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MANUAL FOR A PUNCHED CARD RETRIEVAL SYSTEM FOR ORGANIC PHOSPHORUS COMPOUNDS

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CONTENTS

INTRODUCTION

This manual describes the organic-phosphorus punched card retrieval system mentioned in Patent Office Research and Development Report No. 18, Mechanized Searching of Phosphorus Compounds. It describes the revised "CAMP" (Card Mechanization of Phosphorus) system as applied to the organic phosphorus compounds in Class 260, Subclass 461 (official U. S. Patent Office classification (3)). The card deck to date includes the 1551 patents in Class 260, Subclass 461 and approximately 650 other patents containing organic phosphorus compounds. The machine used in the Patent Office is a Census Multicolumn Sorter but an IBM 101 or a single column sorter may be used to search the CAMP deck.

I—DEFINITION OF TERMS

1. DESCRIPTIVE CHARACTER—an atom or fragment directly attached to a phosphorus atom.

2. FRAGMENT—an element or group of elements treated as a unit. The fragments used in CAMP may be found in the fragment dictionary.

3. FRAGMENT DICTIONARY—the catalog of fragments used in the CAMP system; cols. 65-70 and 78 on the code sheet. All fragments, except descriptive characters, are coded here. All applicable specific and generic terms are used.

4. NODE—a node is composed of two portions; the first, a descriptive character, and the second, a fragment directly or indirectly attached to the descriptive character. This system uses three nodes, the position of a fragment in the structural formula determining in which node, if any, it will be coded. The three classes of nodes are:

   1st NODE —the combination of a descriptive character and a fragment directly attached to it.

   2nd NODE —the combination of a descriptive character and a fragment once removed from it.

   TERMINAL NODE—the combination of a descriptive character and a fragment furthest removed from it; only used in chains that extend beyond the 2nd node.

5. ORGANIC PHOSPHORUS NUCLEUS—a phosphorus atom and all fragments directly connected to it, i.e., a phosphorus atom and all its descriptive characters.

II—GENERAL CODING PRINCIPLES

"CAMP" coding relies on a matrix format to show relationships. Each node has its own matrix. The 1st node is the smallest and least specific of the three; the 2nd and terminal nodes are larger and identical.

Two coding sheets are used in most cases for every document analyzed. Composite coding (2) is used in this system. One coding sheet is used for all the organic phosphate and thiophosphate compounds in the document; the second coding sheet is used for all other organic phosphorus compounds in the document. Therefore, there is a maximum of two cards per document.

Polyphosphates and polythiophosphates are coded on two sheets; as a phosphate nucleus on one sheet, and as an "other phosphorus nucleus" on the second sheet. The terms for the first, second, and terminal nodes, as well as for the fragment dictionary, are coded on both sheets.

	1		1		1		1	1st Node	2	2	3	3	4	4	5	5		6		8		7
									O_1	O_2	O_3	S_1	S_2	S_3	N	Misc A	N		Misc		Mis	
				Cycl	0	Alk	5	Alkyl	12	4	12	4	12	4	12	4			Met	2	C=X	12
				=	1	=	6	Alkenyl	11	5	11	5	11	5	11	5	Pri	12	Si	3	-X-X	11
				Poly	2	Mene	7	Aryl	0	6	0	6	0	6	0	6	Sec	11	P	4	Cycl P	0
Misc	12	0	11	S	3	N	8	Hetero	1	7	1	7	1	7	1	7	Ter	0	Se	5	Mix	1
				Met	4	H	9	H or Met	2	8	2	8	2	8	2	8	=N	1	Te	6	Sa	2
								Misc	3	9	3	9	3	9	3	9			Cl	7	Mis	3

	8		8		9		10	II NODE	11	12	13	14	15	16	17	18	19	20	21	22	23
									O_1	O_2	O_3	S_1	S_2	S_3	N	Alk	Aryl	Met	Misc	CN	R
				Cycl	12	Alk	12	Alkyl	12	12	12	12	12	12	12	12	12	12	12	12	12
				=	11	=	11	Alkenyl	11	11	11	11	11	11	11	11	11	11	11	11	11
				Poly	0	Mene	0	Aryl	0	0	0	0	0	0	0	0	0	0	0	0	0
Mis	12	0	11	S	1	N	1	Hetere	1	1	1	1	1	1	1	1	1	1	1	1	1
				Acyl	2	OH	2	OH	2	2	2	2	2	2	2	2	2	2	2	2	2
		Met	0	O-O	3	OR	3	-O-	3	3	3	3	3	3	3	3	3	3	3	3	3
		Met	1	Acyl	4	SH	4	SH	4	4	4	4	4	4	4	4	4	4	4	4	4
				S-S	5	SR	5	-S-	5	5	5	5	5	5	5	5	5	5	5	5	5
				=S	6	=O	6	=O,=S	6	6	6	6	6	6	6	6	6	6	6	6	6
		Met	2	R	7	H	7	COOR,MET	7	7	7	7	7	7	7	7	7	7	7	7	7
		N◯	3	R	8	H	8	$CONR_2$	8	8	8	8	8	8	8	8	8	8	8	8	8
				R	9	H	9	NR_2	9	9	9	9	9	9	9	9	9	9	9	9	9
	24		24		24		24		25	25	25	26	26	26	27	27	27	28	28	28	29
				NO_2	2	CN	5	NO_2,CN	12	2	6	12	2	6	12	2	6	12	2	6	12
I	12	F	0	BR	3	Cl	6	Hale	11	3	7	11	3	7	11	3	7	11	3	7	11
R	11	N◯	1	SO_2	4	SO	7	$SO,SO_2,SON\begin{matrix}R\\R\end{matrix}$	0	4	8	0	4	8	0	4	8	0	4	8	0
								Misc.	1	5	9	1	5	9	1	5	9	1	5	9	1

54		55		56		57	
12	X=P-(X_3)	12			R	12	Mene Ester
11	$O\rightarrow P\langle^{X}_{X}$	11	X	12	3AR	11	Di-Ester
0		0	1+S	11	2AR	0	Tri Ester
1	=X,O	1	4S	0	1AR	1	Mixed Ester
2	=S,X	2	=S;2S;O	1	3Acyclic	2	Cellulose
3	=O,X	3	=S;S;2-O	2	2Acyclic	3	Resin
		4	=S;3-O	3	1Acyclic	4	Poly-P
		5	=O;3S	4	3Alicyclic	5	Salt
		6	=O;3O	5	2Alicyclic	6	Mene acid
		7	=O;2S;O	6	1Alicyclic	7	Di-acid
		8	=O;S;2-O	7	3Hetero	8	Misc
		9		8	2Hetero		
				9	1Hetero		

