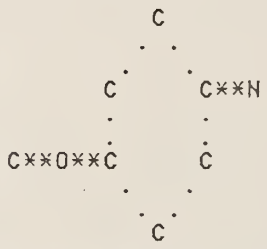
Benzenamine, 2-methoxy- (9CI)
o-Anisidine (8CI)

| 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 |
|---|---|

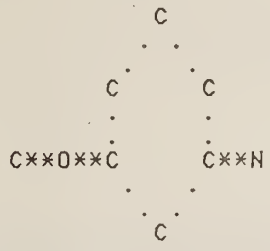



Benzenamine, 4-methoxy- (9CI)
p-Anisidine (8CI)

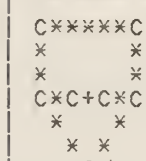
| GB (exp) : 203.9+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 212.3+/-2 kcal/mol | Temperature : 300 K |

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)<br>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.<br>Gas-Phase Basicities of Substituted Anilines. Inferences about the Role of Solvent in Dictating Site of Protonation,<br>J. Am. Chem. Soc. 99, 4585 (1977). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale base on NH3. Ring protonation | |

| C7H10 | CAS REGN : 498-66-8 |
|---|---|



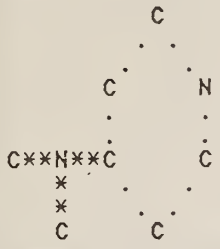
Bicyclo[2.2.1]hept-2-ene (9CI)
2-Norbornene (8CI)

| | |
|---|---|
| | |
| 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 |
|---|---|



4-Pyridinamine, N,N-dimethyl- (9CI)
Pyridine, 4-(dimethylamino)- (8CI)

| GB (exp) : 224.90+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 232.70+/-2 kcal/mol | Temperature : 300 K |

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

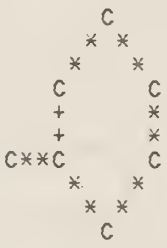
Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

| GB (exp) : >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

| C7H12 | CAS REGN : 591-49-1 |
|---|---|



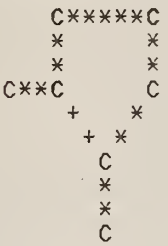
Cyclohexene, 1-methyl- (8CI9CI)

| 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 |
|---|---|



Cyclopentene, 1,2-dimethyl- (8CI9CI)

| GB (exp) : 188.4+/-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

| C7H13N | CAS REGN : 100-76-5 |
|---|---|
|  | |
| 1-Azabicyclo[2.2.2]octane (9CI)<br>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<br>Calculated entropy<br>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.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

Continued on next page

| 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

| C7H17N | CAS REGN : 111-68-2 |
|---|---|

C**C**C**C**C**C**C**N

1-Heptanamine (9CI)
Heptylamine (8CI)

| GB (exp) : 208.2+/-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

| C7H17N | CAS REGN : 4458-31-5 |
|---|---|

```
C**C**N**C**C**C
      *
      *
      C
      *
      *
      C
```

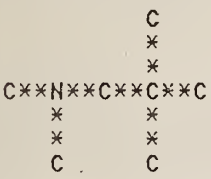
1-Propanamine, N,N-diethyl- (9CI)
Propylamine, N,N-diethyl- (8CI)

| 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 |
|---|---|



1-Propanamine, N,N,2,2-tetramethyl- (9CI)
Propylamine, N,N,2,2-tetramethyl- (8CI)

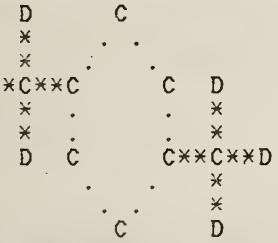
| GB (exp) : 218.6+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 226.4+/-2 kcal/mol | Temperature : 300 K |

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<br>*  *<br>*  *<br>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<br>Equilibrium; scale based on NH3 | |

| C8H4D6 | CAS REGN : 25493-13-4 |
|---|---|



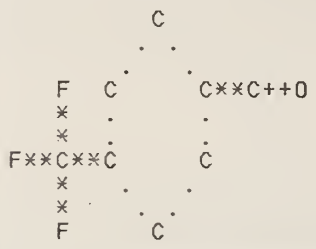
Benzene, 1,4-(dimethyl-d3)-

| GB (exp) : 182.9+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 189.8+/-2 kcal/mol | Temperature : 300 K |

Ausloos, P., and Lias, S. G.
Equilibrium Isotope Effects on the Proton Transfer
Reactions of Methylbenzenes,
J. Am. Chem. Soc. 99, 4198 (1977).

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

| C8H5F3O | CAS REGN : 455-19-6 |
|---|---|



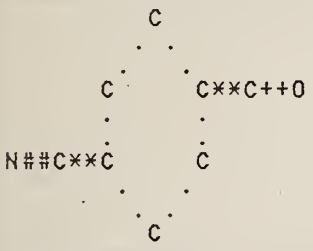
Benzaldehyde, 4-(trifluoromethyl)- (9CI)
p-Tolualdehyde, .alpha.,.alpha.,.alpha.-trifluoro- (8CI)

| GB (exp) : 181.3+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 189.1+/-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

| C8H5NO | CAS REGN : 105-07-7 |
|---|---|



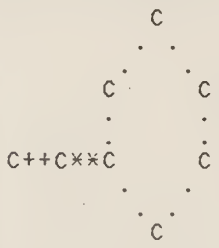
Benzonitrile, 4-formyl- (9CI)
Terephthalaldehydonitrile (8CI)

| 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 |
|---|---|



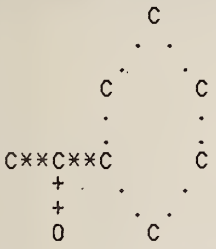
Benzene, ethenyl- (9CI)
Styrene (8CI)

| GB (exp) : 191.5+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 199.3+/-2 kcal/mol | Temperature : 300 K |

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

| C8H8O | CAS REGN : 98-86-2 |
|---|---|



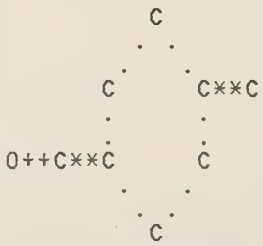
Ethanone, 1-phenyl- (9CI)
Acetophenone (8CI)

| 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 |
|---|---|



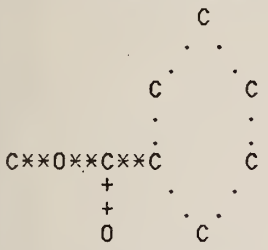
Benzaldehyde, 4-methyl- (9CI)
p-Tolualdehyde (8CI)

| 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 |
|---|---|

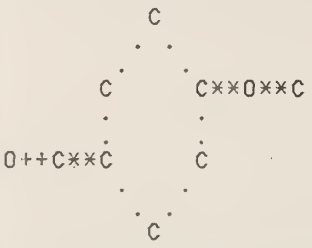


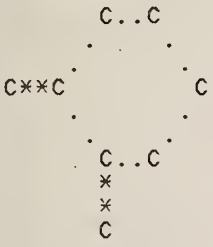
Benzoic acid, methyl ester (8CI9CI)

| GB (exp) : 193.1+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 200.9+/-2 kcal/mol | Temperature : 300 K |

