

A Chemical Fragment Notation Index*

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A new concept is introduced for indexing and computer processing chemical fragments or moieties and functional groups by means of the author's notation system. The notation for each fragment in a molecule is written and cited in essentially the same way as the formula is drawn and its notation assigned. Only a few rules are required for maintaining consistency within the index.

Many systems are described in the literature for classifying and indexing chemicals.⁶⁻⁷ Essentially all have attempted to achieve four objectives: chemical uniqueness, comprehensiveness, and logic for the compounds in the system, and location predictability for new compounds. Most systems, surprisingly, have fallen short in chemical logic. The Beilstein system, which was the first of the widely accepted comprehensive systems, uses a chemical logic that was relevant to Beilstein's time but which is anachronistically complex and illogical in terms of today's chemistry. In fact, no classification system has been able to bridge the generation gaps in chemistry.

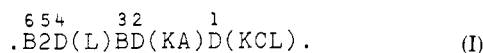
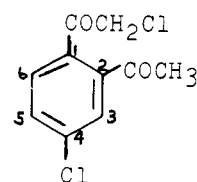
Because indexing by chemical nomenclature is still a challenging problem, there has been considerable activity during the past two decades in new notation systems, fragmentation codes, and connectivity systems. The purpose of the work described in this paper was to apply the notation system, introduced recently by the author,¹⁻⁴ to a computer-manipulatable, chemical fragment index, which also discloses within each index entry the complete chemical structure.

THE NOTATION SYSTEM

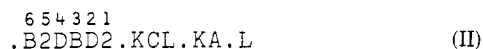
The new notation system employs a set of notation symbols, shown in Table I, that designates the bonding and number of hydrogens associated with carbon in particular and with other atoms in general. In harmony with the predominance of carbon and hydrogen atoms in organic chemistry, 12 notation symbols (single letters of the alphabet) define the three important parameters associated with carbon in organic structures: the number of hydrogens attached to a carbon atom, the kinds of bonds on the carbon atom, and fused or bridgehead carbon atoms. Because of the high occurrence of the carbonyl group, it is assigned a separate notation symbol, viz., K.

Chemical structures are represented in the notation system in an atom-by-atom correspondence with the structural formula as usually drawn—i.e., from left to right with functional groups at the right-end position, or from the atom having the highest position number to the atom in position 1. Thus, the notation system is in accord with accepted numbering schemes—this is particularly advantageous in cyclic structures whose numberings are given in the *Revised Ring Index*.⁵

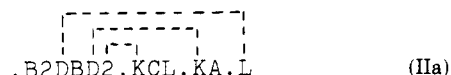
Either of two methods can be used to represent structures with the notation system, as shown below for 2-acetyl-4-chlorophenacyl chloride.



or



Note that in notation II, substituents are cited in the order of attachment from the lowest numbered ring atom to the highest. This is both a matter of convention and of convenience, and allows for a check against possible error, as illustrated in IIa.



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Table I. Notation Symbols




Carbons									
Single-bonded		Double-bonded		Triple-bonded		Fused and Bridgehead			
$-\text{CH}_3$	A	$=\text{CH}_2$	E	$\equiv\text{CH}$	U	$>\text{CH}-$	J		
$>\text{CH}_2$	C	$=\text{CH}-$	B	$\equiv\text{C}-$	V	$>\text{C}<$	T		
$>\text{CH}-$	Y	$=\text{C}<$	D			$=\text{C}<$	R		
$>\text{C}<$	X	$=\text{C}=\text{X}$	X						
Other Elements and Carbonyl									
Carbonyl		Halogen		Oxygen		Nitrogen		Other	
$>\text{C}=\text{O}$	K	$-\text{F}$	F	$-\text{O}-$	Q	$>\text{NH}$	M	$-\text{H}$	H
$-\text{CH}=\text{O}$	KH	$-\text{Br}$	G	$=\text{O}$	Q	$-\text{NH}_2$	MH	$-\text{S}-$	S
				$\begin{array}{c} \text{O} \\ \parallel \\ \text{O} \end{array}$	W	$>\text{N}-$	N	$-\text{SH}$	SH
		$-\text{I}$	I	$-\text{O}-\text{O}-$	Q2	$\equiv\text{N}$	Z	$=\text{S}$	S
		$-\text{Cl}$	L	$-\text{OH}$	QH	$=\text{N}-$	Z	$>\text{SO}$	SQ
						$-\text{N}=\text{O}$	ZQ	$>\text{SO}_2$	SW
						$=\text{NOH}$	ZQH	P	P
						$-\text{NO}_2$	ZW		
Character Symbols									