Other Phespherus Nucleus											
58		59		60		61		62		63		64	
12	P-N	12	P-Hal	12	P-R	12	P-S	12	P=O	12	P=Mise	12	P-(X)-P
11	1	11	1	11	1	11	1	11	1	11	1	11	1
0	2	0	2	0	2	0	2	0	2	0	2	0	2
1	3	1	3	1	3	1	3	1	3	1	3	1	3
2	4	2	4	2	4+	2	4	2	4	2	4	2	4
3	5	3	F	3	P=C	3	5	3	5	3	5	3	5
4	P=N	4	BR							4	Met		
		5	I	4	Cyclic-P	4	P-NR	4	P=O	5	H	4	Phes 3
5	Poly-P	6	Cl	5	3	5	Mene Ester	5	1	6	Se	5	Phes 5
6	2			6	4	6	Di Ester	6	2	7	Te	6	
7	3	7	P-P	7	5	7	Tri Ester			8	Cellulose	7	
8	4	8	Polymer	8	6+	8	Mene Acid	7	P=S	9	Misc	8	
9	5+	9	Resin	9	All C	9	Di Acid	8	1			9	
								9	2				

	30		30		31		32	Ter. NODE	33	34	35	36	37	38	39	40	41	42	43	44	45
									O_1	O_2	O_3	S_1	S_2	S_3	N	Alk	Aryl	Het	Misc	CH	R
				Cycl	12	Alk	12	Alkyl	12	12	12	12	12	12	12	12	12	12	12	12	12
				=	11	=	11	Alkenyl	11	11	11	11	11	11	11	11	11	11	11	11	11
				Poly	0	Mene	0	Aryl	0	0	0	0	0	0	0	0	0	0	0	0	0
Mis	12	0	11	S	1	N	1	Hetero	1	1	1	1	1	1	1	1	1	1	1	1	1
				Acyl	2	OH	2	OH	2	2	2	2	2	2	2	2	2	2	2	2	2
		Met	0	O-O	3	OR	3	-O-	3	3	3	3	3	3	3	3	3	3	3	3	3
		Met	1	Acyl	4	SH	4	SH	4	4	4	4	4	4	4	4	4	4	4	4	4
				S-S	5	SR	5	-S-	5	5	5	5	5	5	5	5	5	5	5	5	5
				=S	6	=O	6	=O,=S	6	6	6	6	6	6	6	6	6	6	6	6	6
		Met	2	R	7	H	7	COOR,MET	7	7	7	7	7	7	7	7	7	7	7	7	7
		N◯	3	R	8	H	8	$CONR_2$	8	8	8	8	8	8	8	8	8	8	8	8	8
				R	9	H	9	NR_2	9	9	9	9	9	9	9	9	9	9	9	9	9
	46		46		46		46		47	47	47	48	48	48	49	49	49	50	50	50	51
				NO_2	2	CN	5	NO_2,CN	12	2	6	12	2	6	12	2	6	12	2	6	12
I	12	E	0	HR	3	Cl	6	Hale	11	3	7	11	3	7	11	3	7	11	3	7	11
R	11	N◯	1	SO_2	4	SO	7	$SO,SO_2,SON\begin{matrix}R\\R\end{matrix}$	0	4	8	0	4	8	0	4	8	0	4	8	0
								Misc	1	5	9	1*	5	9	1	5	9	1	5	9	1

	52	II NODE -52			52				53	Ter. NODE -53											
E	12	=	0	Cycl	2	Alk	5	Alkyl	12	Alk	1	Cycl	4	=	6	E					
				Poly	3	Mene	6	Aryl	11	Mene	2	Poly									
Mis	11	0	1	S	4	N	7	Hetero	0	N	3	S	5	0	7	Misc					

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Fragments								
65								
12	Alkyl	66		68		70		78
11	L	5	Heterocyclic	2	C,O	12	O-Cont	
0	H	6	Sat.-Het.	3	C=O,CHO	11	-O-	6 N Misc
1	Alkylene	7	5M	4	O=C-OH,Met	0	=O	7 O Misc
2	1	8	6M	5	O=C-OR	1	-O-O-	8 S Misc
3	2	9	Other	6	X=C-X-X=Het	2	CH	9 Misc
4	3+ 67	12	Unsat.-Het	7	X=C-X-X-IS	3	O-MET	
5	Alkenyl	11	5-M	8	O=C-N=			
6	C=C	0	6-M	9	C=S,CHS	4	Halogen	
7	Alkinyl	1	Other 69	12	S=C-N=	5	Cl	
8	C=C	2	Unsat-1	11	C=N,ISO	6	Br	
66		3	Unsat-2+			7	I	
12	Aryl			0	S- Cont.	8	F	
11	Bens	4	N-Hetero	1	-S-	9	Polyhalo	
0	Naph	5	S-Hetero	2	=S	78		
1	Cycloalkyl	6	O-Hetero	3	-S-S-	12	Amine	
2	Cyclohexyl	7	Mis-Hetero	4	SH	11	NH_2	
3	Cycloalkenyl	8	Hetero-1	5	S-MET	0	N-Sec	
4	Cyclohexene	9	Hetero-2+	6	SO_3H,MET	1	N-Ter	
	68	12	Same	7	SO_2N=	2	N-Quat	
		11	Diff	8	SO_4	3	NO_2	
		0	Mono R			4	=N imine	
		1	Ring Sys.			5	Amine Salt	

Chemist _____ Pat. No. _____

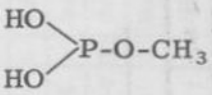
This system has two main features:

(1) division of the compounds into fragments, i.e., NH_2, COOH, SO_3H, etc.

(2) a method of showing relationships between the fragments (matrix).

The fragments used in this system are those ordinarily recognized by chemists. They are listed in the fragment dictionary in columns 65-70 and 78 of the code sheet.

Relationships are shown in this system by the use of matrices. For example, the phosphorus-oxygen-alkyl relationship of



is recorded in the first node as follows:

(punch card columns)	2	2	3	3	
	O_1	O_2	O_3	S_1	← (descriptive characters)
Alkyl	(12)	4	12	4	← (punch card rows)
Alkenyl	11	5	11	5	

The descriptive character O_1 is used to indicate that there is only one P-O-Alkyl relationship in the compound being encoded.

1. FORMAT OF CAMP CODING SHEET

The coding sheet is divided into six sections. The first three sections represent the 1st, 2nd, and Terminal nodes. The fourth section is for the organic phosphorus nucleus for all phosphate and thiophosphate compounds. The fifth section is for the organic phosphorus nucleus for all other organic phosphorus compounds. The sixth section is the fragment dictionary.

The code sheet is based on the 80-column, 12-row tabulating card.

The column numbers in the first node appear on the first line and in the second and terminal node appear on the first line and the fifteenth line. The numbers appearing below the column numbers are the row numbers. The rows, in most cases, are numbered starting with 12, and continuing through 9; i.e., 12, 11, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9.

Ten representative organo-phosphorus structures and their codes are given in the Appendix.

2. CODING PROCEDURE

(a) If the compound to be coded is an organic phosphate or thiophosphate, record all applicable codes in the "Phosphate & Thiophosphate Nucleus" section, $X=P-(X)_3$, cols. 54-57. If the compound is not an organic phosphate or thiophosphate, record all codes in the "Other Phosphorus Nucleus" section, cols. 58-64.

(b) Determine the first node connections, i.e., each descriptive character and the fragment directly attached to it, and code the first node. All specific and generic descriptors that apply are coded.

(c) Determine the second node connections, i.e., each descriptive character and the fragments once removed from it, and record all applicable specific and generic codes. Determine whether the second node fragment is connected to a chain or ring, or both, and use the appropriate code(s) in the last two columns of the 2nd node matrix.