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

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

| C8H8O2 | CAS REGN : 123-11-5 |
|---|---|
|  | |
| Benzaldehyde, 4-methoxy- (9CI)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C8H10 | CAS REGN : 95-47-6 |
|---|---|
|  | |
| Benzene, 1,2-dimethyl- (9CI)<br>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.,<br>Proton Affinities of Benzene, Toluene, and the Xylenes,<br>J. Am. Chem. Soc. 94, 6630 (1972). | |
| Method used : MS<br>Equilibrium relative to CH3SH and (CH3)2O<br>Entropy change assumed zero | |

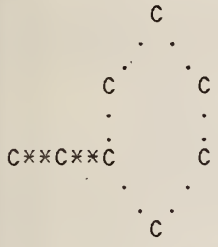
Continued on next page

| | |
|---|---|
| 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)

Continued on next page

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

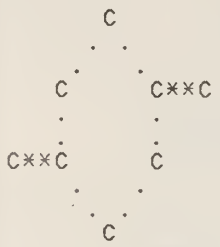
Continued on next page

| | |
|---|---|
| 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 |
|---|---|



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).

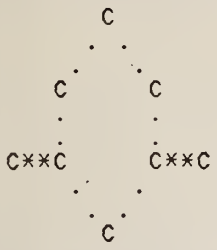
Method used : MS
Equilibrium; scale based on CH3SH and (CH3)2O
Entropy change assumed zero

| 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 |
|---|---|

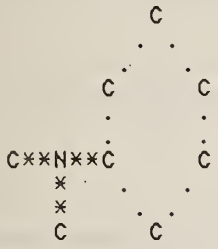
Benzenamine, N-ethyl- (9CI)
Aniline, N-ethyl- (8CI)

| GB (exp) : 203.6+/-2 kcal/mol | Temperature : 600 K |
|---|---|
| PA (exp) : 220.8+/-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 : ICR
Equilibrium; scale based on NH3
Entropy change assumed zero

| C8H11N | CAS REGN : 121-69-7 |
|---|---|



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 |

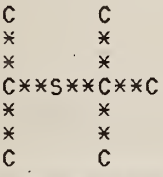
Pollack, S. K., Devlin, J. L., III, Summerhays, K. D., Taft, R. W., and Hehre, W. J.
The Site of Protonation in Aniline,
J. Am. Chem. Soc. 99, 4583 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3. Protonation on the nitrogen

Continued on next page

| | |
|---|---|
| GB (exp) : 206.8+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 224+/-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<br>Equilibrium; scale based on NH3<br>Entropy change assumed zero | |
| 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<br>Bracketing relative to (CH3)2NH | |

| C8H18S | CAS REGN : 107-47-1 |
|---|---|



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

| C8H19N | CAS REGN : 111-92-2 |
|---|---|
| C**C**C**C**N**C**C**C**C | |
| 1-Butanamine, N-butyl- (9CI)<br>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.,<br>Quantitative Proton Affinities, Ionization Potentials,<br>and Hydrogen Affinities of Alkylamines,<br>J. Am. Chem. Soc. 98, 311 (1976). | |
| Method used : ICR<br>Calculated entropy<br>Equilibrium; scale based on CH3NH2 | |

| C8H19N | CAS REGN : 626-23-3 |
|---|---|

```
C**C**C**N**C**C**C
      *     *
      *     *
      C     C
```

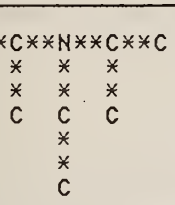
2-Butanamine, N-(1-methylpropyl)- (9CI)
Di-sec-butylamine (8CI)

| 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 |
|---|---|



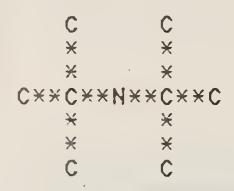
2-Propanamine, N-ethyl-N-(1-methylethyl)- (9CI)
Triethylamine, 1,1'-dimethyl- (8CI)

| 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 |
|---|---|



2-Propanamine, N-(1,1-dimethylethyl)-2-methyl- (9CI)
Di-tert-butylamine (8CI)

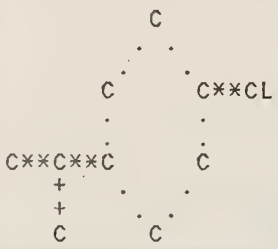
| GB (exp) : 221.7+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 229.9+/-2 kcal/mol | Temperature : 300 K |

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<br>* *<br>* *<br>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<br>Equilibrium; scale based on NH3 | |

| C9H9Cl | CAS REGN : 1712-70-5 |
|---|---|



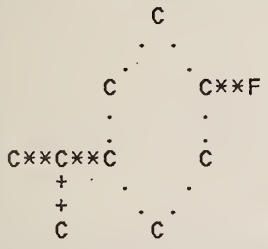

Benzene, 1-chloro-4-(1-methylethenyl)- (9CI)
Styrene, p-chloro-.alpha.-methyl- (8CI)

| 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 |
|---|---|



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 |
|---|---|

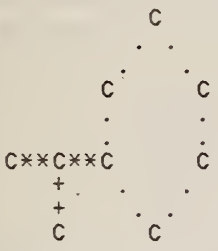
```
C##C**C**N**C**C##C
        *
        *
        C
        *
        *
        C
        #
        #
        C
```

2-Propyn-1-amine, N,N-di-2-propynyl- (9CI)
Tri-2-propynylamine (8CI)

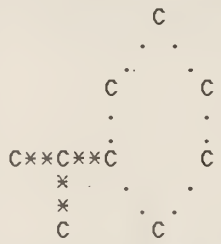
| GB (exp) : 209.3+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 217.1+/-2 kcal/mol | Temperature : 300 K |

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)<br>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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C9H12 | CAS REGN : 98-82-8 |
|---|---|



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)

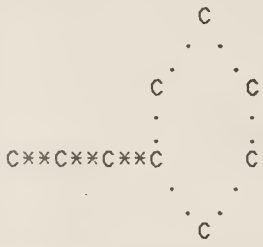
Continued on next page

| | |
|---|---|
| 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)

Continued on next page

| | |
|---|---|
| GB (exp) : 181.8+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 190+/-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).

