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**Part 1**

**Chemical Coding Applications on the IBM Sorter**

NEW CODES FOR HOLLERITH-TYPE PUNCHED CARDS  
TO SORT INFRARED ABSORPTION AND CHEMICAL STRUCTURE DATA\*

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INTRODUCTION

Qualitative infrared analysis involves matching the spectrogram obtained from an unknown compound with one of several thousand known standard spectrograms. The number, size, type, and location of standard spectrograms makes this operation time-consuming. Attempts to simplify the job have resulted in many different systems which usually involve notched cards and needles. Codes and sorting systems using Hollerith cards and International Business Machine sorters have provided a new, simple, fast, accurate, inexpensive, and foolproof means of making universal searches for matching purposes. All operations can be carried out by non-technical personnel on any sorter. The cost of punching master decks of cards to index all available spectrograms is being borne by the author's employer. Duplicate decks are available to all at cost of reproduction. The cooperation of the American Petroleum Institute Research Project 44, the Infrared Punched Card Committee headed by E. Carroll Creitz at the National Bureau of Standards, the American Society for Testing Materials, Samuel P. Sadtler, Inc., and many industrial laboratories has been assured. A similar project for indexing the ASTM x-ray diffraction data card file as well as author-subject search cards for infrared literature is well under way. Cards to index mass spectral data, Raman, ultraviolet, and visible absorption data as well as author-subject cards for x-ray diffraction literature and other fields, all with interlocking codes, are being considered. The savings in time alone resulting from the use of such cards is inestimable.

DISCUSSION

The rapid increase in the number of infrared absorption spectrograms of known compounds that are available to the infrared analyst through publication of catalogs and papers makes the handling of these data increasingly difficult. This is reflected in widespread efforts to make use of notched and other types of punched cards to reduce the time and labor involved. Among many such systems, those reported by Wright<sup>7</sup>,

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\*This article is a reprint in part of Dr. Kuentzel's paper appearing in *Analytical Chemistry*, Vol. 23, No. 10, October, 1951 (a publication of the American Chemical Society). The International Business Machines Corporation wishes to express its appreciation to *Analytical Chemistry* for extending permission to reprint this article - Editor's note.

Stroupe<sup>6</sup>, Brattain<sup>1</sup>, and the Punch Card Committee of the Ohio State University Symposium on Molecular Structure and Spectroscopy<sup>5</sup>, are typical. That none of the systems is widely used results from a number of factors, such as cost of preparation and duplication of the cards, limited simple coding positions, and mechanical problems of sorting. Moreover, such cards and systems were usually designed to fit the problems of a particular laboratory. They have a place in infrared analysis and will continue to be used widely, but there is growing demand for a system that can handle large numbers of cards and be useful in many laboratories.

Hollerith-type cards and sorting machines such as those offered by International Business Machines Corp., provide an answer to many problems that arise in designing a universal system. Such cards and equipment are being used in many phases of scientific endeavor<sup>3</sup>. Their adaptation to the handling of infrared absorption and chemical structure data was the object of the work reported in this paper. The system requires only the use of an IBM sorter<sup>2</sup>.

In general, the codes described herein enable one to prepare cards to sort and correlate infrared absorption data as obtained from sodium chloride and potassium bromide prisms regardless of the form, size, or location of the spectrograms. The cards merely provide an indexing system for matching spectrograms and for correlating chemical structure with absorption data without handling spectrograms themselves. Each card carries punched details of absorptions, chemical structure, physical properties, and a reference to the location of the original data or spectrogram for a given compound, but only the latter reference is printed on the card. The cards enable more or less nontechnical help to make rapid, accurate searches through data on large numbers of cards to locate one or a few pertinent spectrograms which may be removed directly from the file and turned over to competent infrared workers for final analysis. The savings in time, money, and wear and tear on expensive original spectrograms can be considerable. Moreover, such cards are very easily reproduced for exchange and distribution among infrared laboratories and thus provide a very convenient means of indexing spectrograms that are generally available in catalogs, books, and the literature.

Ingenuity and a partial knowledge of the properties or structure of the compound can greatly reduce the number of cards that need be sorted for absorption matching. Sorting for cards bearing particular absorptions can be done simultaneously over as wide or as narrow a range of numbers as necessary, depending upon the width of the absorption or the accuracy with which its position has been determined. The cards may be filed without segregation or according to boiling point range, chemical classification, catalog or library, absorption characteristics, or other systems to provide for card-eliminating selections in the act of removing them from the file for sorting operations.

The codes and sorting operations have been kept as simple as is consistent with a reasonably accurate and specific search. All absorptions exhibiting an intensity of 20% or more absorbed as measured from the adjacent background are punched in to 0.1-micron or 10-cm.<sup>-1</sup> resolution over most of the 2- to 49-micron range. As the system was designed to make the best use of existing spectrograms, which have been obtained under many conditions, no rigid criteria for cell thickness and sample concentration are designated.

Usually the best spectrogram is used for determining which absorptions to punch. Therefore, if one recognizes that a good spectrogram is one in which the strongest absorptions show no transmittance and most of the rest fall between 20 and 70% transmittance, and uses whatever means may be necessary to obtain such a spectrogram, he can be reasonably certain of reliable results in sorting operations with the Wyandotte cards. Conditions that have given good spectrograms in many cases are 30% solution in a 0.1-mm. cell or pure sample in a 0.03-mm. cell. The chemical classification code is based entirely upon structure and elements to eliminate confusion caused by organic names and chemical properties when nontechnical personnel use the cards. However, units in the codes follow common radical types and organic structural arrangements, so that a knowledge of organic chemistry facilitates the use of the codes. The chemical coding system represents a compromise between the extremely complete code devised by the National Research Council<sup>4</sup> and those used on many Keysort systems. Provision is made for expansion of the codes as needs arise. The number of carbon, nitrogen, oxygen, and sulfur atoms, the melting or boiling point, and a serial number or literature reference to the spectrogram are also punched into the card. The latter is printed on the card to facilitate location of the spectrogram for analysis. Finally, space is reserved for the private use of individual laboratories.

### GENERAL CODES

The codes which determine the significance of the punches in the card and thus form the basis for both punching and sorting operations are given below. The location of a punch position in a card is indicated by a column and row designation. The columns are 80 in number and are identified by small numbers 1 through 80 (Figure 1). The horizontal rows are 12 in number and are indicated by numbers 0 through 9 plus two unlabeled overpunches above the 0 row, referred to as x and y in these codes. The y punch is uppermost. As many punches as are necessary may be made in any one column. By using a multiple punch code<sup>2</sup> an entire alphabet can be coded into one column.