(d) Determine the terminal node connections and code similar to the second node. The terminal node is the combination of a descriptive character and the fragment furthest removed from it.

(e) Code all fragments, except descriptive characters, whether included in a node or not, in the fragment dictionary, applying all specific and generic descriptors.

III—DEFINITION OF CODE TERMS

1. PHOSPHATES AND THIOPHOSPHATES

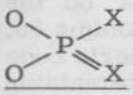
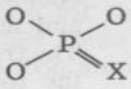
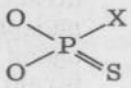
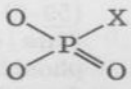
Columns 54-57 are used to encode the phosphate and thiophosphate nuclei. This includes all organic-phosphorus nuclei that have the basic structure $X=P(X)_3$, (col. 54, row 12), where X is either oxygen or sulfur.

Column 54 contains generic descriptors for the $X=P(X)_3$ nucleus. The symbol X designates either oxygen or sulfur whenever it appears.

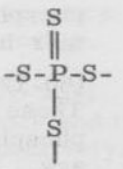
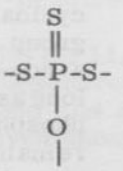
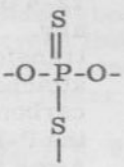
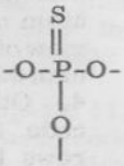
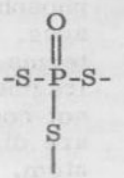
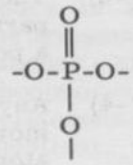
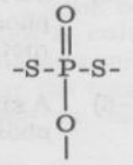
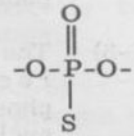
It should be noted that the first six descriptors (code terms) are generic and varying in scope. This enables one to ask the degree of genericity desired.

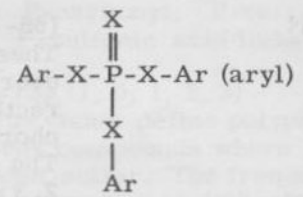
In the codes below, the underlined portion is the column and the numeral after the dash is the row. This convention is used throughout the manual.

$\underline{X=P(X)_3}$ ($\underline{54}$-12)—This is the generic code for this section. All phosphates and thiophosphates receive this code.

Code symbol	Punch location	Definition of code symbol
	(54-11)	Generic phosphate term of lesser scope.
=X,O	(54-1)	
=S,X	(54-2)	
=O,X	(54-3)	

Column 55 contains the specific descriptors for each of the $X=P(X)_3$ nuclei.

1+S	(55-0)	One or more sulfur atoms linked to the phosphorus; either single or double bonded attachments.
4S	(55-1)	
=S;2S;O	(55-2)	
=S;S;2-O	(55-3)	
=S;3-O	(55-4)	
=O;3S	(55-5)	
=O;3-O	(55-6)	
=O;2S;O	(55-7)	
=O;S;2-O	(55-8)	

3 Ar	(56-12)	These codes designate the generic nature of the fragment attached to the three non-double bonded oxygen or sulfur elements of the nucleus. The terms are Ar (aryl), acyclic, alicyclic, and hetero (heterocyclic). The frequency of attachment of each of these is provided for by repeating the terms for 1, 2, and 3 occurrences. For example:  is coded (56-12).
2 Ar	(56-11)	
1 Ar	(56-0)	
3 Acyclic	(56-1)	
2 Acyclic	(56-2)	
1 Acyclic	(56-3)	
3 Alicyclic	(56-4)	
2 Alicyclic	(56-5)	
1 Alicyclic	(56-6)	
3 Hetero	(56-7)	
2 Hetero	(56-8)	
1 Hetero	(56-9)	
Mono Ester	(57-12)	Esters—These codes indicate the number of ester linkages through the three non-double bonded oxygen of sulfur atoms. If all the ester groups are not similar, the "Mixed Ester" code is recorded. An ester linkage is formed whenever an oxygen or sulfur of the nucleus is attached to a non-carbonyl carbon.
Di-Ester	(57-11)	
Tri-Ester	(57-0)	
Mixed-Ester	(57-1)	
Cellulose	(57-2)	Organic-phosphorus nucleus directly connected to a cellulose moiety.

Resin (57-3) The phosphorus nucleus is part of a repeating unit in a polymeric structure.

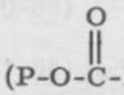
Poly-P (57-4) Any compound containing more than one phosphorus atom.

Salt (57-5) Salts of the organic-phosphorus nucleus, e.g., metal, amine, ammonium.

Mono-Acid (57-6) A single -XH radical on the phosphorus nucleus.

Di-Acid (57-7) Two -XH groups on the phosphorus nucleus.

Misc. (57-8) The Misc. descriptor is recorded whenever the phosphate or thiophosphate nucleus is attached to a group not defined by the terms in column 57, rows 12-7, e.g., a carbonyl group attached to the nucleus,



(P-O-C-R) .

2. OTHER PHOSPHORUS NUCLEUS

Columns 58-64 record the presence of non-phosphate or thiophosphate nuclei. The valence of the phosphorus atom may be either 3 or 5.

P-N (58-12, 11, 0, 1, 2, 3) These codes are used whenever a nitrogen atom is directly attached to the phosphorus atom by single bond. The column 58, rows 11, 0, 1, 2, 3 codes are used to indicate the number of nitrogen atoms attached to a particular phosphorus atom.

P=N (58-4) Double bonded phosphorus-nitrogen linkage.

Poly-P (58-5, 6, 7, 8, 9) The Poly-P codes are employed whenever there is more than one phosphorus atom in a compound, regardless of the nature of the phosphorus containing groups. This includes polyphosphates and polythiophosphates. The column 58, rows 6-9 codes are used to indicate the number of phosphorus atoms in the molecule.

P-Hal (59-12, 11, 0, 1, 2, 3, 4, 5, 6) These descriptors identify halogen substituents on the phosphorus atom, column 59, row 12 being the generic code for the series. The remaining codes indicate the frequency and nature of the halo group. The frequency codes represent the total number of halogens directly attached to a given phosphorus atom. These halogens may be the same or different.

P-P (59-7) This code is used when two phosphorus atoms are linked directly to each other.

Polymer (59-8) This code is recorded when a phosphorus atom participates in a repeating unit of a polymeric structure.

Resin (59-9) The resin code is used when a phosphorus containing polymer has resinous properties.

P-R (60-12, 11, 0, 1, 2, 3) These codes describe the phosphorus-hydrocarbon linkage. This includes alkyl, alkenyl, alkinyl, aryl, and cycloalkyl. The hydrocarbon group may be substituted with a non-hydrocarbon moiety so long as the carbon to which the phosphorus atom is attached remains definable under column 65 and column 66, rows 12-4 of the fragment dictionary. Thus if the substituent transforms the phosphorus-attached carbon to a part of a carbonyl or a carboxy group, the P-R code is not applicable. After fragmenting, the carbon attached to the phosphorus atom must fall within the purview of one of the codes in column 65 and column 66, rows 12-4. Otherwise, the "P-Misc" code is applied (column 63, rows 12-3). Column 60, row 3 represents double bonded phosphorus-hydrocarbon linkages. NOTE: Although the R terms are definable in the fragment dictionary, they are not coded there because they are directly attached to a P atom.