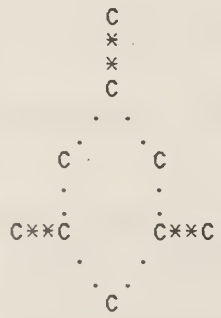
Method used : MS
Calculated entropy
Equilibrium; scale based on C6H6(Benzene)

| | |
|---|---|
| GB (exp) : 182.6+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 190.4+/-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

| C9H12 | CAS REGN : 108-67-8 |
|---|---|



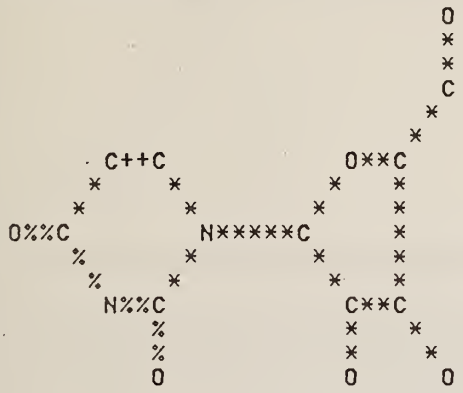
Benzene, 1,3,5-trimethyl- (9CI)
Mesitylene (8CI)

| GB (exp) : 191.3+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 198.4+/-2 kcal/mol | Temperature : 300 K |

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 benzene

| C9H12N2O6 | CAS REGN : 58-96-8 |
|---|---|



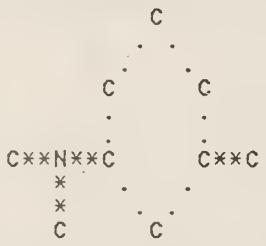
Uridine (8CI9CI)

| | |
|---|---|
| | |
| 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.

| C9H13N | CAS REGN : 121-72-2 |
|---|---|



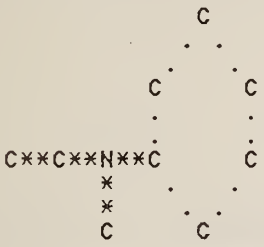
Benzenamine, N,N,3-trimethyl- (9CI)
m-Toluidine, N,N-dimethyl- (8CI)

| | |
|---|---|
| | |
| 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 |
|---|---|



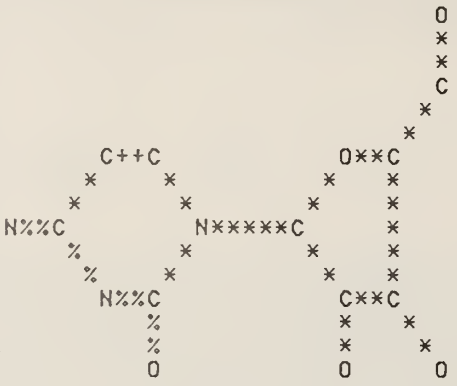
Benzenamine, N-ethyl-N-methyl- (9CI)
Aniline, N-ethyl-N-methyl- (8CI)

| GB (exp) : 209.40+/-2 kcal/mol | Temperature : 600 K |
|---|---|
| PA (exp) : 226.60+/-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 NH3

| C9H13N3O5 | CAS REGN : 65-46-3 |
|---|---|



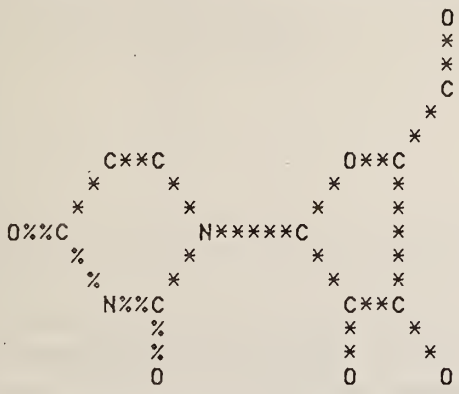
Cytidine (9CI)

| | |
|---|---|
| | |
| 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.

| C9H14N2O6 | CAS REGN : 5627-05-4 |
|---|---|



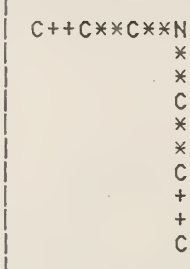
Uridine, 5,6-dihydro- (9CI)
Hydrouracil, 1-.beta.-D-ribofuranosyl- (8CI)

| | |
|---|---|
| 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.

| C9H15N | CAS REGN : 102-70-5 |
|---|---|



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 |
|---|---|

```
C**C**C**N**C**C**C
         *
         *
         C
         *
         *
         C
         *
         *
         C
```

1-Propanamine, N,N-dipropyl- (9CI)
Tripropylamine (8CI)

| GB (exp) : 223.1+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 230.9+/-2 kcal/mol | Temperature : 300 K |

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

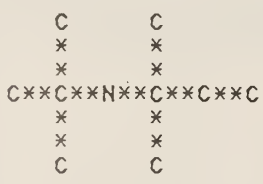
Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

| GB (exp) : 222.8+/-2 kcal/mol | Temperature : 298 K |
|---|---|
| PA (exp) : 230.60+/-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

| C9H21N | CAS REGN : 2085-66-7 |
|---|---|



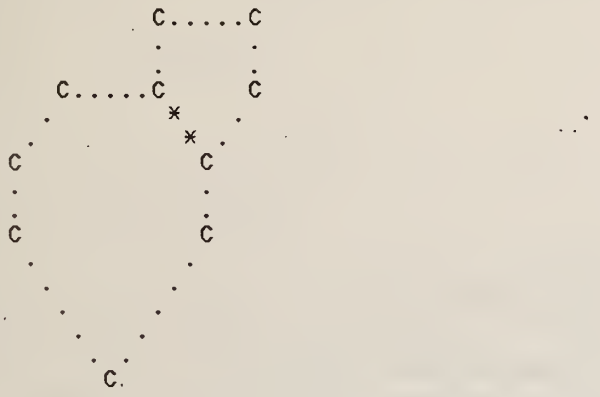
Propylamine, N-tert-butyl-1,1-dimethyl- (8CI)

| 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 |
|---|---|



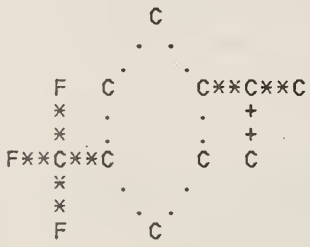
Azulene (8CI9CI)

| 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 |
|---|---|



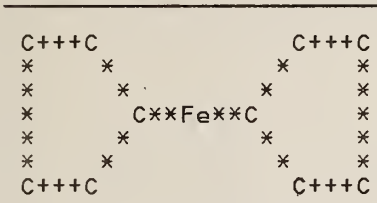
Benzene, 1-(1-methylethenyl)-4-(trifluoromethyl)- (9CI)

| GB (exp) : 189.3+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 197.1+/-2 kcal/mol | Temperature : 300 K |

