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MOGADOC: A Bibliographic Numerical Resource for Gasphase Molecular Spectroscopy and Structure

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A machine-readable literature compilation on free molecules has been established for microwave spectroscopy, molecular radio astronomy, and gas-phase electron diffraction. The inhouse database, which can be run on personal computers with the well known Messenger retrieval language, enables the users to trace back literature by means of bibliographic, chemical, and physical search terms. As a special feature the database also contains structural formulas, conformational descriptions, and numerical data sets for structural parameters such as internuclear distances and bond angles. © 1992 Academic Press, Inc.

The purpose of this publication is to announce the availability of a new bibliographic numerical resource.

Molecular physical and structural chemical investigations on gas-phase molecules are often published in special, not well known sources and consequently are quite often overseen. Many of these papers cannot even be located by means of databases, which generally cover chemistry and physics or which are specialized in particular fields. Thus, in order to facilitate the access to structural and related properties of free molecules, the Sektion für Spektren- und Strukturdokumentation at the University of Ulm has compiled and critically evaluated for more than 2 decades literature in the field of high-resolution molecular spectroscopy (especially in the long-wavelength region) and gas-phase electron diffraction (*1–7*).

This complete and worldwide unique compilation has been the basis for the computerized database MOGADOC (*8*). The acronym stands for Molecular Gas-Phase Documentation. The project has been carried out in cooperation with Fachinformationszentrum in Karlsruhe, the European host for STN International online databases.

The information has been compiled from scientific journals, periodicals, and books. Moreover, a lot of gray literature such as dissertations, theses, reports, and conference proceedings is also included. In particular, relevant abstracts from the Austin Symposia on Molecular Structure and Ohio Symposia on Molecular Spectroscopy, as well as from the European High Resolution Molecular Spectroscopy Conferences, are taken into account. The literature is recorded back to:

—1930 for gas-phase electron diffraction,
—1945 for microwave spectroscopy, and
—1960 for molecular radio astronomy.

In total about 17 200 references (until 1991) are presently included for about 5200 inorganic, organic, and organometallic compounds as well. The database covers the following topics:

—rotational constants and rotation vibration interaction,

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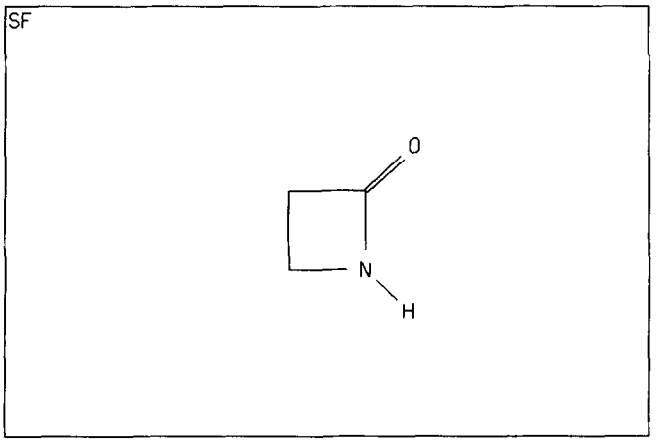
a

L1 ANSWER 1 OF 4

CN 100600
MF C3 H5 N O
RN 930-21-2
NA 2-Azetidinone



Method of study : Electron Diffraction
Microwave Spectroscopy
Theoretical Calculations