Cyclic P (60-4, 5, 6, 7, 8, 9)
These codes are used when the phosphorus atom is a member of a ring. The codes in rows 5, 6, 7 and 8 refer to the number of members in the ring. Column 60, row 9 is recorded when all the ring members, other than phosphorus, are carbon atoms.

P-S (61-12, 11, 0, 1, 2, 3)
Phosphorus-sulfur single bond and its frequency for a given phosphorus atom.

P-XR (61-4, 5, 6, 7)
This code is applied when a hydrocarbon ring or chain is directly connected to an oxygen or sulfur atom attached to a phosphorus atom. The R group must fall within one of the hydrocarbon fragment definitions in column 65 and column 66, rows 12-4. The codes in rows 5, 6, and 7 indicate the frequency of the P-XR relationship.

Mono Acid, Di Acid (61-8, 9)
One- and two-XH groups, respectively, attached directly to a phosphorus atom, where X is either oxygen or sulfur.

P-O (62-12, 11, 0, 1, 2, 3)
Phosphorus-oxygen single bond and its frequency for a given phosphorus atom.

P=O (62-4, 5, 6)
Double-bonded phosphorus-oxygen linkage. Rows 5 and 6 record the frequency for a particular phosphorus atom.

P=S (62-7, 8, 9)
Double-bonded phosphorus-sulfur linkage. Rows 8 and 9 record the frequency for a particular phosphorus atom.

P-Misc (63-12, 11, 0, 1, 2, 3)
These codes are applied when any radical directly attached to a phosphorus atom is not defined by the specific codes in columns 58-62 of the "Other Phosphorus Nucleus" section. This includes P=Misc as well as P-Misc. The P-Misc code applies to all the codes in column 63, rows 4-9. The codes in rows 11-3 indicate the frequency of total miscellaneous substitutions on a phosphorus atom. The miscellaneous groups need not be identical.

NOTE: Any code in column 63, rows 4-9 must be accompanied by a code in column 63, row 12, and the appropriate frequency code for the total P-Misc substitution on the phosphorus atom.

Met (63-4)
A metal or NH_4 group attached directly to the phosphorus atom.

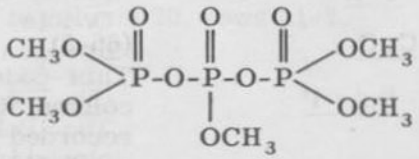
H (63-5)
Hydrogen directly attached to a phosphorus atom.

Se,Te (63-6, 7)
Selenium and tellurium linked to phosphorus.

Cellulose (63-8)
Phosphorus-cellulose linkage.

Misc (63-9)
This code is recorded for any group attached to a phosphorus atom that is not defined elsewhere in the Other Phosphorus Nucleus section. Examples are P-carbonyl, P-carboxy, and P-sulfonic acid linkages.

P-(X)-P (64-12, 11, 0, 1, 2, 3)
These codes define polyphosphorus compounds where X is oxygen, sulfur. The frequency of occurrence is indicated in rows 11-3. A phosphorus atom may participate in more than one P-(X)-P group as in



which is assigned a frequency of 2 (column 64, row 0).

Phos 3 (64-4)
Phosphorus with a valence of 3.

Phos 5 (64-5)
Phosphorus with a valence of 5.

3. FRAGMENT DICTIONARY

The fragment dictionary contains codes for all the fragments used in the system. All fragments in an organic-phosphorus compound except those directly attached to a phosphorus atom (descriptive characters) are coded in the fragment dictionary whether they are included in one of the nodal relationships or not. All applicable specific and generic terms are coded for each fragment. The fragment dictionary encompasses columns 65-70 and 78 on the CAMP code sheet.

Alkyl (65-12)
Saturated, terminal, hydrocarbon chains, e.g., methyl, ethyl, dodecyl.

L (65-11)
Lower alkyl (1-7 members) further defines column 65, row 12.

H (65-0)
Higher-alkyl (8 or more members) further defines column 65, row 12.

Alkylene (65-1, 2, 3, 4)
Substituted alkyl chain, e.g., methylene, ethylene. Rows 2, 3 and 4 indicate the number of carbons in the alkylene group.

Alkenyl (65-5)
Hydrocarbon chain containing a double bond.

C=C (65-6)
This code is specific under column 65, row 5 and is recorded when the alkenyl group is ethenyl.

Alkinyl (65-7)
Hydrocarbon chain containing a triple bond.

C≡C (65-8)
This code is specific under column 65, row 7 and is recorded when the alkinyl group is acetylene.

Aryl (66-12, 11, 0)
Organic radical derived from an aromatic hydrocarbon ring by the removal of at least one hydrogen. It is further defined in rows 11 (benzene) and 0(naphthalene).

Cycloalkyl (66-1)
Saturated hydrocarbon ring.

Cyclohexyl (66-2)
This code further defines column 66, row 1.

Cycloalkenyl (66-3)
Unsaturated, non-aromatic hydrocarbon ring.

Cyclohexene (66-4)
This code further defines column 66, row 3.

Heterocyclic (66-5)
Generic heterocyclic code.

Sat.-Het. (66-6)
Saturated hetero ring.

5M (66-7)
Five membered saturated hetero ring.

6M (66-8)
Six membered saturated hetero ring.

Other (66-9)
Saturated hetero ring with other than 5 or 6 members.

Unsat.-Het. (67-12)
Unsaturated hetero ring.

5M (67-11)
Five membered unsaturated hetero ring.

6M (67-0)
Six membered unsaturated hetero ring.

Other (67-1)
Unsaturated hetero ring with other than 5 or 6 members.

Unsat - 1 (67-2)
Unsaturated hetero ring with one double bond.

Unsat - 2+ (67-3)
Unsaturated hetero ring with 2 or more double bonds. This includes aromatic hetero rings, e.g., pyridine.

N-Hetero (67-4)
Nitrogen containing heterocyclic.

S-Hetero (67-5)
Sulfur containing heterocyclic.

O-Hetero (67-6)
Oxygen containing heterocyclic.

Mis-Hetero (67-7)
Heterocyclic where the hetero atom is not nitrogen, sulfur, or oxygen.

Hetero-1 (67-8)
One hetero ring member.

Hetero-2+ (67-9)
Two or more hetero ring members.

Same (68-12) See 68-11.

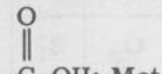
Different (68-11)
These codes refer only to column 67, row 9. If the hetero atoms are identical, row 12 is recorded; if different, row 11 is recorded.

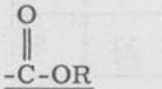
Mono R (68-0)
Mono-ring heterocyclic.

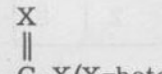
Ring System (68-1)
Poly-ring heterocyclic. Only one of the rings need be hetero.

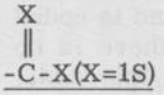
C,O (68-2)
A fragment containing carbon and oxygen. Rings are excluded.

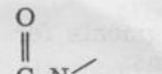
C=O,CHO (68-3)
Carbonyl, aldehyde.


(68-4)
Carboxy group and its metal salts.