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

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

| C10H10Fe | CAS REGN : 102-54-5 |
|---|---|



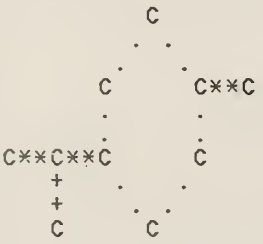
Ferrocene (8CI9CI)

| | |
|---|---|
| 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 |
|---|---|



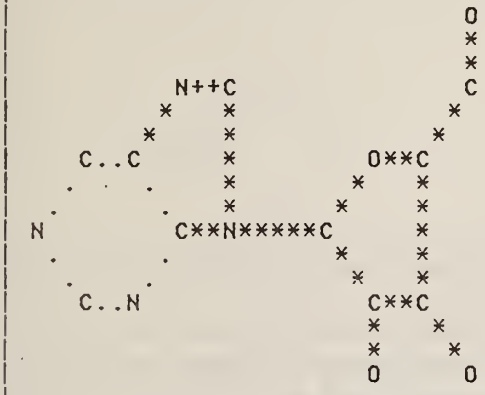
Benzene, 1-methyl-4-(1-methylethenyl)- (9CI)
Styrene, p,.alpha.-dimethyl- (8CI)

| 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

| C10H12N4O4 | CAS REGN : 550-33-4 |
|---|---|



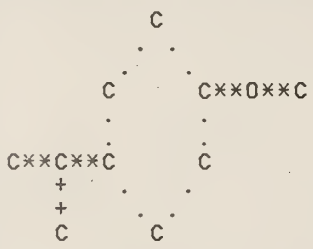
9H-Purine, 9-.beta.-D-ribofuranosyl- (8CI9CI)

| | |
|---|---|
| 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.

| C10H12O | CAS REGN : 1712-69-2 |
|---|---|



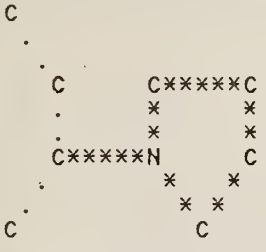
Benzene, 1-methoxy-4-(1-methylethenyl)- (9CI)
Anisole, p-isopropenyl- (8CI)

| 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 |
|---|---|



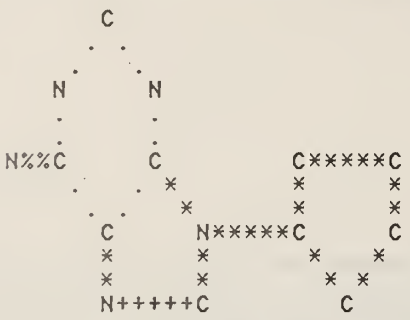
Pyrrolidine, 1-phenyl- (8CI9CI)

| 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

| C10H13N5 | CAS REGN : 715-91-3 |
|---|---|



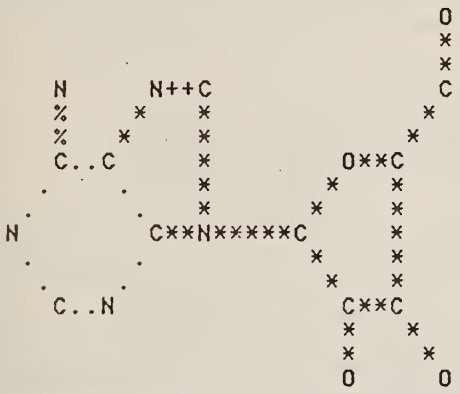
9H-Purin-1-amine, 9-cyclopentyl- (9CI)
Adenine, 9-cyclopentyl- (8CI)

| | |
|---|---|
| | |
| PA (exp) : >222.1 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

| C10H13N5O4 | CAS REGN : 58-61-7 |
|---|---|



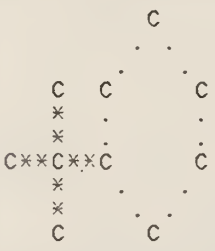
Adenosine (8CI9CI)

| | |
|---|---|
| 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.

| C10H14 | CAS REGN : 98-06-6 |
|---|---|



Benzene, (1,1-dimethylethyl)- (9CI)
Benzene, tert-butyl- (8CI)

| GB (exp) : 183.2+/-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)

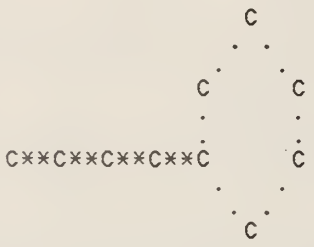
Continued on next page

| | |
|---|---|
| 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 |
|---|---|



Benzene, butyl- (8CI9CI)

| 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)

Continued on next page

| | |
|---|---|
| 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).

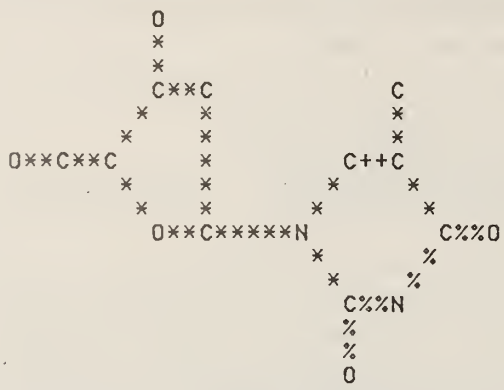
Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

| | |
|---|---|
| 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)

| C10H14N2O5 | CAS REGN : 50-89-5 |
|---|---|



Thymidine (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.

| 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 |
|---|---|

1-Azabicyclo[3.3.3]undecane (9CI)

| | |
|---|---|
| PA (exp) : 227.9+/-2 kcal/mol | Temperature : 298 K |

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).