INFRARED ABSORPTIONS		TO LO MICRON	CHEMICAL CLASSIFICATIONS (SEE CODE CHART)		ATOMS		- + B.P.		IDENTIFICATION	
TO O.I. MICRON			A	B	C	N O S	- +	M.P.	JOURNAL	SERIAL NO.
0	0	0	0	0	0	0	0	0	0	0
1	2	3	4	5	6	7	8	9	10	11
1	1	1	1	1	1	1	1	1	1	1
2	2	2	2	2	2	2	2	2	2	2
3	3	3	3	3	3	3	3	3	3	3
4	4	4	4	4	4	4	4	4	4	4
5	5	5	5	5	5	5	5	5	5	5
6	6	6	6	6	6	6	6	6	6	6
7	7	7	7	7	7	7	7	7	7	7
8	8	8	8	8	8	8	8	8	8	8
9	9	9	9	9	9	9	9	9	9	9

THIS INDEXING SYSTEM  
 WAS DEVELOPED IN THE  
 PHYSICS RESEARCH LABORATORIES  
 RESEARCH AND DEVELOPMENT DIVISION  
 WYANDOTTE CHEMICALS CORPORATION  
 WYANDOTTE, MICHIGAN

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80  
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 I 6 4 B A  
 JOURNAL VOL. PAGE SERIAL NO. LIBRARY TYPE  
 IBM 501



1. Column 1.

A y overpunch indicates that absorptions have been punched in as wave numbers in reciprocal centimeters. No overpunch signifies that the absorptions were punched as wave lengths in microns.

2. Columns 1 through 5

Infrared absorptions punched in as wave numbers in reciprocal centimeters are coded here. Headings above the columns indicate wave number divided by 1000. Numbers punched into these columns indicate wave numbers to hundreds. Thus, a 5 punched in column 3 headed by the number 4.0 means 4500 reciprocal centimeters. Punching resolution is 100 reciprocal centimeters.

3. Columns 6 through 23

Same as No. 2, except that punches indicate wave numbers to 10 reciprocal centimeters. Thus, a 5 punched in column 15 headed by the number 1.0 means 1050 reciprocal centimeters. Punching resolution is 10 reciprocal centimeters.

4. Columns 1 through 25.

(No overpunch at y in column 1.) Infrared absorptions punched in at wave-length positions in microns occupy these columns. The column number indicates the whole number value. Tenths are punched into the column. Thus, a punch at 5 in column 12 means 12.5 microns. Punching resolution is 0.1 micron.

5. Columns 26 through 28

Same as No. 4, except that column headings indicate values to tens and the units are punched into the column. Thus a punch at 5 in column 27, which is headed by the number 30, means 35 microns. Punching resolution is 1 micron. Digits 0 through 5 of column 26 are to be used for coding organometallic and inorganic cards to be issued later.

6. Columns 29 through 31

No use has been assigned to these columns. They are reserved for future expansion as agreed upon by a majority of those using the cards.

7. Columns 32 through 57

This section is used for punching in chemical composition and structure (see the accompanying Chemical Classification Code, Table I). A compound is coded by inspecting a structural formula and punching in all applicable codes. A special code for inorganic and organometallic compounds will be issued later.

8. Columns 58 through 62

The number of carbon, nitrogen, oxygen, and/or sulfur atoms are punched in these columns. In columns 60, 61, and 62, overpunches are used to indicate numbers over 9 according to the schedule in the accompanying Miscellaneous Codes.

9. Columns 63, 64, and 65.

One value of a melting point or a boiling point at 760-mm. pressure (or near thereto) in degrees centigrade is punched here. The hundreds digit is punched into column 63, the tens into 64, and the units into column 65. Identification of the number is achieved by means of overpunches in columns 64 and 65 according to the schedule in the schedule in the Miscellaneous Code.

10. Columns 66 through 70

These are reserved for each individual laboratory to use as it sees fit. Private codes and numbering systems may be punched into these columns at will without conflicting with any master code.

### 11. Columns 71 through 79

These columns are used to identify the source of the infrared spectrogram from which the absorption data punched into the card were obtained. If the curve came from a publication, the identity of the journal or book is given by a code punched into columns 71 and 72 (see the Miscellaneous Code). Volume and page numbers are punched in columns 73 through 78. If the spectrogram is from a regular library of infrared curves, the library will be identified by a letter punched into column 79 according to the schedule in the Miscellaneous Code and the serial number of the spectrogram punched into columns 74 through 78. Column 73 will be used for coding subdivisions of any particular library not involving literature references. Letters are used and a different code for each library is permissible. The owner or publisher of each library is responsible for this code and it will be made known to users as needed.

### 12. Column 80

The type of information punched into the card will be indicated by punches in this column (see the Miscellaneous Code).

Data punched into columns 71 through 80 are printed at the top of the card for ease in reading.

Table I. Chemical Classification Code Chart

Part A					
Row	Column 32, Elements	Column 34, Basic Structure	Column 36, Substitutions	Column 38, Miscellaneous	Row
—	C, H only	Saturated aliphatic	Unsubstituted	Not used	—
0	O	Unsaturated aliphatic	Monosubstituted	Solid	0
1	N	Saturated monocyclic	Disubstituted	Liquid	1
2	S	Unsaturated monocyclic	Trisubstituted	Gas	2
3	F	Saturated polycyclic	Higher substituted	Organometallic	3
4	Cl	Unsaturated polycyclic	Alpha substituted	Isotopic	4
5	Br, I	Benzo aromatic	Beta substituted	Indeterminate	5
6	P, As, Sb, Bi	Polybenzo aromatic	Gamma substituted	Inorganic	6
7	Si, Ge, Sn, Pb	Fused ring aromatic	Delta substituted	Polymer	7
8	Se, Te	3 or 4 atom ring			8
9	B, Al	5 or 6 atom ring			9
z		7 or more atom ring			z
y	Other	Other			y

Row	Column 33, Unsaturation	Column 35, Rings—Chains	Column 37, Substitutions	Column 39	Row
0	>C=C<		Internal		0
1	1	1	1		1
2	2	2	2		2
3	3	3	3		3
4	4	4	4		4
5	5	5	5		5
6	6	6	6		6
7	7	7	7		7
8	8	8	8		8
9	9	9	9		9
z	—C=C—	10	10		z
y	Internal	11 or more	Other		y