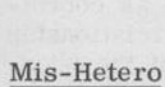

(68-5)
Carboxylic acid ester; R represents hydrocarbon chain or ring.


(68-6)
X represents oxygen, sulfur, nitrogen, and heterocyclic, with at least one X heterocyclic.


(68-7)
X represents oxygen, sulfur, nitrogen, with at least one X sulfur.


(68-8)
Carboxylic acid amide.

C=S, CHS (68-9)
Analogous to column 68, row 3.


(69-12)
Thiocarboxylic acid amide.

C≡N; Iso (69-11)
Cyanide; isocyanide.

S-Cont (69-0)
Generic "sulfur-containing" code for the specific fragments in column 69, rows 1-8.

-S- (69-1)
Thioether.

=S (69-2)
Double bonded sulfur attached to a ring. When not attached to a ring the =S is considered along with the carbon to which it is attached and coded in column 68.

-S-S- (69-3)
Disulfide.

-SH (69-4)
Mercapto.

S-Met (69-5)
Sulfur-metal, e.g., -S-Na.

SO_3R, Met (69-6)
Sulfonic acid and its derivatives. R represents hydrogen or an organic radical.

$SO_2N=$ (69-7)
Sulfonamide.

SO_4 (69-8)
Sulfate.

O-Cont. (70-12)
Generic "oxygen-containing" code for the specific fragments in column 70, rows 11-3.

-O- (70-11)
Ether.

=O (70-0)
Keto attached to a ring. When not attached to a ring, the =O is considered along with the carbon to which it is attached and coded in column 68.

-O-O- (70-1)
Peroxide.

-OH (70-2)
Hydroxy.

-O-Met (70-3)
Oxygen-metal, e.g., -O-Na.

Halogen (70-4, 5, 6, 7, 8)
Row 4 is the generic halogen code; rows 5-8 indicate the specific halogens.

Polyhalo (70-9)
More than one halogen, the same or different, in the compound.

Amine (78-12)
Generic code for the specific fragments of column 78, rows 11-5.

NH_2 (78-11)
Primary amine.

N-Sec (78-0)
Secondary amine.

N-Ter (78-1)
Tertiary amine.

N-Quat (78-2)
Quaternary amine.

NO_2 (78-3)
Nitro

=N, imine (78-4)
An imine; includes substituted (=N-R) and unsubstituted (=N-H).

Amine salt (78-5)

N-Misc (78-6)
O-Misc (78-7)
S-Misc (78-8)
Nitrogen, oxygen, and sulfur containing radicals, respectively, not specifically provided for in the fragment dictionary.

Misc (78-9)
Radicals not provided for in the fragment dictionary. Fragments coded under column 78, rows 6, 7, or 8 are not recorded here.

4. THE NODES

The remaining sections of the code sheet (columns 1-53) contain the 1st, 2nd, and terminal nodes. Nodal relationships are coded in matrices comprising descriptive characters (O_1, O_2, O_3, etc.) and generic chemical fragments as coordinates. The 1st node indicates the relationship between the descriptive characters of the phosphorus nucleus and the fragments directly linked to the descriptive characters. The 2nd node records the combination of the descriptive characters and the fragment(s) once removed from them. The terminal node represents the relationship between the descriptive characters and the fragments furthest removed from them.

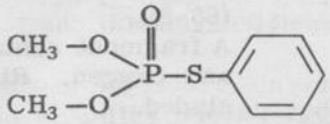
The matrix principle is the same for all the nodes. The second and terminal nodes are identical and differ from the 1st node only in the use of more descriptive characters and chemical fragments.

Attached to all the nodes to the left of the generic chemical fragments is a supplemental dictionary which further defines the fragments. Some of the descriptive characters are further defined to the right of the 1st node (columns 6 and 7) and at the bottom of the code sheet (columns 52 and 53).

A. The 1st Node

The 1st node records the combination of a descriptive character and the fragment(s) attached to it.

Example:



1st Node

Columns		2	2	3	3
Descriptive Characters		O_1	O_2	O_3	S_1
Chemical Fragments	Alkyl	12	(4)	12	4
	Alkenyl	11	5	11	5
	Aryl	0	6	0	(6)
	H or Met	2	8	2	8

The nodal relationship of oxygen-methyl appears twice so the descriptive character O_2 is used and column 2, row 4 is recorded. The 1st node combination of sulfur-aryl appears once and is coded by recording column 3, row 6. Since there is no nodal relationship beyond the 1st node, this completes the nodal codings for this compound.

The descriptive characters and fragments for the 1st node have the following definitions:

1. Descriptive Characters

O_1 —a single oxygen-fragment nodal relationship.

O_2 —two identical oxygen-fragment nodal relationships on the same phosphorus atom. The fragments of the two combinations need be identical only with reference to the generic fragment definitions listed under "1st Node" on the code sheet. Thus P-O-CH_3 and P-O-cyclopentyl are both "Alkyl" and the O_2 code is used. But P-O-CH_3 and P-O-$CH{=}CH_2$ are classified separately under "Alkyl" and "Alkenyl" so the O_1 descriptive character is used for both.

O_3 —three identical oxygen-fragment nodal relationships on the same phosphorus atom. Fragments classified under the same generic fragment definition (Alkyl, Alkenyl, Aryl, Hetero, H or Met, and Misc.) are considered identical.

The S_1, S_2, and S_3 definitions are analogous to the O_1, O_2, and O_3 definitions.

N — nitrogen attached to the phosphorus atom. This descriptive character is further defined in column 6, rows 12, 11, 0, and 1 (primary, secondary, tertiary, and imino, respectively). This includes a heterocyclic N directly attached to the P atom.

Misc A — any atom attached to phosphorus other than oxygen, sulfur, or nitrogen. This term is further defined in column 6, rows 2-7 and column 7, rows 12-3.

Met (6-2) metal.

Si (6-3) silicon.

B (6-4) boron.

Se (6-5) selenium.

Te (6-6) tellurium.

(6-7) X is oxygen or sulfur.

C=X (7-12) X is oxygen or sulfur.

X-X (7-11) X is oxygen or sulfur.

Cycl P (7-0) phosphorus as a ring member.

Mix (7-1) refers to "Cycl P" where other ring members are not identical to each other.

Sa (7-2) refers to "Cycl P" where other ring members are the same.

Mis (7-3) miscellaneous; any Misc. term not included in column 6, rows 2-7 or column 7, rows 12-2.

2. Fragments

The generic fragment categories are found listed directly under "1st Node" on the code sheet. Specific descriptors that further define the fragment being coded, are found to the left of these terms. In defining the terms below, the generic term definitions are immediately followed by definition of their specific descriptors:

Alkyl — saturated hydrocarbon chain and saturated or unsaturated hydrocarbon ring (aromatics excluded).

Alk (1-5) saturated hydrocarbon chain.

Cycl (1-0) saturated or unsaturated hydrocarbon ring (aromatics excluded).

Alkenyl — unsaturated hydrocarbon chain, either double or triple bond.

= (1-6) hydrocarbon chain containing a double bond.

≡ (1-1) hydrocarbon chain containing a triple bond.

Aryl — aromatic hydrocarbons, e.g., phenyl, naphthyl.

Mono (1-7) mono aromatic ring, i.e., phenyl.