Method used : ICR
Equilibrium; scale based on CH3NH2
Van't Hoff plot

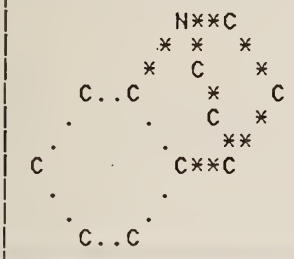
| C10H23N | CAS REGN : 2016-57-1 |
|---|---|
| N**C**C**C**C**C**C**C**C**C**C | |
| 1-Decanamine (9CI)<br>Decylamine (8CI) | |
| GB (exp) : >209.7 kcal/mol | Temperature : 423-473 K |
| | |

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<br>*  *<br>*  *<br>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<br>Equilibrium; scale based on NH3 | |

| C11H13N | CAS REGN : 4363-25-1 |
|---|---|



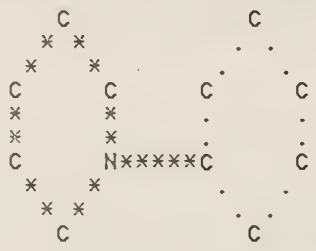
2H-1,4-Ethanoquinoline, 3,4-dihydro- (8CI9CI)

| 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 |
|---|---|



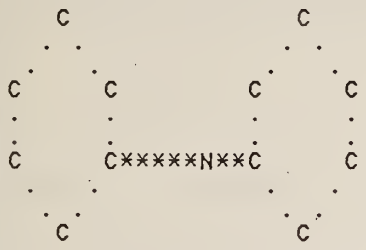
Piperidine, 1-phenyl- (8CI9CI)

| 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 REGN : 122-39-4 |
|---|---|



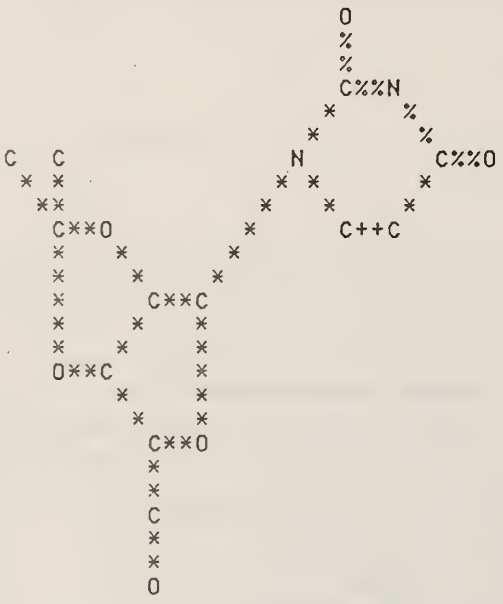
Benzenamine, N-phenyl- (9CI)
Diphenylamine (8CI)

| 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

| C12H16N2O6 | CAS REGN : 362-43-6 |
|---|---|

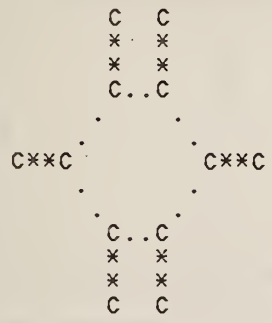


Uridine, 2',3'-O-(1-methylethylidene)- (9CI)
Uridine, 2',3'-O-isopropylidene- (8CI)

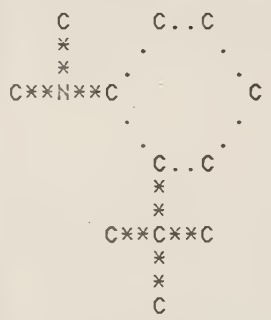
| | |
|---|---|
| PA (exp) : 207+/-5 kcal/mol | Temperature : |

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 CH3NH2 and NH3.

| C12H18 | CAS REGN : 87-85-4 |
|---|---|
|  | |
| 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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

| C12H19N | CAS REGN : 22025-87-2 |
|---|---|



Benzenamine, 2-(1,1-dimethylethyl)-N,N-dimethyl- (9CI)
Aniline, o-tert-butyl-N,N-dimethyl- (8CI)

| GB (exp) : 218+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : 225.8+/-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

| C12H27N | CAS REGN : 102-82-9 |
|---|---|

```
C**C**C**C**N**C**C**C**C
          *
          *
          C
          *
          *
          C
          *
          *
          C
          *
          *
          C
```

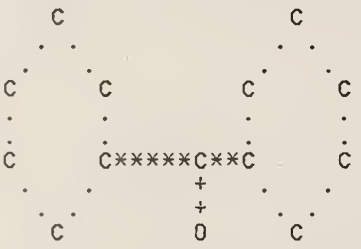
1-Butanamine, N,N-dibutyl- (9CI)
Tributylamine (8CI)

| GB (exp) : 224.1+/-2 kcal/mol | Temperature : 298 K |
|---|---|
| PA (exp) : 232+/-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

| C13H10O | CAS REGN : 119-61-9 |
|---|---|



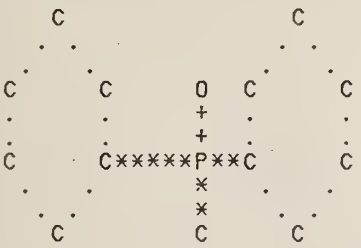
Methanone, diphenyl- (9CI)
Benzophenone (8CI)

| GB (exp) : ~200.7+/-2 kcal/mol | Temperature : 300 K |
|---|---|
| PA (exp) : ~208.1+/-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

| C13H13OP | CAS REGN : 2129-89-7 |
|---|---|



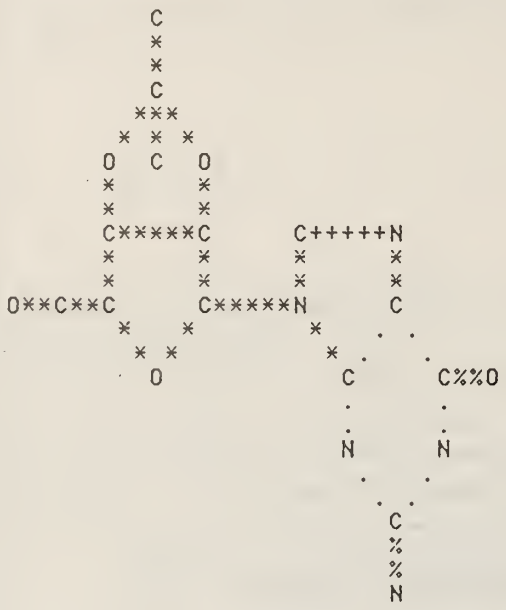
Phosphine oxide, methyldiphenyl- (8CI9CI)

| | |
|---|---|
| PA (exp) : 220+/-3 kcal/mol | Temperature : ~400 K |

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).