\cdot	\sim	Cyclic moiety
$:$	\sim	Atoms between bridgeheads in a cyclic moiety
@	@	Spiro atom
*		Fused or bridgehead atom other than carbon
=		Ionic form
@		Symbol for condensed ring moieties
$\left[\sim \right]$		Polymer repeating unit
&		Used to denote atoms (other than above) with atomic symbol—e.g., & NA for sodium
		Cis, beta (rosins and steroids), exo, and axial designation
-		Trans, alpha (rosins and steroids), endo, and equatorial designation

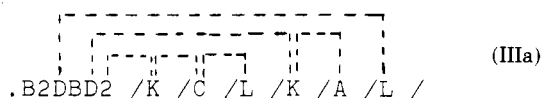
When cited in this order, the dotted lines between the substituents and the ring atoms in IIa do not cross. The advantage of this check will be discussed more fully later.

FRAGMENT NOTATION INDEX

2-Acetyl-4-chlorophenacyl chloride contains the following seven important fragments:

- A trisubstituted benzene: C_6H_3 
- A keto radical attached to benzene: $-\text{C}-$ 
- A methylene radical attached to the keto: $-\text{CH}_2-$
- A chloro radical attached to the methylene: $-\text{Cl}$
- A keto radical attached to benzene: $-\text{C}-$ 
- A methyl radical attached to the keto: $-\text{CH}_3$
- A chloro radical attached to benzene: $-\text{Cl}$

These fragments can be delineated in a permutable form as follows:



The order of citing notations in the fragment notation

index is much the same as used in writing the chemical notation. Starting with the main chain or cyclic moiety, the notation is started with the atom having the highest position number and ended with the atom having the lowest position number, or, in the case of noncyclic structures until a functional group occurs. Substituents attached to a cyclic moiety are cited in the order of from the lowest to the highest numbered atom of the cyclic moiety. Fragments within the substituent are cited consecutively from the attachment atom or fragment to the one farthest removed. It is obvious that IIIa and IVa are isomers and that the fragments follow:

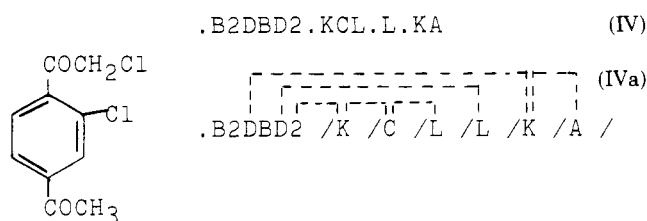
- $\begin{array}{c} 4 \quad 2 \quad 1 \\ \text{B2DBD2} \end{array}$ a 1,2,4-trisubstituted benzene to which
- $-\text{K}-$ (keto group) is attached in position 1 [the K, in turn, is attached to
- $-\text{C}-$ (methylene group), which, in turn is attached to
- $-\text{L}-$ (chloro group)];
- $-\text{K}-$ (keto group) is attached in position 2 [the K, in turn, is attached to
- $-\text{A}$ (methyl group)]; and
- $-\text{L}$ (chloro group) is attached in position 4

Connections between the trisubstituted benzene moiety and the three substituents and within the substituent radicals are shown by dotted lines in IIIa (compare with IIa). If the notations for the benzene moiety and each of the fragments are cited in the correct order, no dotted line will cross

Table II. Notations for Functional Groups or Radicals

Function	Formula	Notation
Acid chloride or chloroformyl-	-COCl	KL
Alcohol or hydroxy-	-OH	QH
Aldehyde or formyl-	-CHO	KH
Acid amide or formamido-	-CONH ₂	KMH
Amine or amido-	-NH ₂	MH
Carboxylic acid or carboxy	-COOH	KQH
Ether or oxy-	-O-	Q
Hydrazide or hydrazino-	-NHNH ₂	MMH or M2H
Hydrazone or hydrazono-	=NNH ₂	ZMH
Hydroperoxide or hydroperoxy-	-OOH	QQH or Q2H
Hydroxylamine or hydroxyamino-	-NHOH	MQH
Imine or imino-	=NH	M
Isocyanate or isocyanato-	-NCO	ZK
Isocyanide or isocyano-	-NC	ZV
Isothiocyanate or isothiocyano-	-NCS	ZXS
Ketone or carbonyl	-CO-	K
Nitrate or nitrate-	-ONO ₂	QZW
Nitrile or cyano-	-CN	VZ
Nitrilo-	-N<	N
Nitro-	-NO ₂	ZW
Nitroso-	-NO	ZQ
Oxime or hydroxyimino-	=NOH	ZQH
Peroxide or peroxy-	-O-O-	QQ or Q2
Sulfate or sulfato-	-OSO ₂ OH	QSWQH
Sulfonamide or sulfonamido-	-SO ₂ NH ₂	SWMH
Sulfone or sulfonyl-	-SO ₂ -	SW
Sulfonic acid or sulfo-	-SO ₂ OH	SWQH
Sulfoxide or sulfinyl	-SO-	SQ
Thiocyanate or thiocyanato	-SCN	SVZ