Poly (1-2) two or more fused aromatic hydrocarbon rings, e.g., naphthyl, phenanthryl.

Hetero — heterocyclic.

N (1-8) nitrogen containing heterocyclic.

S (1-3) sulfur containing heterocyclic.

O (1-11) oxygen containing heterocyclic.

Misc (1-12) hetero atom other than oxygen, nitrogen or sulfur.

H or Met — hydrogen, metal, or ammonium.

H (1-9) hydrogen.

Met (1-4) metal or ammonium.

B. 2nd and Terminal Nodes

The 2nd node records the relationship of a descriptive character and the fragment(s) once removed from it. The terminal node indicates the combination of descriptive character and its terminal fragments, or those furthest removed from it. The terminal node is used only for terminal fragments beyond the 2nd node.

Since the code sheet format and the definitions are identical for both nodes, definitions are given only for terms in the 2nd node.

1. Descriptive Characters

The first seven descriptive characters are also used in the 1st node where they have already been defined, (O_1, O_2, O_3, S_1, S_2, S_3, N). Note that the 2nd node does not carry supplemental specific terms for the N descriptive character as does the 1st node in column 6, rows 12, 11, 0, and 1.

The remaining descriptive characters in the 2nd node are Alk, Aryl, Het, and Misc.

Alk — hydrocarbon chain or ring, saturated or unsaturated, aromatics excluded. It is further defined in column 52 (bottom left of code sheet).

- ≡ (52-12) hydrocarbon chain containing a triple bond.
- = (52-0) hydrocarbon chain containing a double bond.
- Cycl (52-2) cycloalkyl, saturated or unsaturated, aromatics excluded.
- Alk (52-5) saturated hydrocarbon chain.

Aryl — aromatic hydrocarbon. It is further defined in column 52.

- Poly (52-3) polyaromatic; two or more fused aromatic rings.
- Mono (52-6) monoaromatic, i.e., phenyl.

Het — heterocyclic. Further defined in column 52.

- N (52-7) nitrogen containing.
- S (52-4) sulfur containing.
- O (52-1) oxygen containing.
- Misc (52-11) hetero atom other than nitrogen, sulfur, or oxygen.

Misc — fragment attached to phosphorus not defined by the other descriptive characters.

2. Chain-Connected and Ring-Connected

Columns 22 and 23 in the 2nd node record the nature of the direct attachments to the chemical fragment component of the nodal combination. The term CH (column 22) denotes a chain connection, and the term R (column 23) indicates a ring connection. CH includes bonds to any fragment that is not cyclic. Either or both of these codes must be assigned to each non-descriptive character fragment coded in the 2nd node.

3. Fragments

The generic fragment categories are found listed directly under "2nd node" on the code sheet. Specific descriptors are found to the left of each generic term. Each generic term defined below is immediately followed by definitions of its specific descriptors.

The first four generic fragments (alkyl, alkenyl, aryl, hetero) and their specific descriptors also appear in the 1st node and have been defined in that section of the manual.

OH — hydroxy or O-acyl.

- OH (10-2) hydroxy.
- Acyl (9-2) the oxygen of an -O-acyl group.

-O- — ether, peroxide, or the oxygen of an -O-metal group.

- OR (10-3) ether oxygen.
- -O-O- (9-3) peroxide.
- Met (8-0) the oxygen of an -O-metal group.

SH — mercapto, S-acyl, or S-metal.

- SH (10-4) mercapto.
- Acyl (9-4) the sulfur of an -S-acyl group.
- Met (8-1) the sulfur of an -S-metal group.

-S- — thioether, or disulfide.

- SR (10-5) thioether.
- S-S (9-5) disulfide.

=O, =S oxo and thioxo.

- =O (10-6) oxo.
- =S (9-6) thioxo.

COOR, Met carboxy and its esters and salts.

- H (10-7) carboxy.
- R (9-7) carboxylic acid ester.
- Met (8-2) carboxylic acid salt.

$CXNR_2$ carboxylic acid amide; R is hydrogen or any organic radical. X is oxygen or sulfur.

- H (10-8) R is hydrogen.
- R (9-8) any radical except when the two R's form a cyclic group.
- N⁀ (8-3) the nitrogen is a heterocyclic ring member.

NR_2 primary, secondary, or tertiary amine.

- H (10-9) primary or secondary amine.
- R (9-9) secondary or tertiary amine.

NO_2, CN nitro or cyano.

- CN (24-5)
- NO_2 (24-2)

Halo halogen.

- Cl (24-6)
- Br (24-3)
- F (24-0)
- I (24-12)

SO, SO_2, SON(R)(R) all sulfur containing fragments not provided for elsewhere in the node.

- SO (24-7) sulfoxide.
- SO_2 (24-4) sulfone.
- N⁀ (24-1) SON(R)(R) where the nitrogen is a heterocyclic ring member.
- R (24-11) any fragment other than N-heterocyclic.

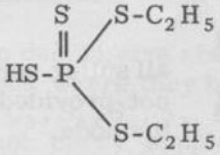
Misc fragment not included within the purview of any of the terms of the node.

NOTE: When a chain is terminated by COOR, OR, or SR, where the R group is unsubstituted hydrocarbon, the terminal node for that chain is COOR, OR, or SR, rather than the R group involved. See the terminal node coding in Example 5.

APPENDIX

EXAMPLES

1. PHOSPHATE AND THIOPHOSPHATE NUCLEUS



Thiophosphate Nucleus

Col. 54, Row 12	$X=P-(X)_3$
Col. 55, Row 0	1+S
Col. 55, Row 1	4S
Col. 56, Row 2	2 Acyclic
Col. 57, Row 11	Di-ester
Col. 57, Row 6	Monoacid

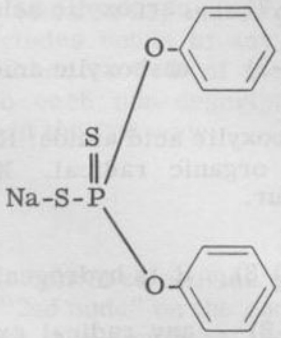
1st Node

Col. 1, Row 5	Alkyl
Col. 4, Row 12	$S_2 \rightarrow$ Alkyl
Col. 1, Row 9	Hydrogen
Col. 3, Row 8	$S_1 \rightarrow$ H or Met

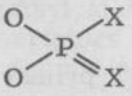
Fragment Dictionary

Col. 65, Row 12	Alkyl
Col. 65, Row 11	Low Alkyl

2. PHOSPHATE AND THIOPHOSPHATE NUCLEUS



Thiophosphate Nucleus

Col. 54, Row 12	$X=P-(X)_3$
Col. 54, Row 11	
Col. 54, Row 2	=S,X
Col. 55, Row 0	1+S
Col. 55, Row 3	=S,S,2-O
Col. 56, Row 11	2 Aryl
Col. 57, Row 11	Diester
Col. 57, Row 5	Salt

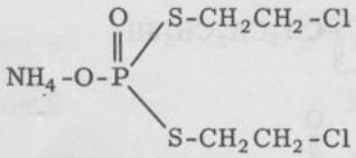
1st Node

Col. 1, Row 7	Monoaryl
Col. 2, Row 6	$O_2 \rightarrow$ Aryl
Col. 3, Row 8	$S_1 \rightarrow$ H or Met
Col. 1, Row 4	Metal