Method used : MS
Bracketing relative to pyridine and Me3N scale based
on NH3

| C13H17N5O5 | CAS REGN : 362-76-5 |
|---|---|



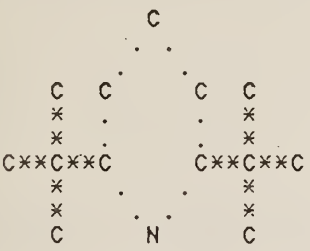
Guanosine, 2',3'-O-(1-methylethylidene)- (9CI)
Guanosine, 2',3'-O-isopropylidene- (8CI)

| | |
|---|---|
| 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 |
|---|---|



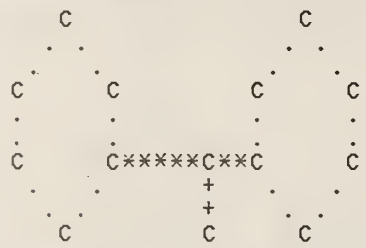
Pyridine, 2,6-bis(1,1-dimethylethyl)- (9CI)
Pyridine, 2,6-di-tert-butyl- (8CI)

| 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 |
|---|---|



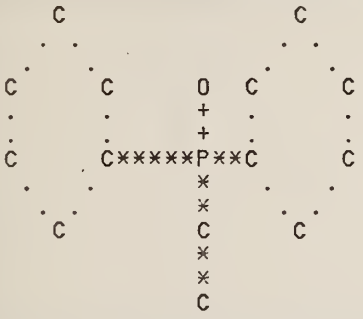
Benzene, 1,1'-ethenylidenebis- (9CI)
Ethylene, 1,1-diphenyl- (8CI)

| 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

| C14H15OP | CAS REGN : 1733-57-9 |
|---|---|



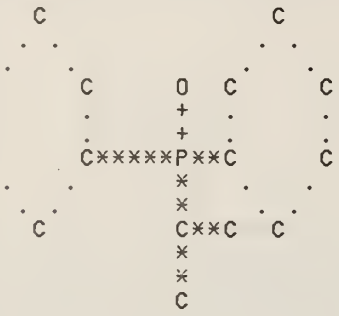
Phosphine oxide, ethyldiphenyl- (8CI9CI)

| | |
|---|---|
| PA (exp) : 220+/-3 kcal/mol | Temperature : ~400 K |

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).

Method used : MS
Bracketing relative to pyridine and Me3N; scale based
on NH3

| C15H17OP | CAS REGN : 2959-75-3 |
|---|---|



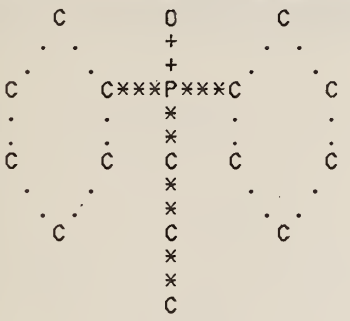
Phosphine oxide, (1-methylethyl)diphenyl- (9CI)
Phosphine oxide, isopropyldiphenyl- (8CI)

| | |
|---|---|
| PA (exp) : 220+/-3 kcal/mol | Temperature : ~400 K |

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).

Method used : MS
Bracketing relative to pyridine and Me3N; scale
based on NH3

| C15H17OP | CAS REGN : 4252-88-4 |
|---|---|



Phosphine oxide, diphenylpropyl

| | |
|---|---|
| PA (exp) : 220+/-3 kcal/mol | Temperature : ~400 K |

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).

Method used : MS
Bracketing relative to pyridine and Me3N; scale based
on NH3

| C16H19OP | CAS REGN : Not available |
|---|---|

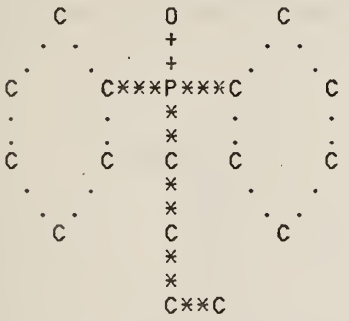
Phosphine oxide, isobutyldiphenyl-

| | |
|---|---|
| PA (exp) : 220+/-3 kcal/mol | Temperature : ~400 K |

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).

Method used : MS
Bracketing relative to pyridine and Me3N; scale based
on NH3

| C16H19OP | CAS REGN : 4233-13-0 |
|---|---|



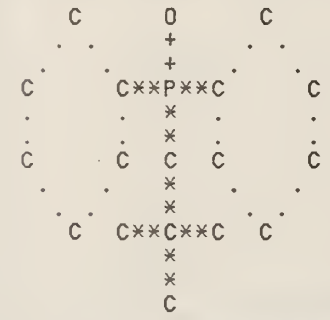
Phosphine oxide, butyldiphenyl-

| | |
|---|---|
| PA (exp) : 220+/-3 kcal/mol | Temperature : ~400 K |

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).

Method used : MS
Bracketing relative to pyridine and Me3N; scale
based on NH3

| C17H21OP | CAS REGN : Not available |
|---|---|



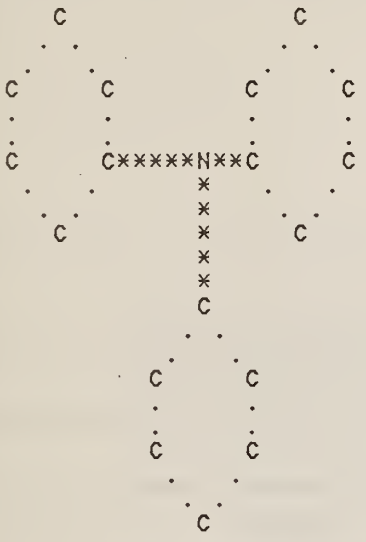
Phosphine oxide, neopentyldiphenyl-

| | |
|---|---|
| PA (exp) : 220+/-3 kcal/mol | Temperature : ~400 K |

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).

Method used : MS
Bracketing relative to pyridine and Me3N scale based
on NH3

| C18H15N | CAS REGN : 603-34-9 |
|---|---|



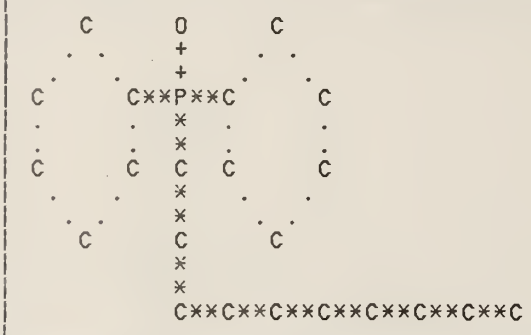
Benzenamine, N,N-diphenyl- (9CI)
Triphenylamine (8CI)

| GB (exp) : >202.9 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 CH3NH2

| C22H31OP | CAS REGN : Not available |
|---|---|



Phosphine oxide, decanyldiphenyl-

| | |
|---|---|
| PA (exp) : 220+/-3 kcal/mol | Temperature : ~400 K |

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).