Part B						
Row	Column 40, Carbon-Hydrogen	Column 42, Oxygen	Column 44, Nitrogen	Column 46, Sulfur	Column 48, Nitrogen-Oxygen	Row
0	—CH <sub>3</sub> , Methyl	—C(=O)OH Acid, anhydride	—C(=NH)N< Amidine	—C(=S)S— Thionothioic	>NC(=O)O— Carbamyl	0
1	—C <sub>2</sub> H <sub>5</sub> , Ethyl	—C(=O)OR Ester, salt	>NC(=NH)N< Guanidine	—C(=S)H Thioaldehyde	>NC(=O)N< Ureido, ureylene	1
2	—C <sub>3</sub> H <sub>7</sub> , n-Propyl	—C(=O)H Aldehyde	—C≡N Nitrilo, cyano	>C=S Thione, thioketo	—C(=O)N< Amide	2
3	—C <sub>4</sub> H <sub>9</sub> , Isopropyl	>C=O Ketone	—N≡C Isonitrilo	—SC(=S)S— Trithiocarbonate	—N=C=O Isocyanate	3
	—C <sub>4</sub> H <sub>9</sub> , n-Butyl	—OC(=O)— Carbonate	—NH <sub>2</sub> n-Amine	—SH Thiol	—OC≡N Cyanate	4
	—C <sub>4</sub> H <sub>9</sub> , Isobutyl	C(OH) <sub>2</sub> Ortho carbonate	>NH sec-Amine	—S— Sulfide	>N—NO <sub>2</sub> Nitro amine	5
	—C <sub>4</sub> H <sub>9</sub> , sec-Butyl	—C(OH) <sub>2</sub> Ortho carboxylate	>N tert-Amine	—SS— Polysulfide	>N—N=O Nitrosoamine	6
7	—C <sub>4</sub> H <sub>9</sub> , tert-Butyl	—OH Alcohol, phenol	=NH Imine	—H <sub>2</sub> S <sup>+</sup> Sulfonium	—N=N(=O)— Azoxy	7
8	—C <sub>4</sub> H <sub>11</sub> , n-Pentyl	—O— Ether, oxy	>N—N< Hydrazone, hydrazine	=S=S Perthio	—ONO <sub>2</sub> Nitrate	8
9	—C <sub>6</sub> H <sub>5</sub> , Phenyl	—OO— Peroxide	—N=N— Other		—ONO Nitrite	9
z		Other Heterocyclic	Heterocyclic	Other Heterocyclic	Other Heterocyclic	z
y						y

**Table I. Part B (Continued)**

Row	Column 41	Column 43, Oxygen	Column 45, Nitrogen	Column 47	Column 49, Nitrogen-Oxygen	Row	
0		-H <sub>2</sub> O <sup>+</sup> Oxonium	-N=N-N< HN=N <sup>+</sup> ≡N <sup>+</sup>	Triazine Diazonium Quaternary ammonium		-NO <sub>2</sub> Nitro	0
1						-N-O Nitroso	1
2						>NO- Isonitroso, oxime	2
3			>N< >NCN	Ammonium Cyanamide		>N=O Amino oxide	3
4							4
5							5
6							6
7							7
8							8
9							9
z							z
y							y

Row	Column 50 Nitrogen-Sulfur	Column 52, Oxygen-Sulfur	Column 54, Nitrogen-Oxygen-Sulfur	Column 56, Other Elements	Row
0	>NC(=S)N< Thiourido	-OC(=S)S- Dithiocar- -SC(=O)S- bonate	-C(=O)NS- Carboxamido sulfide	F	0
1	>NC(=S)S- Thiocarbonyl	-OC(=S)O- Thiocar- -OC(=O)S- bonate	>NC(=S)O- Thiocar- >NC(=O)S- bamate	Cl	1
2	-C(=S)N< Thio amide	-C(=S)O- Thiolic, -C(=O)S- thionic	-C(=O)SCN Acyl thio- cyanate	Br.	2
3	-C(=NH)S- Thio imide	-S(O <sub>2</sub> )O- Sulfonate	-C(=O)NCS Acyl isothio- cyanate	P	3
4	-SCN Thiocyno	-S(O)O- Sulfinate	>NS(O <sub>2</sub> )N< Sulfamide	As, Sb	4
5	-NCS Isothiocyno	-S(=O)S- Thiosulfi- -S(=S)O- nate	>NS(O <sub>2</sub> )O- Azo sulfo- nate	B	5
6	>NSN< Diamino sulfide	>S <sub>2</sub> O <sub>3</sub> (x=1-4) Thionate	>NS(O <sub>2</sub> )- Sulfonyl amine	Si	6
7	>NS Sulfime, etc.	>SO <sub>2</sub> Sulfone	>NS(=O)O- Amino sulfinate		7
8	-N=S Sulfamino	>S=O Sulfoxy, sulfanyl	-N=S=O Sulfanyl amine		8
9	>S=N- Sulfimine	-OSO- Sulfenate	-N(SO <sub>2</sub> H) <sub>2</sub> Amino disulfate		9
z	Other Heterocyclic	Other Heterocyclic	Other Heterocyclic	Other Heterocyclic	z
y					y

Row	Column 51	Column 53, Oxygen-Sulfur	Column 55, Nitrogen-Oxygen-Sulfur	Column 57, Inorganic Esters	Row
0		>SO <sub>2</sub> Sulfate	-S(O <sub>2</sub> )N< Sulfonamide	Carbonic, etc.	0
1		>SO <sub>3</sub> Sulfite	-S(=O)N< Sulfinamide	Sulfuric, etc.	1
2				Nitric, etc.	2
3				Phosphoric, etc.	3
4				Boric, etc.	4
5					5
6					6
7					7
8					8
9					9
z					z
y					y

## CODES FOR CHEMICAL CLASSIFICATION

Table I is the Chemical Classification Code Chart.

### General Instructions.

#### Part A.

1. All elements in the compound being coded are punched into column 32 according to the schedule in the chart. Thus a compound containing carbon, hydrogen, oxygen, sulfur, and chlorine would require punches at 0, 2, and 4 in this column. As other charts will be prepared for metalorganic and inorganic compounds, only those elements most commonly found in organic compounds are included in this chart.
2. Column 34 is used to code major structural features of the compound. This may involve several punches to codify complex molecules completely. When an inspection of the structural formula reveals structures that can be characterized by any of the codes, they should be so punched into the card.
3. Column 33 provides for identifying types and location of unsaturated bonds. If there is a 2 and/or 4 punch in column 34, punches in this column locate unsaturation in rings.

Otherwise, the code locates unsaturation in chains. The type of unsaturation is indicated by punches at 0 or x.

4. Column 35 is used to indicate the number or length of rings or carbon chains. If punches in column 34 indicate two or more rings, the number punched into column 35 records the total number of rings. If only one ring, or no rings, are present the number indicates the length of the longest carbon-carbon chain.

5. Columns 36 and 37 indicate the degree and location of substitutions upon the basic structures. The code is not adequate for large complex molecules, but with these there are usually many other coding possibilities which provide means for sorting them. The numbers in column 37 may be used to indicate substitution positions on rings or chains.