Fragment Dictionary

Col. 66, Row 12	Aryl
Col. 66, Row 11	Benzene

3. PHOSPHATE AND THIOPHOSPHATE NUCLEUS



Thiophosphate Nucleus

Col. 54, Row 12	$X=P-(X)_3$
Col. 55, Row 0	1+S
Col. 55, Row 7	=O,2S,O
Col. 56, Row 2	2 Acyclic
Col. 57, Row 11	Di-ester
Col. 57, Row 5	Salt

1st Node

Col. 1, Row 5	Alkyl
Col. 4, Row 12	$S_2 \rightarrow$ Alkyl
Col. 1, Row 4	Metal
Col. 2, Row 2	$O_1 \rightarrow$ H or Met

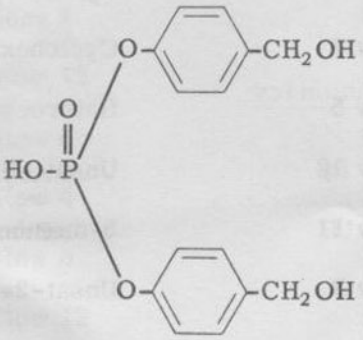
2nd Node

Col. 24, Row 6	Chlorine
Col. 26, Row 3	$S_2 \rightarrow$ Hal
Col. 28, Row 7	Hal $\rightarrow$ Chain

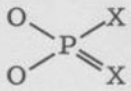
Fragment Dictionary

Col. 65, Row 1	Alkylene
Col. 65, Row 3	Ethylene
Col. 70, Row 4	Halogen
Col. 70, Row 5	Chlorine
Col. 70, Row 9	Polyhalo

4. PHOSPHATE AND THIOPHOSPHATE NUCLEUS



Phosphate Nucleus

Col. 54, Row 12	$X=P-(X)_3$
Col. 54, Row 11	
Col. 54, Row 1	=X,O
Col. 54, Row 3	=O,X
Col. 55, Row 6	=O,30
Col. 56, Row 11	2 Aryl
Col. 57, Row 11	Di-ester
Col. 57, Row 6	Monoacid

1st Node

Col. 1, Row 9	Hydrogen
Col. 2, Row 2	$O_1 \rightarrow$ H or Met
Col. 1, Row 7	Monoaryl
Col. 2, Row 6	$O_2 \rightarrow$ Aryl

2nd Node

Col. 10, Row 12	Alkyl
Col. 12, Row 12	$O_2 \rightarrow$ Alkyl
Col. 22, Row 12	Alkyl $\rightarrow$ Chain
Col. 23, Row 12	Alkyl $\rightarrow$ Ring

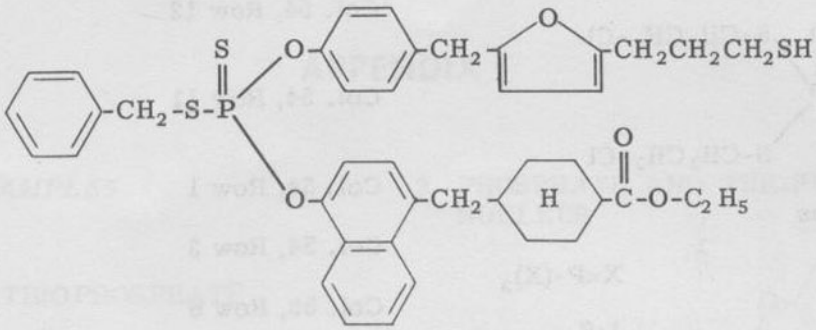
Terminal Node

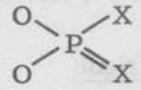
Col. 32, Row 2	OH
Col. 34, Row 2	$O_2 \rightarrow$ OH
Col. 44, Row 2	OH $\rightarrow$ Chain

Fragment Dictionary

Col. 66, Row 12	Aryl
Col. 66, Row 11	Benzene
Col. 65, Row 1	Alkylene
Col. 65, Row 2	Methylene
Col. 70, Row 12	O-containing
Col. 70, Row 2	OH

5. PHOSPHATE AND THIOPHOSPHATE NUCLEUS

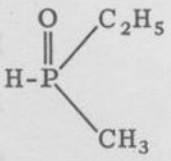


Thiophosphate Nucleus		Terminal Node	
Col. 54, Row 12	$X{=}P{-}(X)_3$	Col. 32, Row 4	SH
Col. 54, Row 11		Col. 33, Row 4	$O_1 \rightarrow SH$
		Col. 44, Row 4	$SH \rightarrow$ Chain
Col. 54, Row 2	=S,X	Col. 31, Row 7	COOR
Col. 55, Row 0	1+S	Col. 33, Row 7	$O_1 \rightarrow$ COOR, Met
Col. 55, Row 3	=S,S,2-0	Col. 45, Row 7	COOR, Met $\rightarrow$ Chain
Col. 56, Row 3	1 Acyclic	Fragment Dictionary	
Col. 56, Row 11	2 Aryl	Col. 65, Row 1	Alkylene
Col. 57, Row 0	Tri-ester	Col. 65, Row 2	Methylene
Col. 57, Row 1	Mixed-ester	Col. 65, Row 4	Propylene
1st Node		Col. 66, Row 12	Aryl
Col. 1, Row 5	Alkyl	Col. 66, Row 11	Benzene
Col. 3, Row 4	$S_1 \rightarrow$ Alkyl	Col. 66, Row 0	Naphthalene
Col. 1, Row 2	Poly Aryl	Col. 69, Row 0	S-containing
Col. 1, Row 7	Mono Aryl	Col. 69, Row 4	SH
Col. 2, Row 6	$O_2 \rightarrow$ Aryl	Col. 68, Row 2	C,O
2nd Node		Col. 68, Row 5	O=C-OR
Col. 10, Row 12	Alkyl	Col. 66, Row 1	Cycloalkyl
Col. 12, Row 12	$O_2 \rightarrow$ Alkyl	Col. 66, Row 2	Cyclohexyl
Col. 23, Row 12	Alkyl $\rightarrow$ Ring	Col. 66, Row 5	Heterocyclic
Col. 10, Row 0	Mono Aryl	Col. 67, Row 12	Unsat.-Het.
Col. 14, Row 0	$S_1 \rightarrow$ Aryl	Col. 67, Row 11	5-membered
Col. 22, Row 0	Aryl $\rightarrow$ Chain	Col. 67, Row 3	Unsat-2+

Fragment Dictionary (Continued)

Col. 67, Row 6	O-Hetero
Col. 67, Row 8	1 Hetero Atom
Col. 68, Row 0	Mono Ring
Col. 65, Row 12	Alkyl
Col. 65, Row 11	Lower Alkyl

6. OTHER PHOSPHORUS NUCLEUS

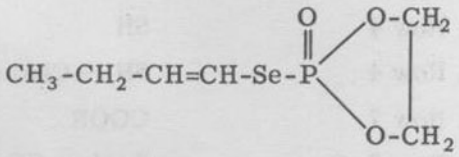


Other Phosphorus Nucleus

Col. 62, Row 4	P=0
Col. 62, Row 5	P=0 once
Col. 60, Row 12	P-R
Col. 60, Row 0	P-R twice
Col. 63, Row 12	P-Misc
Col. 63, Row 11	P-Misc once
Col. 63, Row 5	Misc.=H
Col. 64, Row 5	Phos 5

No other codes for this compound.