another. This simple check is particularly useful in very complex structures. It is also a convenience in learning to use the notation system for the notation fragment index. Consider, for example, the fragment notation index (IVa) for 4-acetyl-1-chlorophenacyl chloride (IV), an isomer of II.

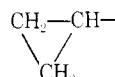
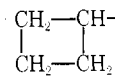
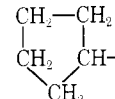
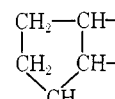
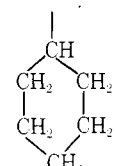
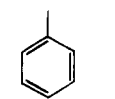
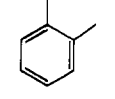
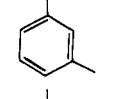
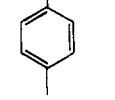
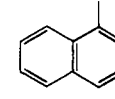
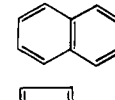
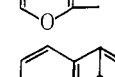
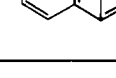


It is obvious that IIIa and IVa are isomers and that the fragment notation index for each is both unique and discriminatory. Relatively little time is required for a chemist to become expert in visualizing each radical and the fragments and their relationships within each radical and how each radical is connected to the benzene ring (or main chain in acyclic compounds). Until experience is gained, the use of the dotted line connectors enhances the structural visualization.

The virgule or slanted line symbol is used in the computer program for permuting or wrapping around, so that from the one input there are as many index entries as there are fragments, as in the following:

.B2DBD2 /K /C /L /K /A /L / (IIIa) (Input)
 K /C /L /K /A /L / .B2DBD2 / (IIIb)
 C /L /K /A /L / .B2DBD2 /K / (IIIc)
 L /K /A /L / .B2DBD2 /K /C / (IIId)
 K /A /L / .B2DBD2 /K /C /L / (IIIe)

Table III. Notations for Cyclic Moieties

Cyclic Moiety	Formula	Notation
Cyclopropyl		.C2Y /
Cyclobutyl		.C3Y /
Cyclopentyl		.C4Y /
1,2-Cyclopentylene		.C3Y2 /
Cyclohexyl		.C5Y /
Phenyl		.B5D /
<i>o</i> -Phenylene		.B4D2 /
<i>m</i> -Phenylene		.B3DBD /
<i>p</i> -Phenylene		.B2DB2D /
1-Naphthyl		.B4R2@B3D /
2-Naphthyl		.B4R2@B2DB /
2-Furyl		.B3DQ /
1,4-Methanonaphthalen-2-yl		.B4R2@RBDR:C /

A /L / .B2DBD2 /K /C /L /K / (IIIe)
 L / .B2DBD2 /K /C /L /K /A / (IIIg)

The input entry, IIIa, and each of the permuted entries, IIIb to IIIg, are retrieval keys for the chemical structure from the following viewpoints:

1,2,4-Trisubstituted benzene (IIIa)
 Keto attached to position 1 of C₆H₃ and to -CH₂Cl (IIIb)
 Methylene attached to 1 -C₆H₃CO- and Cl (IIIc)
 Chloro attached to 1 -C₆H₃COCH₂- (IIId)
 Keto attached to position 2 of C₆H₃ and to -CH₃ (IIIe)
 Methyl attached to 2 -C₆H₃CO- (IIIg)
 Chloro attached to position 4 of C₆H₃ (IIIg)

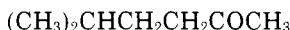
A CHEMICAL FRAGMENT NOTATION INDEX

Each entry, furthermore, discloses the total molecular structure.