6. Column 38 codes the physical state and other miscellaneous classifications. Unfilled sections in the chart provide for expansion.

#### Part B.

1. Column 40 codes the simplest carbon-hydrogen groups.

2. Except for columns 56 and 57 (discussed below) the rest of Part B is concerned with coding reactive groups or radicals. A reactive group as used in this code is defined as a combination of atoms containing no more than one carbon atom and/or atoms of oxygen, nitrogen, and/or sulfur, with or without hydrogen which usually function together to impart special properties to a compound. For the most part they may be considered organic radicals. The more complex radicals involving two or more carbon atoms can usually be coded as a combination of two or more of the simple groups. As several punches may be made in any one column, it is possible to code all the groups that may be present in even very large molecules. Coding is based entirely on structure. The names included in the chart are merely exemplary and are not meant to restrict the use of a particular punch.

Heterocyclic rings are coded with y punches in the proper column, depending upon what elements other than carbon are present. Whether the ring is saturated or not and the size of it are revealed by punches in column 34.

3. Column 56 codes radicals or reactive groups containing other elements in combination with oxygen, nitrogen, or sulfur. The other elements by themselves are not considered groups or radicals. Thus, chlorobenzene would be coded by a 4 punched in column 32 and a 5 in column 34 but nothing punched into Part B.

4. Column 57 provides for organic esters of inorganic acids. All esters of related acids are given the same punch. Thus, esters of phosphoric, phosphorous, pyrophosphoric, metaphosphoric, hypophosphoric, etc., acids would all be coded with a punch at 3 in column 57.

Blank spaces may be used for additions to the code. Anyone desiring to suggest additions should communicate with the author, so that codes will not become mixed through duplication.

Use of the chemical classification code chart is illustrated with a few examples of coding. It is intended that the codes be applied on a strict structural basis without regard to chemical names or properties. This may result in some duplication, such as

the coding of 2-thiopseudouric acid in the examples. Here the sulfur atom is coded both as a thio-keto group (column 46, punch 2) and as a part of a thiourido group (column 50, punch 0). Large groups or radicals usually can be coded by using two or more of the simpler ones. Thus, a thiocarbohydrazone,  $R:NNHC(:S)-NHNH_2$ , could be coded as a thio amide, a hydrazine, and an amine. The general practice is to start with a central carbon atom, tie as much to it as can be done in using the code, then add other codes to identify the rest of the group. It is better to overcodify than to use too few code designations in describing a compound. An understanding that such an attitude was used in punching the cards will assist the user in obtaining maximum usefulness from them. (See table II)

Coded Examples					Table II
	Column	Punch			
1. <i>p</i> -Chlorophenol	32 34 36 37 38 42	0,4 5 1 1,4 0 7			$C_6H_4OH$
2. Isoprene	33 34 35 36 37 38 40	0,1,3 0 4 0 2 1 0			$CH_2=C(CH_3)-CH=CH_2$
3. 2-Thiopseudouric acid	32 34 36 37 38	0,1,2 1,9 0 2 0	Column 42 44 46 48 50	Punch 3 y 2 1 0	
4. Sulfamethylthiazole	32 34 35 36 38	0,1,2 1,5,9 2 3 0	40 44 50 54	0 4 y 6	
5. Potassium salt of $\gamma$ - <i>p</i> -chlorophenoxy crotylmercaptomethyl penicillin	32 33 34 35 36 37	0,1,2,4,y 0,2 3,5,8,9 3 3,6 1,4	38 40 42 44 46 48 50	0 0 1,3,8 y 5 2 y	$CH_3(C_6H_4O)C=CHCH_2SCH_2C(=O)NHCH_2CH(S)(C(CH_3)_3)CH_2COOK$

## MISCELLANEOUS CODES

1. Provision for indicating a larger number of atoms than 9 in columns 60, 61, and 62 is achieved by use of overpunches. A y overpunch adds 10 to the value punched in the column, an x adds 20, and a 0 punch adds 30 to the punched-in number. Thus, for example, an x and a 5 punched in column 61 indicate 25 oxygen atoms. All numbers over 38 are punched as 39.
2. The code for identifying the number punched in columns 63, 64, and 65 is as follows:

y punched in column 64 indicates boiling point below zero.  
y punched in column 65 indicates boiling point above zero.  
x punched in column 65 indicates melting point above zero.  
x punched in column 64 indicates melting point below zero.

These overpunches remove plus or minus signs on the card, so that interpretation is easy. Only one number for a given compound can be punched into a card.

3. A code list of books and journals for punching references into columns 71 and 72 follows:

<u>No.</u>	<u>Journal or Book</u>
1	Analytical Chemistry
2	Journal of the American Chemical Society
3	Journal of the Optical Society of America
4	Journal of Research of the National Bureau of Standards
5	Transactions of the Faraday Society
6	"Infrared Determination of Organic Structures," Randall

Others will be added as needed, and all users of the cards notified.

4. The code list of libraries as punched into column 79 follows:

<u>Letter</u>	<u>Library</u>
A	American Petroleum Institute Research Project 44
B	User's own library
C	Sadtler Library of Spectrograms
D	National Bureau of Standards Cards (Creitz)

Others will be added as needed.

5. A code list of types of data to be punched into column 80 follows:

<u>Letter</u>	<u>Type of Data</u>
A	Infrared absorption (2 to 50 microns)
B	X-ray diffraction (ASTM powder data)
C	Ultraviolet absorption
D	Raman
E	Mass spectroscopic

Others will be added as needed, including bibliographies.

The ways in which cards punched according to these codes can be sorted are almost limitless. As each punch is a direct, independent code, a sort at any given position will

segregate all cards having the property or character coded by the position. Further sorts of the cards segregated by the first sort isolate groups of cards that represent compounds having two, three, or more features in common. Such sorting can be carried as far as available information permits. The order in which the sorts are made often determines the speed with which unwanted cards are eliminated. Usually a well-chosen first sort eliminates 90% or more of the cards from further consideration. Thus, when sorting absorptions it is time-saving to make the first sort on an absorption that appears to be unique or characteristic. It is easy to segregate cards coding melting or boiling points in as wide or as narrow a range as desired. Private codes further classifying compounds into such groups as wetting agents, dyes, sugars, plastics, etc., depending upon local interests are useful. Finally, having the spectrogram serial numbers punched into the cards enables one to sort the cards quickly into numerical sequence for a periodic check for missing cards.

As the sorting is practically effortless and automatic, human error is reduced to a minimum. It is possible to make quick and accurate comparisons or correlations between all types of data punched into the card. The number of uses to which the coded information can be put grows with increased familiarity with the code and sorting system. Decks of punched cards indexing all published infrared spectrograms have been prepared and are available at very low cost from publishers of catalogs of spectrograms.