Method used : MS
Bracketing relative to pyridine and Me3N scale based
on NH3

| | |
|---|---|
| Ca | CAS REGN : 7440-70-2 |
| CA | |
| Calcium (8CI9CI) | |
| | |
| PA (exp) : >211 kcal/mol | Temperature : ~800 K |
| Eslava, L. A., and Porter, R. F.<br>A Kinetic Study of Proton Transfer Reactions of NH4+,<br>CH3NH3+, and PH4+ with Calcium Atoms,<br>Chem. Phys. Letters 52 368 (1977). | |
| Method used : MS<br>Bracketing relative to NH3, PH3 and MeNH2 | |

| ClH | CAS REGN : 7647-01-0 |
|---|---|
| CL | |
| Hydrochloric acid (8CI9CI) | |
| | |
| PA (exp) : 140+/-3 kcal/mol | Temperature : |
| Haney, M. A., and Franklin, J. L.,<br>Mass Spectrometric Determination of the Proton Affinities<br>of Various Molecules,<br>J. Phys. Chem. 73, 4328 (1969). | |
| Method used : MS<br>Absolute PA value estimated by assuming that<br>for reaction RH+ + RH -> R + RH2+ the delta<br>H ~5X TC.<br>TC = measured translational energy of the products. | |
| | |
| PA (exp) : >120 kcal/mol | Temperature : 297 K |
| Fehsenfeld, F. C., and Ferguson, E. E.<br>Rate Constants for the Reactions Cl+ + H2 -> HC+ + H<br>and ClH+ + H2 -> ClH2+ + H,<br>J. Chem. Phys. 60, 5132 (1974). | |
| Method used : FAG<br>Found reaction ClH+ + H2 -> ClH2+ + H react rapidly.<br>Since reaction Cl+ + H2 -> HCl+ + H + .22eV has a<br>low exothermicity, they assumed HCl+ to be in ground<br>vibrational state. | |

| 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.,<br>Proton Affinities of the Alkali Hydroxides,<br>J. Am. Chem. Soc. 91, 2810 (1969). | |
| Method used : MS<br>PA derived from delta H of reaction M+ +<br>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.,<br>Woessner, P. J., and Leventhal, J. J.,<br>Binding Energy of H3+,<br>J. Chem. Phys. 59, 6181 (1973). | |
| Method used : MS<br>Threshold measurement of CID of D3+ + HE->D2 +<br>D+ + HE. Correction for collision energies distribution. | |

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

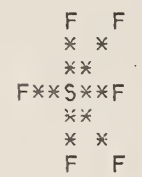
| | |
|---|---|
| D2O | CAS REGN : 7789-20-0 |
| O | |
| Water-d2 (9CI)<br>Water, heavy (D2O) (8CI) | |
| PA (exp) : 167+/-3 kcal/mol | Temperature : |
| Cotter, R. J., and Koski, W. S.,<br>Reaction of D3O+ with D2: Proton Affinity of Water,<br>J. Chem. Phys. 59, 784 (1973). | |
| Method used : MS<br>Correction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

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

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

| F3N | CAS REGN : 7783-54-2 |
|---|---|
| F**N**F<br>*<br>*<br>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.,<br>Basicity of Nitrogen Trifluoride in the Gas Phase by Ion Cyclotron Resonance,<br>Inorg. Chem. 10, 201 (1971). | |
| Method used : ICR<br>Bracketing relative to C2H4 AND HCL. | |

| F6S | CAS REGN : 2551-62-4 |
|---|---|



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 -> R + RH2+; the delta H
~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<br>PA value derived from delta H of reaction:<br>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<br>PA value derived from delta H of reaction<br>M+ + H2O -> (MOH2)+ | |

| HNaO | 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.,<br>Proton Affinities of the Alkali Hydroxides,<br>J. Am. Chem. Soc. 91, 2810 (1969). | |
| Method used : MS<br>PA value derived from delta H of reaction<br>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.,<br>Correlation Studies on H3+. I. The Wavefunctions,<br>J. Chem. Phys. 55, 4270 (1971). | |
| Method used : TC<br>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 |
| O | |
| 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 : |

Sherman, J.,
Crystal Energies of Ionic Compounds and Thermochemical Applications,
Chem. Rev. 11, 93 (1932).

Method used : CLE
Using thermochemical cycle the value of PA(H2O) was calculated from PA(NH3).

| | |
|---|---|
| PA (exp) : 171+/-2 kcal/mol | Temperature : 296,355,426 K |

Hopkins, J. M., and Bone, L. I.,
Relative Proton Affinities of Hydrogen Sulfide and Water,
J. Chem. Phys. 58, 1473 (1973).

Method used : MS
Van't Hoff plot
Equilibrium relative to H2S. Assume steady state kinetics.

| | |
|---|---|
| PA (exp) : 165.8+/-1.8 kcal/mol | Temperature : 0 K |

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).

Method used : PI
AP of $H_3O^+$ from $(H_2O)_2$. No temperature correction was applied in this supersonic expansion

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| | |
|---|---|
| GB (exp) : 153.3+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 169.3+/-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

| | |
|---|---|
| GB (exp) : 162.3+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 170.3+/-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

| | |
|---|---|
| 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 |
| Freeman, C. G., Harland, P. W., and McEwan, M. J. The Equilibrium H3S+ + HCN = H2CN+ +H2S and the Relative Proton Affinities of HCN and H2S, Intern. J. Mass Spectrom. Ion Phys. 27, 77 (1978). | |
| Method used : FAG<br>Equilibrium relative to HCN; scale based on NH3 | |
| | |
| PA (exp) : 173.3+/-2 kcal/mol | Temperature : 296,355,426 K |
| Hopkins, J. M., and Bone, L. I., Relative Proton Affinities of Hydrogen Sulfide and Water, J. Chem. Phys. 58, 1473 (1973). | |
| Method used : MS<br>Equilibrium relative to H2O<br>Van't Hoff plot | |

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

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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 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 H and S at 300 k were derived. Equilibrium; scale based on NH3

| H2Se | CAS REGN : 7783-07-5 |
|---|---|
| SE | |
| Hydrogen selenide (H2Se) (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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

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

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| | |
|---|---|
| GB (exp) : 185.1+/-2 kcal/mol | Temperature : 600 K |
| PA (exp) : 202.3+/-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 : 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.<br>Proton Affinities and Cluster Ion Stabilities in CO2 and CS2. Application in Martian Ionspheric Chemistry,<br>J. Chem. Phys. 66, 4527 (1977). | |
| Method used : CLE<br>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.,<br>The Proton Affinity of Gaseous Ammonia, the Charge Distribution on the NH4+ Ion and the Lattice Energies of NH4Cl, NH4Br, and NH4I,<br>Mol. Phys. 21, 761 (1971). | |
| Method used : CLE<br>Using thermochemical cycle the PA is derived from crystal lattice energy and the distributed charge on NH4+. | |

| H3P | CAS REGN : 7803-51-2 |
|---|---|
| P | |
| Phosphine (8CI9CI) | |
| | |
| PA (exp) : 200+/-10 kcal/mol | Temperature : 298 K |
| Wendlendt, W.,<br>Proton Affinity of Phosphine in the Phosphonium Halides,<br>Science 122, 831 (1955). | |
| Method used : CLE<br>Using thermochemical cycle calculate the PA value<br>from crystal lattice energy. | |
| | |
| PA (exp) : 156.2+/-3 kcal/mol | Temperature : |
| Wada, Y., and Kiser, R. W.,<br>A Mass Spectrometric Study of Some Alkyl-Substituted<br>Phosphines,<br>J. Phys. Chem. 68, 2290 (1964). | |
| Method used : EI<br>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 -> RH2+ + R.