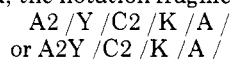
Computer alphabetization yields printouts in which IIIa is associated with all other 1,2,4-trisubstituted benzenes, alphabetically sorted by the substituent on position 1, then by the substituent on position 2 (for those with the same 1-substituent), and then by the substituent on position 3 (for those with the same 1- and 2-substituents). In a similar manner, the other III's would appear in the following order: IIIf in the methyl or A group; IIIc in the methylene or C group; IIIe in the keto or K group attached to a methyl or A group; IIb in the keto or K group attached to a methylene or C group; IIg in the chloro or L group attached to benzene; and finally IIId in a chloro miscellaneous group. Obviously, monovalent fragments, such as chloro- and methyl-, are not always meaningful in a left to right alphabetization. When they are the first term in a permuted fragment index, they should be inspected in association with the last term or terms of the entry.

DEFINITION OF FRAGMENTS

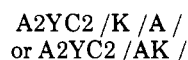
There is no question about the need for retrieving chemicals by functionality, such as those listed in Table II, or by cyclic moieties, such as those listed in Table III. Opinions may vary, however, on the need for retrieving parts of *vs.* the entire acyclic radical. For example, in isopentyl methyl ketone,



in addition to the carbonyl fragment, there are the following: methyl, isopropyl, and ethylene fragments. If deep indexing is required, the notation fragment index would be:



if the isopropyl is to be designated as a fragment. For most retrieval needs, however, the following fragment notation index would be sufficient:



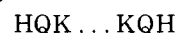
if the acetyl group is to be designated as a fragment.

Whereas saturated acyclic radicals are considered as entities, olefinic and acetylenic fragments are reasonable candidates for indexing to differentiate among classes of chemicals, such as vinyls, allyls, olefins, conjugated dienes, acetylenes, etc. Table IV illustrates the notation fragment index for several alkyl, olefinic, and acetylenic compounds. Thus, vinyls or terminal olefins are characterized by fragments beginning with E: such as E2 / for ethylene itself; EB / for terminal olefins of the class $-\text{CH}=\text{CH}_2$; ED / for terminal olefins of the class $-\text{C}(\text{R})=\text{CH}_2$; EB3 (or higher) / for conjugated terminal diolefins, triolefins, etc.; EB /C / for allyls; and ED(A) /C / for methallyls. Nonterminal olefins are characterized by fragments such as /B2 / for $-\text{CH}=\text{CH}-$; /D2 / for $> \text{C}=\text{C}<$; /BD / for $-\text{CH}=\text{C}<$; /B4 / for $-\text{CH}=\text{CH}-\text{CH}=\text{CH}-$; and /B2 /C /B2 / for $-\text{CH}=\text{CH}-\text{CH}_2-\text{CH}=\text{CH}-$.

Strictly speaking, notations for terminal olefins and acetylenes should be in the reverse order than that shown in Table IV. The EB and UV order was selected to emphasize these classes of compounds and to ensure, for example, that terminal olefins would be with ethylene itself and with methylene cyclic compounds—e.g., methylenecyclopentane.

A number of radicals containing double-bonded and triple-bonded carbons are illustrated in Table V.

In designating notations for radicals, particularly in polyfunctional or complex compounds, it is important to cite the radicals in a consistently retrievable order, rather than in the order they may be cited in the notation. For example, in dicarboxylic acids having terminal functional groups, the notation would be



The notation for each carboxylic acid group would be KQH in the notation fragment index, so that the carboxylic acid functional group can be consistently indexed and retrieved

Table IV. Notations and Notation Fragment Index for Compounds Containing Alkyl, Olefinic, and Acetylenic Fragments