#### LITERATURE CITED

1. Brattain, R., private communication, March 1951.
2. Eckert, W., J. Chem. Education, 24, 54-7 (1947).
3. Ferris, L., Taylor, K., Perry, J., and Torok, M., "Bibliography on the Uses of Punched Cards," Punched Card Committee, American Chemical Society.
4. National Research Council, Washington, D. C., Chemical-Biological Coordination Center, "Method of Coding Chemicals for Correlation and Classification," 1950.
5. Ohio State University, Punch Card Committee, Report, June 1950.
6. Stroupe, J., private communication, June 1950.
7. Wright, Norman, Abstracts of Papers, 108th Meeting, Am. Chem. Soc., p. 6L, New York, September 1944.

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INSTRUCTIONS AND CODES FOR WYANDOTTE PUNCHED CARDS  
INDEXING X-RAY DIFFRACTION DATA

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GENERAL

Wyandotte X-Ray Punched Cards were designed to facilitate the matching of powder data obtained from unknown compounds with identifying data in the file of x-ray diffraction data cards published by the Joint Committee on Chemical Analysis by X-Ray Diffraction Methods and to provide a means for using a partial knowledge of the chemical nature or physical properties of the unknown to assist in the matching operations for qualitative analysis. Moreover, it is an object in the use of these cards to provide a fool-proof method for non-technically trained personnel to carry out the actual sorting operations on an International Business Machines sorter at a high rate of speed. Finally, the ease and accuracy with which decks of such cards can be reproduced or duplicated provides punched cards at very low cost which can be distributed widely for the common good.

The design of the present card, the sorting system and codes were an outgrowth of similar work done in the field of infrared absorption and the cooperative effort of Dr. F. W. Matthews, other members of the Indexing Sub-Committee of the above-mentioned A. S. T. M. joint group and the writer. Whereas, the need for such cards and sorting procedures in the infrared absorption field was acute resulting in widespread and immediate acceptance of the new techniques, the excellent filing system and indexes developed for the x-ray diffraction data cards as well as the new Keysort type cards now available have made the need for machine sorting of x-ray data less acute, nevertheless, it is felt that any attempt to make x-ray analysis less time-consuming, more reliable, more flexible and less expensive for both cards and salary of sorting personnel merits thorough investigation and testing. It is believed that Research Departments using machine sorting for other purposes such as infrared absorption, ultraviolet and visible absorption, mass spectroscopic and raman analysis as well as subject-author literature searches and laboratory note records will find it convenient to handle x-ray diffraction analysis the same way.

The present punched cards were designed to handle x-ray diffraction powder data. No provision is made for the intensities of the lines but all spacing or "d" values of lines having a relative intensity of 10 or more are punched into the cards. Lines of less intensity are punched in if there are less than ten lines in the pattern having the required





of 7.32 angstroms would be coded by a punch of 3 in column 31 which is headed by the number 7. The last two columns have a punching resolution of 1.0 angstroms, so that a value of 23.7 would be punched in as 4 in column 35 headed by the number 20. All values 29 or greater are punched in as 29.

2. Columns 43 through 62. This space is allotted to punching in chemical classifying data. Section A provides for coding the identify of all elements in the compound according to the schedule in the "Elements Code" which is given in detail later. Section B is used to code the common radicals of inorganic chemistry. See the "Radicals Code" on page 19 for details. Section C provides for some indication of the type of organic compound and Section D contains miscellaneous information. See "Organic Code", page 20, and "Miscellaneous Code", page 20, for identity of punch positions in these sections.

3. Columns 63, 64 and 65. This space may be used to record the melting point of the compound being coded. This is accomplished by rounding off the number to the nearest whole number and punching the units value into column 65, the tens into 64 and the hundreds into column 63. All melting points of 999° C. or higher are punched in as 999.

4. Columns 71 through 79. Information punched into this section serves to identify the source of the x-ray data punched into the card. If this involves a journal or book reference, such space is indicated and a code list of such periodicals will be made up and punched into columns 71 and 72, as the need arises. However, at present the only source of such data is the A.S.T.M. Card File of X-Ray Diffraction Data so that the serial number is punched in. The simple serial number, running from 0001 up in each set, was used with the exception that instead of using a digit to indicate whether the set was "original", "first supplement" or "second supplement" this was indicated by using letters A, B or C respectively and placing the letter after the number. Thus, a card from the second supplement (set No. 3) bearing the number 3-0255 was actually punched in as 255C with the C falling in column 79. This number is printed at the top of each card.

5. Column 80. To provide a means of separating cards of various types by machine, a letter code is used in this column to identify the type of data punched into the card. See the "Type Code", page 21, for details.

6. Columns 66 through 70. This space is reserved for each individual laboratory to use as it sees fit. Special codes may be used here without interfering with any of the master codes.

7. Columns 36 through 42. These columns provide for additional punching space should the need arise in the future. Use of this space is subject to approval by the Joint Committee for the common good of those utilizing such cards for sorting purposes.

#### SPECIFIC CODES

##### 1. Elements Code. Chemical Classification. Section A.

Each element is assigned a punch position in this section. Since each punch position is independent, any number of different elements can be coded, and sorted for, independently. There is no provision for indicating the number of any particular kind of atom since this

is not known when sorting is being done. It is intended that pre-sorts based on knowledge of the presence of certain metal elements as might be obtained from emission spectroscopy may reduce the number of cards that need be handled in spacing sortings. The punch positions are indicated by a column number and a digit or letter locating the punch in the column. Thus, copper is coded by punching number 9 in column 44. This list is in both numerical and alphabetical arrangement.