7. OTHER PHOSPHORUS NUCLEUS



Other Phosphorus Nucleus

Col. 60, Row 4	Cyclic P
Col. 60, Row 7	5-membered
Col. 62, Row 12	P-O
Col. 62, Row 0	P-O twice
Col. 62, Row 4	P=0
Col. 62, Row 5	P=0 once
Col. 63, Row 12	P-Misc
Col. 63, Row 11	P-Misc once
Col. 63, Row 6	Misc = Se
Col. 64, Row 5	Phos 5

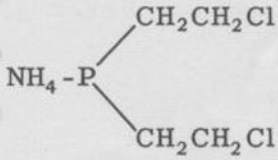
1st Node

Col. 1, Row 5	Alkyl
Col. 2, Row 4	$O_2 \rightarrow$ Alkyl
Col. 1, Row 6	Alkenyl
Col. 5, Row 5	Misc A → Alkenyl
Col. 6, Row 5	Se
Col. 7, Row 0	Cycl P
Col. 7, Row 1	Mixed Cycl P

Fragment Dictionary

Col. 65, Row 1	Alkylene
Col. 65, Row 3	Ethylene
Col. 65, Row 5	Alkenyl

8. OTHER PHOSPHORUS NUCLEUS



Other Phosphorus Nucleus

Col. 63, Row 12	P-Misc.
Col. 63, Row 11	P-Misc. once
Col. 63, Row 4	Misc.=Metal
Col. 64, Row 4	Phos 3
Col. 60, Row 12	P-R
Col. 60, Row 0	P-R twice

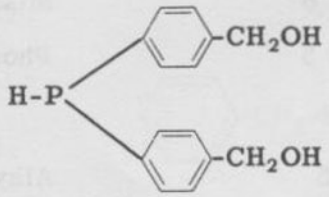
1st Node

Col. 5, Row 9	Misc A → Misc.
Col. 7, Row 3	Miscellaneous

Fragment Dictionary

Col. 70, Row 4	Halogen
Col. 70, Row 5	Chlorine
Col. 70, Row 9	Polyhalo

9. OTHER PHOSPHORUS NUCLEUS



Other Phosphorus Nucleus

Col. 64, Row 4	Phos 3
Col. 63, Row 12	P-Misc.
Col. 63, Row 11	P-Misc. once
Col. 63, Row 5	Misc=Hydrogen
Col. 60, Row 12	P-R
Col. 60, Row 0	P-R twice

1st Node

Col. 1, Row 5	Alkyl
Col. 5, Row 4	Misc A → Alkyl

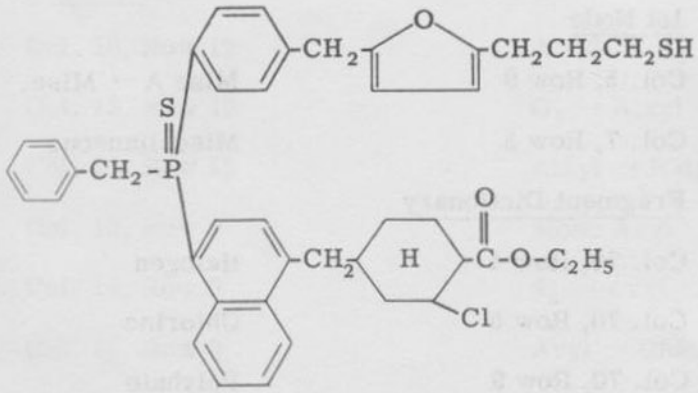
2nd Node

Col. 19, Row 2	Aryl → OH
Col. 10, Row 2	OH
Col. 22, Row 2	OH → chain
Col. 52, Row 6	Monoaryl

Fragment Dictionary

Col. 65, Row 1	Alkylene
Col. 65, Row 2	Methylene
Col. 70, Row 12	O-containing
Col. 70, Row 2	OH

10. OTHER PHOSPHORUS NUCLEUS



Other Phosphorus Nucleus

Col. 62, Row 7	P=S
Col. 62, Row 8	P=S once
Col. 64, Row 5	Phos 5
Col. 60, Row 12	P-R
Col. 60, Row 1	P-R three times

1st Node

Col. 1, Row 7	Monoaryl
Col. 5, Row 6	Misc A → Aryl
Col. 1, Row 5	Alkyl
Col. 5, Row 4	Misc. A → Alkyl

2nd Node

Col. 19, Row 1	Aryl → Heterocycle
Col. 8, Row 11	O-Heterocyclic
Col. 22, Row 1	Hetero → Chain
Col. 9, Row 12	Cycloalkyl
Col. 19, Row 12	Aryl → Alkyl
Col. 22, Row 12	Alkyl → Chain
Col. 52, Row 6	Mono Aryl
Col. 52, Row 3	Poly Aryl

Terminal Node

Col. 41, Row 4	Aryl → SH
Col. 32, Row 4	SH
Col. 44, Row 4	SH → Chain
Col. 31, Row 7	COOR
Col. 41, Row 7	Aryl → COOR, Met
Col. 45, Row 7	COOR-Ring
Col. 46, Row 6	Chlorine
Col. 49, Row 7	Aryl → Halo
Col. 51, Row 11	Halo → Ring
Col. 53, Row 11	Mono Aryl
Col. 53, Row 2	Poly Aryl

Fragment Dictionary

Col. 66, Row 12	Aryl
Col. 66, Row 11	Benzene

Fragment Dictionary (Continued)

Col. 65, Row 11	Lower Alkyl
Col. 65, Row 1	Alkylene
Col. 65, Row 4	Propylene
Col. 65, Row 2	Methylene
Col. 65, Row 12	Alkyl
Col. 66, Row 1	Cycloalkyl
Col. 66, Row 2	Cyclohexyl
Col. 66, Row 5	Heterocyclic
Col. 67, Row 12	Unsat.-Het.
Col. 67, Row 11	5-membered
Col. 67, Row 3	Unsat.-2+
Col. 67, Row 6	O-Hetero
Col. 67, Row 8	1 Hetero Atom
Col. 68, Row 0	Mono Ring
Col. 68, Row 2	C, O
Col. 68, Row 5	O=C-OR
Col. 69, Row 0	S-containing
Col. 69, Row 4	SH
Col. 70, Row 4	Halogen
Col. 70, Row 5	Chlorine

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1. Frome, Julius. "Mechanized Searching of Phosphorus Compounds." Patent Office Research and Development Report No. 18. Washington 25, D. C., Department of Commerce, 1961.
2. Frome, Julius and Leibowitz, Jacob. "A Punched Card System for Searching Steroid Compounds." Patent Office Research and Development Report No. 7. Washington 25, D. C., Department of Commerce, 1957.
3. Classification Bulletin, Class 260, Chemistry, Carbon Compounds. No. 200 Rev. 1, U.S. Patent Office, Department of Commerce, Washington 25, D. C., pp. 260-79.

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