Compound	Notation	Notation Fragment Index
1. $\text{CH}_2=\text{CH}_2$	E2	E2 /
2. $\text{CH}=\text{CH}$	U2	U2 /
3. $\text{CH}_3\text{CH}=\text{CH}_2$	ABE	A /EB /
4. $\text{CH}_3\text{C}\equiv\text{CH}$	AVU	A /UV /
5. $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$	ACBE	AC /EB /
6. $\text{CH}_3\text{CH}=\text{CHCH}_3$	AB2A	A,2 /B2 /
7. $\text{CH}_2=\text{CHCH}=\text{CH}_2$	EB2E	EB,2 /
8. $\text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$	AB3E	A /B2 /EB /
9. $\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CHCH}_2\text{CH}_3$	AC2B2CA	AC2 /B2 /AC /
10. $(\text{CH}_3)_2\text{CHCH}=\text{CHCH}_2\text{CH}_3$	A2YB2CA	A2Y /B2 /AC /
11. $(\text{CH}_3)_2\text{CHOH}$	A2YQH	A2Y /QH /
12. $\text{CH}_2=\text{CHCH}_2\text{OH}$	EBCQH	EB /C /QH /
13. $\text{CH}_2=\text{CHCH}_2\text{Cl}$	EBCL	EB /C /L /
14. $(\text{CH}_3)_2\text{CHCH}_2\text{OH}$	A2YCQH	A2YC /QH /
15. $(\text{CH}_3)_3\text{COH}$	A3XQH	A3X /QH /
16. $\text{CH}_2=\text{CHCOOH}$	EBKQH	EB /KQH /
17. $\text{CH}_2=\text{C}(\text{CH}_3)\text{COOH}$	ED(A)KQH	ED(A) /KQH /
18. $\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_7\text{COOH}$	AC7B2C7KQH	AC7 /B2 /C7 /KQH /
19. $\text{CH}_3(\text{CH}_2)_{14}\text{CH}=\text{CHCOOH}$	AC14B2KQH	AC14 /B2 /KQH /
20. $\text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CHCH}=\text{CH}(\text{CH}_2)_7\text{COOH}$	AC5B4C7KQH	AC5 /B4 /C7 /KQH /
21. $\text{NCCH}=\text{CHCH}=\text{CHCN}$	ZVB4VZ	VZ,2 /B4 /
22. $\text{CH}_2=\text{CHCH}(\text{CH}_3)\text{CH}_2\text{COOH}$	EBY(A)CKQH	EB /AYC /KQH /
23. $\text{CH}_2=\text{CHC}(\text{CH}_3)_2\text{COOH}$	EBX(A2)KQH	EB /A2X /KQH /
24. $(\text{CH}_3)_2\text{CHCH}=\text{CHCOOH}$	A2YB2KQH	A2Y /B2 /KQH /
25. $\text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$	EBCBE	EB,2 /C /

Table V. Notations for Radicals Containing Double-Bonded and Triple-Bonded Carbons

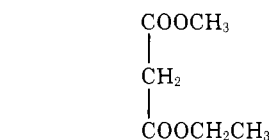
Radical	Formula	Notation	Notation Fragment Index
Acryloyl	$\text{CH}_2=\text{CHCO}-$	EBK—	EB /K /
Allyl	$\text{CH}_2=\text{CHCH}_2-$	EBC—	EB /C /
π -Allyl	$\text{CH}_2 \leftrightarrow \text{CH} \leftrightarrow \text{CH}_2-$	EB2(H)—	EB2(H) /
Allylidene	$\text{CH}_2=\text{CH}-\text{CH}<$	EBY<	EB /Y /
1,3-Butadienediylidene	$>\text{C}=\text{CHCH}=\text{C}<$	$>\text{DB2D}<$	/DB2D /
Butadienyl	$\text{CH}_2=\text{CHCH}=\text{CH}-$	EB3—	EB3 /
Butadiynylene	$-\text{C}\equiv\text{C}-\text{C}\equiv\text{C}-$	—V4—	/V4 /
Butenyl	$\text{CH}_3\text{CH}=\text{CHCH}_2-$	AB2C—	A /B2 /C /
Butenylene	$-\text{CH}_2\text{CH}=\text{CHCH}_2-$	—CB2C—	/C /B2 /C /
Butynylene	$-\text{CH}_2\text{C}\equiv\text{CCH}_2-$	—CV2C—	/C /V2 /C /
Cinnamoyl	$\text{C}_6\text{H}_5\text{CH}=\text{CHC}\equiv\text{O}$.B5D.B2K—	.B5D /B2 /K /
Ethenediylidene	$>\text{C}=\text{C}<$	$>\text{D2}<$	/D2 /
Ethynyl	$\text{HC}\equiv\text{C}-$	UV—	UV /
Ethynylene	$-\text{C}\equiv\text{C}-$	—V2—	/V2 /
Isopropenyl	$\text{CH}_2=\text{C}(\text{CH}_3)-$	ED(A)—	ED(A) /
Methallyl	$\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2-$	ED(A)C—	ED(A) /C /
3-Methyl-1-butenyl	$(\text{CH}_3)_2\text{CHCH}=\text{CH}-$	A2YB2—	A2Y /B2 /
Methylene	$\text{CH}_2=$	E—	E /
2-Methyl propenyl	$(\text{CH}_3)_2\text{C}=\text{CH}-$	A2DB—	A,2 /DB /
Oleoyl	$\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_7\text{C}\equiv\text{O}$	AC7B2C7K—	AC7 /B2 /C7 /K /
2-Pentenyl	$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2-$	ACB2C—	AC /B2 /C /
Vinyl	$\text{CH}_2=\text{CH}-$	EB—	EB /
Vinylene	$-\text{CH}=\text{CH}-$	—B2—	/B2 /
Vinylidene	$\text{CH}_2=\text{C}<$	ED<	ED /