#### ELEMENTS

43-0 Actinium - Ac	45-9 Holmium - Ho	48-4 Rhodium - Rh
43-1 Aluminum - Al	45-x Hydrogen - H	48-5 Rubidium - Rb
43-2 Americium - Am	45-y Indium - In	48-6 Ruthenium - Ru
43-3 Antimony - Sb	46-0 Iodine - I	48-7 Samarium - Sm
*43-4 Argon - A	46-1 Iridium - Ir	48-8 Scandium - Sc
43-5 Arsenic - As	46-2 Iron - Fe	48-9 Selenium - Se
43-6 Astatine - At	43-4 Krypton - Kr	48-x Silicon - Si
43-7 Barium - Ba	46-3 Lanthanum - La	48-y Silver - Ag
43-8 Beryllium - Be	46-4 Lead - Pb	49-0 Sodium - Na
43-9 Bismuth - Bi	46-5 Lithium - Li	49-1 Strontium - Sr
43-x Boron - B'	46-6 Lutecium - Lu	49-2 Sulfur - S
43-y Bromine - Br	46-7 Magnesium - Mg	49-3 Tantalum - Ta
44-0 Cadmium - Cd	46-8 Manganese - Mn	49-4 Technetium - Tn
44-1 Calcium - Ca	46-9 Mercury - Hg	49-5 Tellurium - Te
44-2 Carbon - C	46-x Molybdenum - Mo	49-6 Terbium - Tb
44-3 Cerium - Ce	46-y Neodymium - Nd	49-7 Thallium - Tl
44-4 Cesium - Cs	43-4 Neon - Ne	49-8 Thorium - Th
44-5 Chlorine - Cl	47-0 Neptunium - Np	49-9 Thulium - Tm
44-6 Chromium - Cr	47-1 Nickel - Ni	49-x Tin - Sn
44-7 Cobalt - Co	47-2 Nitrogen - N	49-y Titanium - Ti
44-8 Columbium - Cb	47-3 Osmium - Os	50-0 Tungsten - W
44-9 Copper - Cu	47-4 Oxygen - O	50-1 Uranium - U
44-x Curium - Cm	47-5 Palladium - Pd	50-2 Vanadium - V
44-y Dysprosium - Dy	47-6 Phosphorus - P	43-4 Xenon - Xe
45-0 Erbium - Er	47-7 Platinum - Pt	50-3 Ytterbium - Yb
45-1 Europium - Eu	47-8 Plutonium - Pu	50-4 Yttrium - Yt
45-2 Fluorine - F	47-9 Polonium - Po	50-5 Zinc - Zn
45-3 Francium - Fr	47-x Potassium - K	50-6 Zirconium - Zr
45-4 Gadolinium - Gd	47-y Praseodymium - Pr	50-7 Unassigned
45-5 Gallium - Ga	48-0 Prometheum - Pm	50-8 "
45-6 Germanium - Ge	48-1 Proactinium - Pa	50-9 "
45-7 Gold - Au	48-2 Radium - Ra	50-x "
45-8 Hafnium - Hf	43-4 Radon - Rn	50-y "
43-4 Helium - He	48-3 Rhenium - Re	

\* Also Helium, Krypton, Neon, Radon and Xenon

## 2. Radicals Code. Chemical Classification Section B.

Herein, an attempt is made to further identify the type of compound being considered. It was felt that a place should be provided for making additional card-eliminating pre-sorts based upon partial knowledge of the unknown compound obtained from various qualitative chemical tests. Since the kinds and degrees of accuracy of such tests are quite numerous, it was decided to confine coding to the name of the compound itself in the hope that whatever chemical tests might be made upon it the net result would be a partial revelation of the name. The following inorganic radicals have been sufficient in kind to code all compounds listed in the present x-ray diffraction file. Additions will be made as needed. The use of prefixes and suffixes to further qualify these radicals has not been attempted so one will find, for example, that all phosphates, whether, pyro-, ortho- etc., will be coded by a punch at number 6 in column 54.

### RADICALS

51-0 aluminate	53-0 ferrite	55-0 selenate	57-0 chromite
51-1 ammonium	53-1 fluoride	55-1 selenide	57-1 gallate
51-2 antimonate	53-2 fulminate	55-2 selenite	57-2 palladite
51-3 antimonite	53-3 germanate	55-3 silicate	
51-4 arsenate	53-4 hafniate	55-4 silicide	
51-5 arsenide	53-5 hexammine	55-5 stannate	
51-6 arsenite	53-6 hydride	55-6 stannide	
51-7 bismuthate	53-7 hydroxide	55-7 sulphate	
51-8 borate	53-8 iodate	55-8 sulphide	
51-9 boride	53-9 iodide	55-9 sulphite	
51-x bromate	53-x manganate	55-x tantalate	
51-y bromide	53-y molybdate	55-y telluride	
52-0 carbamate	54-0 nitrate	56-0 tellurite	
52-1 carbide	54-1 nitride	56-1 thionate	
52-2 carbonate	54-2 nitrite	56-2 titanate	
52-3 cerate	54-3 osmate	56-3 thorate	
52-4 chlorate	54-4 oxide	56-4 tungstate	
52-5 chloride	54-5 pentammine	56-5 uranate	
52-6 chlorite	54-6 phosphate	56-6 vanadate	
52-7 chromate	54-7 phosphide	56-7 zincate	
52-8 cyanamid	54-8 phosphite	56-8 zirconate	
52-9 cyanate	54-9 plumbate	56-9 zirconyl	
52-x cyanide	54-x plumbide	56-x platinate	
52-y ferrate	54-y rhenate	56-y platinitite	

(Column 58 available for expansion)

3. Organic Code. Chemical Classification. Section C.

Since the number of organic compounds in the x-ray diffraction data file is growing rapidly, it was deemed advisable to provide some breakdown of this class of compounds. The code below provides this and is based entirely upon structure and is thus divorced both from chemistry and names. Such a code may be useful for some time to come. However, when it becomes desirable to classify the organic compounds more precisely, a code developed for cards handling infrared absorption and chemical structure data can be adapted to fit x-ray punch cards.

ORGANIC

59-0 Saturated aliphatic  
59-1 Unsaturated aliphatic  
59-2 Saturated monocyclic  
59-3 Unsaturated monocyclic  
59-4 Saturated polycyclic  
59-5 Unsaturated polycyclic  
59-6 Benzo aromatic  
59-7 Polybenzo aromatic  
59-8 Fused ring aromatic  
59-9 Heterocyclic  
59-x Unassigned  
59-y Unassigned

(Column 60 available for expansion)

4. Miscellaneous Code. Chemical Classification. Section D.

The general class of the compound being coded is indicated here. The list is self-explanatory.

MISCELLANEOUS

61-0 Hydrated  
61-1 Inorganic  
61-2 Organic  
61-3 Metal organic  
61-4 Unassigned  
61-5 “  
61-6 “  
61-7 “  
61-8 “  
61-9 “  
61-x “  
61-y “

(Column 62 available for expansion)

5. Type Code. Column 80.

Letters punched into this column indicate the type of data the card bears. This makes it possible to separate the various cards should they become mixed. Thus, all cards dealing with x-ray diffraction powder data will have a "B" punched into this column.

TYPE

80-A Infrared Absorption (2 to 40 microns)

80-B X-Ray Diffraction (Powder Patterns)

80-C Ultraviolet Absorption

80-D Raman

(Others will be added as needed, including bibliographies)

The punched card shown in Figure 1 illustrates the manner in which the codes are applied. This card indexes the data on card number 152 of the first supplement as indicated by the first "B". The second "B" over column 80 means that the card indexes x-ray diffraction data. The three punches in the A Section of Chemical Classification codes elements carbon (44-2), hydrogen (45-x) and oxygen (47-4). Punches in Sections C and D indicate that an organic compound containing a benzene ring is involved. The spacing values are punched into the left half of the card. The compound involved is phthalic anhydride.