Temperature : 408-421 K

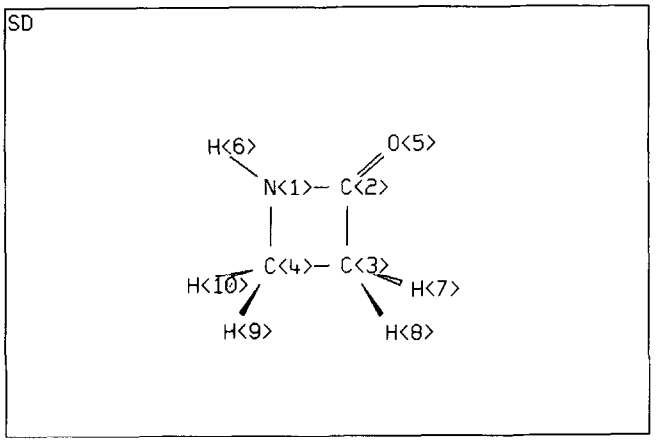


FIG. 1. Printout of a compound entry in the MOGADOC database. The example lists the gross formula in Hill system, the CAS registry number, the compound name, the structural formula, the methods and the temperature range of the quoted structure determination, a stereo drawing for the definition of internuclear distances and bond angles, tables of refined distances and angles with error limits, tables for important dependent parameters, and last, but not least, assumptions on which the structure determination is based.

—structure of free molecules,
—nuclear quadrupole and electronic hyperfine structure,
—Stark and Zeeman effects,
—collisional effects (i.e., pressure broadening, line shifts, etc.),

b

Refined geometrical parameters

Errors of values are parenthesized in units of the last digit.

Structure type for distances: r(g)

Parameter(s)	Value(s) (Angstroem)	Note(s)
N1-C2	1.380 (2)	
C2-C3	1.537 (3)	
C3-C4	1.553 (5)	
N1-C4	1.479 (3)	
C2-O5	1.201 (1)	
N1-H6	0.990 (3)	
C3-H7	1.105 (5)	

Structure type for angles: r(alpha)

Parameter(s)	Value(s) (degrees)	Note(s)
C2-C3-C4	86.0 (2)	
C3-C2-O5	136.6 (3)	
C4-N1-H6	131.0 (6)	
C4-C3-H7	114.5 (9)	
H7-C3-H8	110.0 (3)	

Important dependent parameters

Errors of values are parenthesized in units of the last digit.

Structure type for angles: r(alpha)

Parameter(s)	Value(s) (degrees)	Note(s)
N1-C2-C3	91.1 (2)	
N1-C4-C3	87.6 (1)	
C4-N1-C2	95.3 (2)	
C2-C3-H7	115.1 (8)	
N1-C4-H9	114.4 (9)	

Dihedral and other angles

Parameter(s)	Value(s) (degrees)	Note(s)
H7-C3-C2-O5	64.8 (10)	
H9-C4-N1-H6	64.1 (9)	

Other relevant information:

Assumptions:
C(s) symmetry.
The bond distances C3-H7, C3-H8, C4-H9 and C4-H10 are equal.

FIG. 1—*Continued*

—large-amplitude motion (internal rotation, ring puckering, inversion, quasilinear and quasisymmetric top molecules, loosely bound molecules), and
—astrophysical and environmental observations.

The MOGADOC database is not accessible online, that is, by international computer network. However, it was developed as an inhouse database, which can be run on IBM-compatible personal computers with the Messenger retrieval language, well known from STN online databases. The inhouse database enables the users to trace back literature by means of bibliographic, chemical, and physical search terms. Nested Boolean expressions may be applied. The database structure, computational details, and retrieval features have been developed over many years and are the result of extensive and very valuable interactions with the community of prospective users (*9, 10*).

As a special feature the MOGADOC database contains structural and stereo formulas, conformational descriptions, and numerical data sets for structural parameters such as internuclear distances and angles (Fig. 1). Presently about 800 numerical data sets are available in MOGADOC. It is emphasized that no other parameters are given numerically. However, keywords, which form a hierarchical, controlled vocabulary, give hints to appropriate references for rotational and centrifugal distortion constants, hyperfine structure parameters, dipole moments, internal rotation potential, mean amplitudes of vibration, etc.

Now the MOGADOC database is available and can be distributed by floppy diskettes (3.5″ or 5.25″). Plans have been made to update the database once every year. Hereby the implementation of further recent and even older structural numerical data will be continued. Furthermore, high-resolution infrared spectroscopic publications are being added to MOGADOC. Further information may be obtained from the author.

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