under KQH /. Similarly, terminal divinyls, whose notation would be

EB . . . BE

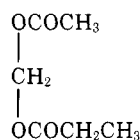
are consistently indexed and retrieved under EB/, as illustrated in Table IV for compounds 3, 5, 7, 8, and 25.

The value of fragment notation consistency is further illustrated by the following three esters:



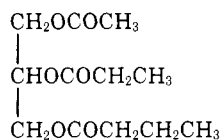
Notation: C(KQA)KQCA

Index: C /KQ,2 /A /AC /



ACKQCQKA

A /AC /KQ,2 /C /



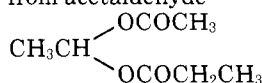
AC2KQCY(QKCA)CQKA

A /AC /AC2 /KQ,3 /CYC /

Carboxy or KQ is the important functional group in esters, and should be given precedence, to the degree possible, in the notation. In the fragment notation, however, the carboxy group must be assigned KQ consistently. Thus, the above three esters would have the following index entries under KQ:

KQ,2 /A /AC /C / malonate
KQ,2 /C /A /AC / acetal
KQ,3 /CYC /A /AC /AC2 / glyceride

It is obvious that KQ,2 /C / . . . is an acetal and not a dicarboxylic acid derivative. Similarly, the analogous acetal from acetaldehyde



Notation: ACKQY(A)QKA

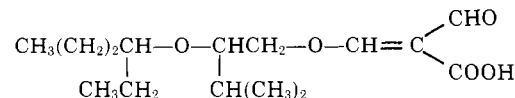
Index: A /AC /KQ,2 /AY /

would have the following index entry under KQ:

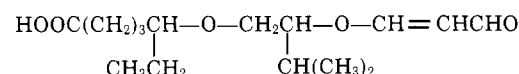
KQ,2 /AY /A /AC /

Again, it is obvious that KQ,2 /AY / . . . is an acetal and not a dicarboxylic acid derivative.

Alkyl radicals are indexed in the fragment notation index as entities, and consequently may appear in two forms (mirror images) as illustrated in the following two isomers:



AC2Y(CA)QY(YA2)CQBD(KH)KQH



HQKC3Y(CA)QCY(YA2)QB2KH

The fragment notation indexes would be as follows:

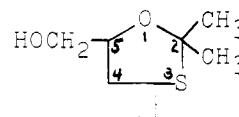
AC2YCA /Q /A2Y2C /Q /BD /KH /KQH / Va
KQH /C3YCA /Q /CY2A2 /Q /B2 /KH / VIa

KH /B2 /Q /A2Y2C /Q /ACYC3 /KQH / Vlb

DISCUSSION

The chemical fragment notation index has the advantages of fragmentation codes without their disadvantages. Its main disadvantage, from the viewpoint of individual chemists, is the need to learn a notation system. The notation system utilized for the fragment index, however, is relatively simple and compact as illustrated in Table I. Because notations are written essentially as structures are drawn and numbered, and the notation symbol includes the bonding and number of hydrogens, the notation system is oriented conceptually to the way chemists consider or view chemical structures. The fragment notation index is

Although several conventions for writing notations and assigning fragment notation indexes are noted in this paper, the absence of inflexible rules allows a versatility directed to retrieval needs. For example, this paper suggests writing notations of moieties from the highest to the lowest numbered atom. In a retrieval system which is heavily involved with heterocyclic moieties and for which there is merit in emphasizing the hetero atom or atoms, the reverse order might be preferable, as illustrated below for 2,2-dimethyl-5-hydroxymethyl-1,3-oxathiolane.



or .QX(A2)SCY(CQH).

Index: . QXSCY /C /QH /A2 /

.D2BDB2.L.KA.KCL

II Reversed

1 2 3 4 5 6
D2BDB2 /L /K /A /K /C /L / IIIa Reversed

LITERATURE CITED

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