SORTING TECHNIQUES

The IBM sorter operates upon one column at a time and normally deposits cards in a pocket corresponding to the highest number punched into the column. However, by using selector switches, it is possible to segregate all cards punched at any one or more positions in a column regardless of what other numbers may also be punched. This makes possible the coding of a large mass of data in a form that is relatively easy to sort. Each punch is independent of all others and may be sorted for independently. Since this is the case, the order in which various punched positions are sorted has no effect upon the final results but the time required to make a series of sorts can be lessened considerably by an intelligent search program. Thus, in so far as it can be determined, the most characteristic or unique data should be sorted first. This eliminates the largest number of cards which need not be handled again. Such a beginning sort may be a diffraction line, not necessarily one of the strongest, which has a rather uncommon value. Or, it may be that the identity of a rather uncommon element is known so that a beginning sort can be made via the elements section. Each sort for a specific punch position eliminates many cards and retains those cards representing compounds having the punched-for data in common. The first sort usually eliminates about 90% of the cards and the number of cards normally reduces to a half dozen or less in 4 or 5 sorts.

When sorts involving the angstrom spacing values are made, it should be remembered that numbers from 1.00 through 3.49 were rounded off to the nearest hundredth (to the nearest tenth for values from 3.4 through 9.9 and to the nearest unit from 10 through 29)

when the data was punched into the cards. So, if there is any doubt as to the exact value of a line being measured on an unknown pattern, sorting should be carried out over a broad enough range to insure inclusion of the line in question. Thus, a value of 2.576 angstroms would be punched into the card as 2.58 and if a value for the same line as measured in an unknown pattern gave 2.574 and sorting was done for a value of 2.57 the card would be missed. Since it is possible to sort for 2.57 and 2.58 simultaneously, or over wider ranges if desired, this should be done in all cases where there is some doubt as to the exact value of the line being sorted. One may always extend the range arbitrarily over which sorting may be made in order to insure including the particular line being sorted.

Since the cards wear out with use and are subject to accidental loss or damage, it is advised that spare decks of punched cards be kept on hand for rapid replacement. Wyandotte Chemicals Corporation will continue to supply decks of punched cards at a price that reflects little more than the actual cost of reproduction and handling so that they may be considered expendable. Also, rigid uniformity of reproduction will be maintained by having the same master decks used at all times. This is necessary in order to maintain the usefulness of both cards and codes. Other projects of a similar nature in other fields of science have been invalidated by promiscuous reproduction of cards and alteration of codes on the part of many users. In an attempt to prevent such from occurring to the present project, Wyandotte Chemicals Corporation has copyrighted all cards and codes prepared in our laboratories. This should not be construed as an attempt to restrict use of the cards in any sense as it is a safety measure only. Persons desiring to reproduce copyrighted cards for their own use should apply to Wyandotte Chemicals Corporation for permission. However, it is hoped that the cost of punched cards available to users through distributors will be sufficiently low so as to make such reproduction economically unattractive.

Finally, unpunched, printed cards which bear no reference to Wyandotte Chemicals Corporation copyright are available at cost and handling charges to laboratories that wish to punch cards to index x-ray data in their own private libraries. Also, Wyandotte Chemicals Corporation will assist any laboratory desirous of having their own unpublished x-ray data indexed on Wyandotte Cards. All that is required is a list of the compounds, formulae and line and intensity data, and such other pertinent data as may be available. The data are to remain the property of Wyandotte Chemicals Corporation which agrees not to further reproduce or distribute them without permission of the original owner.

Part 2

Application of the IBM Type 602-A Calculating Punch



CALCULATION OF SQUARE ROOTS  
ON THE  
IBM TYPE 602-A CALCULATING PUNCH

John J. Herz

Square roots may be calculated on the IBM Type 602-A Calculating Punch by an algebraic method similar to that used with desk calculating machines. This method depends on the fact that the sum of an arithmetic progression whose first term is 1 and whose common difference is 2, is equal to the square of the number of terms.

The radicand is broken up into groups of two digits each, starting with the units and tens position and going left. The highest order group is considered first.

The sum of the first five terms of the progression 1, 3, 5, etc., is 25. If 25 is subtracted from any number between 0 and 99, the sense of the remainder is an indication of the size of the square root of that number. If the remainder is negative, the square root lies between 0 and 4; if it is positive or zero, the root lies between 5 and 9. In the former case, the terms of the series 9, 7, 5, 3, 1, are added successively to the remainder until the sum again becomes positive or zero. In the other case, the remainder is first made negative by subtracting 75 from it, and then the terms of the series 19, 17, 15, 13, 11, are added to it until the sum is positive or zero. In either case, the number of additions performed is subtracted from 5 or 10, respectively, to find the square root.

The square root of 121,104, for example, would be found in the following manner:

12		
<u>-25</u>	<u>+5</u>	
= -13	=5	Remainder is negative; no further subtraction is necessary.
+ 9	-1	
<u>+ 7</u>	<u>-1</u>	
= 3	=3	Remainder is positive; no further addition takes place.

This completes the first iteration. The number of additions performed during this iteration, subtracted from 5, is 3. This is the high order digit of the root.

Before proceeding with the second iteration, three things must be done:

- a) Multiply the remainder by 100 and add the next two digits of the radicand to the product.  $(100 \times 3) + 11 = 311$ .
- b) Multiply the last addend by 10 and decrease the product by 10.  $(10 \times 7) - 10 = 60$ .
- c) Multiply the square root, as far as it has been developed, by 10.  $10 \times 3 = 30$ .
- On the second iteration, the subtrahend consists of the sum of the first five terms of the progression 1, 3, 5, etc., namely 25, plus five times the result of (b).

	311	30	
$(5 \times 60) + 25$	<u>-325</u>	<u>+5</u>	
	=-14	=35	Remainder is negative.
60 + 9	<u>+69</u>	<u>-1</u>	
	=55	=34	Sum is positive.

- a)  $(100 \times 55) + 04 = 5504$ .
- b)  $(10 \times 69) - 10 = 680$ .
- c)  $10 \times 34 = 340$ .

Third iteration.

	5504	340	
$(5 \times 680) + 25$	<u>-3425</u>	<u>+5</u>	
	=2079	=345	Remainder is positive.
$(5 \times 680) + 75$	<u>-3475</u>	<u>+5</u>	
	=-1396	=350	
680 + 19	<u>+699</u>	<u>-1</u>	
	=-697	=349	
680 + 17	<u>+697</u>	<u>-1</u>	
	=0	=348	Sum is zero (positive).