Continued on next page

| | |
|---|---|
| GB (exp) : 178.8+/-2 kcal/mol | Temperature : 300 K |
| PA (exp) : 187.4+/-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<br>Calculated entropy<br>Equilibrium; scale based on NH3 | |

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

| H4Si | CAS REGN : 7803-62-5 |
|---|---|
| SI | |
| Silane (8CI9CI) | |
| | |
| PA (exp) : 155+/-3 kcal/mol | Temperature : |
| Cheng, T. M. H., and Lampe, F. W.,<br>SiH5+ and the Proton Affinity of Monosilane,<br>Chem. Phys. Letters 19, 532 (1973). | |
| Method used : MS<br>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.,<br>Proton Affinity of Atoms and Ions,<br>Zh. Obshch. Khim. 44, 2297 (1974). | |
| Method used : TC<br>Using thermochemical cycles. | |

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| | |
|---|---|
| | |
| PA (exp) : 42 kcal/mol | Temperature : |
| Beauchamp, J. L.,<br>Interactions between Ions and Molecules,<br>Ed. P. Ausloos, (Plenum Press, New York and London,<br>1975) p. 413. | |
| Method used : HE<br>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.,<br>Reactions of Gaseous Ions. XVI. Effects of Additives<br>on Ionic Reactions in Methane,<br>J. Am. Chem. Soc. 87, 4243 (1965). | |
| Method used : MS<br>Bracketing relative to H2 and CH4. | |

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| | |
|---|---|
| | |
| PA (exp) : 100.3+/-0.5 kcal/mol | Temperature : |
| 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 H3+ + Kr = KrH+ + H2 and the Relative Proton Affinity of Kr and H2, J. Chem. Phys. 63, 149 (1975). | |
| Method used : FAG<br>Equilibrium relative to H2. Delta S estimated from the entropies of the particles. | |

| | |
|---|---|
| Mg | CAS REGN : 7439-95-4 |
| MG | |
| Magnesium (8CI9CI) | |
| | |
| PA (exp) : ~198 kcal/mol | Temperature : 350 K |
| Po, P. L., and Porter, R. F. High-Temperature Ion-Molecule Chemistry. A Kinetic Study of Gas-Phase Reactions of Magnesium Atoms with D3+, Methanium, Ammonium, and tert-C4H9+ Ions, J. Am. Chem. Soc. 99, 4922 (1977). | |
| Method used : MS<br>Bracketing relative to (CH3)2C=CH2 and NH3 | |

| | |
|---|---|
| Mg2 | 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) =
Mg2H+ and using PA (Mg) = 196 and delta Hf(H+) = 365.7

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

| | |
|---|---|
| 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.,<br>Flowing Afterglow Studies at York University,<br>Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975). | |
| Method used : FAG<br>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.<br>The Heat of Formation of N2H2 and the Proton Affinity of N2,<br>Can. J. Chem. 54, 1 (1976). | |
| Method used : EM<br>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.,<br>Flowing Afterglow Studies at York University,<br>Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975). | |
| Method used : FAG<br>Calculated entropy<br>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.,<br>To be published. | |
| Method used : PI<br>Photoionization of H2O2. | |

Continued on next page

| | |
|---|---|
| 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.

| O3S | CAS REGN : 7446-11-9 |
|---|---|
| O++S++O<br>+<br>+<br>O | |
| Sulfur trioxide (8CI9CI) | |
| | |
| PA (exp) : 142+/-2 kcal/mol | Temperature : |
| Munson, B., Smith, D., and Polley, C.<br>The Mass Spectrum, Proton Affinity and Ion-Molecule Reactions of SO3,<br>Intern. J. Mass Spectrom. Ion Phys. 25, 323 (1977). | |
| Method used : MS<br>Bracketing relative to HBr and CO. Use delta Hf(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 H400 = delta H298
Entropy change assumed zero

| | |
|---|---|
| Xe | CAS REGN : 7440-63-3 |
| XE | |
| Xenon (8CI9CI) | |
| | |
| PA (exp) : 118+/-11 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<br>Bracketing relative to CH4 and reaction XE+(2P1/2) + CH4. | |
| | |
| PA (exp) : 113.2+/-1.5 kcal/mol | Temperature : 800 K |
| 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). | |
| Method used : FAG<br>Van't Hoff plot<br>Equilibrium relative to N2; scale based on PA (N2) = 112.6 | |

| | |
|---|---|
| 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 |
| 166.9 | 19,267 |
| 167.0 | 267 |
| 167.2 | 22 |
| 167.3 | 54 |
| 167.8 | 270 |
| 169.5 | 96 |
| 169.6 | 13 |
| 169.7 | 43 |
| 169.8 | 65 |
| 170.1 | 60 |
| 171.2 | 52,83,246 |
| 171.8 | 57,66 |
| 171.9 | 25 |
| 172.0 | 269 |
| 172.2 | 69 |
| 172.3 | 2,116,144 |
| 172.4 | 456 |
| 172.5 | 97 |
| 172.7 | 247 |
| 173.0 | 98 |
| 173.1 | 47,154,248 |
| 173.4 | 249-250 |
| 173.7 | 251 |
| 173.9 | 119,257 |
| 174.1 | 252,334 |
| 174.2 | 264 |
| 174.3 | 254 |
| 174.4 | 34,255 |
| 174.5 | 85,266 |
| 174.7 | 269 |
| 175.1 | 370 |
| 175.4 | 151 |
| 175.6 | 123 |
| 176.1 | 174 |
| 176.4 | 217 |
| 176.6 | 294 |
| 176.7 | 268 |
| 177.1 | 157 |
| 177.2 | 64 |
| 177.4 | 162 |
| 177.5 | 34 |
| 177.6 | 361 |
| 178.1 | 35 |

| | |
|---|---|
| 227.7 | 358 |
| 229.3 | 383 |

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Literature 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 of 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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