#### Planning Chart and Wiring\*

This illustration shows how to extract a six-digit square root from a twelve-digit radicand.

Read. The two highest digits of the radicand are added in counters 3, 4, 5, which are coupled to make one counter-group (the B counter), over storage transfer exits 2R, 2L, 1R, 3R, 3L, and the normal points of co-selectors 1 and 2. The rest of the radicand is entered in storage units 1R, 2L, 2R, 3L, 3R. A read cycles impulse is taken to program skip 2.

Program Step 1. This step is skipped.

Program Step 2. Co-selector 1 is picked up from the program couple. A 9 from the digit emitter is added in counter 1 (the A<sub>1</sub> counter) over the transferred points of co-selector 1 and the normal of co-selector 3. 25 is subtracted in

\*Planning charts follow this paper

the B counter over the transferred points of co-selector 1 and the normal of co-selector 2. 5 is added in counter 6 (the R counter) over the transferred points of co-selector 1 and the normal of co-selector 2. The B counter is tested at the end of this program. If it is negative, the negative balance will cause a skip to program step 5.

Program Step 3. This step has no significance on the first iteration, since counter 2 (the  $A_2$  counter) is clear.

Program Step 4. These exits, as well as program exits 3, emit impulses only if the B counter was positive at the end of program step 2. Co-selector 2 is picked up from the program couple. 10 is added in both A counters, whose entries are common, over the transferred points of co-selector 2 and the normal of co-selector 5. 75 is subtracted in the B counter over the transferred points of co-selector 2. 5 is added in the R counter over the normal points of co-selector 1 and the transferred of co-selector 2.

Program Step 5. Co-selector 3 is picked up from the program couple. The number in the  $A_1$  counter is added in the B counter and also entered in storage unit 4L. 7 is added in the  $A_2$  counter over the transferred points of co-selector 3. 1 is subtracted in the R counter over the transferred points of co-selector 3 and the normal of co-selector 4. A digit impulse is led over the transferred points of co-selector 3 to the D pickup hub of pilot selector 1, which is coupled with co-selector 4. The balance test is explained below.

Program Steps 6-9. 4 is subtracted alternately in the two A counters over the transferred points of co-selector 4 and the normal of co-selectors 1 and 3. The numbers in these counters are alternately added in the B counter and also entered in storage unit 4L. 1 is subtracted in the R counter on each of these steps over the normal points of co-selector 3 and the transferred of co-selector 4. The B and R counters and storage unit 4L are controlled by all cycles impulses taken over the transferred points of co-selector 4.

Since the negative balance impulse is timed exactly like an X impulse, a positive balance in the B counter is indicated by pilot selector 7 being normal at X time. In that case a hot X is led over the normal points of that pilot selector, and when either co-selector 3 or 4 is transferred (in other words, on program steps 5-9), the X will cause skipping to program step 10 and will also drop out pilot selector 1 and co-selector 4. If the hot X were entered into pilot selector 7 directly, it might go through the normal points in the split second the pilot selector requires to become transferred. To prevent this, the hot X is delayed by leading it over the transferred points of pilot selector 8, which is itself picked up by a hot X. A co-selector may be used instead of pilot selector 8.

Program Step 10. The B counter is read into storage unit 6, the R counter into 7R, and all counters are reset.

This completes the first iteration. The remainder of the radicand is in storage

unit 6, the last addend used is in storage unit 4L, and the first digit of the root is in storage unit 7R.

Program steps 11 and 12 will set up the counters for the second iteration.

Program Step 11. 10 is subtracted in both A counters over the normal side of co-selector 2 and the transferred side of co-selector 5, which is picked up from the program couple. An all cycles impulse is taken over the transferred points of co-selector 5 to read out storage unit 7R, which is added in the R counter, shifted one position. The same impulse is also used to read out storage unit 6, which contains the remainder of the radicand. This remainder is added in the B counter, shifted two positions. A digit impulse is taken over the transferred points of co-selector 5 to the D pickup hub and the high C hub of pilot selector 2. An all cycles impulse is taken to the low C hub of pilot selector 2, also over the transferred points of co-selector 5. From the N hub of the lower part, this impulse reads out storage unit 1R (wire A), which contains the second highest pair of digits of the radicand. This is added in the B counter, also. Pilot selector 2 will transfer at the end of this program.

Program Step 12. The last addend used is read out of storage unit 4L and added in both A counters, shifted one position.

Program Step 13. The number in the  $A_2$  counter is subtracted five times in the B counter, by impulsing the  $\times 5$  hub.

Program Step 14. Same as program step 2.

Program Step 15. Same as program step 13.

Program Steps 16-22. Same as program steps 4-10.

Program Step 23. Program step 23 is the same as program step 11, but since pilot selector 2 is now transferred, storage unit 2L will be read out instead of storage unit 1R. Also, pilot selector 3 receives an impulse to transfer, so that storage unit 2R can be read out on program step 35, etc.

The remaining program steps are repetitions of the two iterations just described. Each iteration will develop one digit of the root.

On program steps 12, 24, 36, etc., the last addend used is added in the A counters from storage unit 4L, shifted one position. At the end of the fifth iteration, this number may have six digits, in which case the highest digit cannot be added in the A counters. Instead, it is stored in storage unit 1L and read into the B counter on program steps 61, 63, and 65-69.

On program step 60, pilot selector 6 receives an impulse to transfer, and on program step 70 an impulse from program exit 10 taken over the transferred points of pilot selector 6 will cause the machine to punch the result and read the next card.

If a half adjustment is desired, the "reset to 5" impulse must be taken to the units position of the R counter over the transferred points of a selector coupled with pilot selector 5, and the normal of pilot selector 6. Pilot selector 6 is coupled with another

co-selector. The five low positions of counter exit 6 are taken to the normal points of that co-selector, the five high positions to the transferred points, and the common points to storage entry 7R.

On a machine with all possible counters and at least eight pilot selectors, seven-digit square roots may be calculated. Conversely, to get a five-digit root, the wiring for pilot selector 6 and storage units 1L and 3R are omitted. Pilot selector 5 then assumes the function of terminating the problem.

Digits in Square Root	Estimated Speed		Ratio	Square Roots per Hour (Algebraic Method)
	Analytic Method *	Algebraic Method		
6	86	52	1.7	231
5	80.6	43	1.9	279
4	75.2	34	2.2	353
3	69.8	25	2.8	480
2	64.4	16	4.0	750

\* The method described in the Principles of Operation manual for the IBM Type 602-A Calculating Punch.

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# IBM CALCULATING PUNCH TYPE 602A PLANNING CHART

APPLICATION \_\_\_\_\_ PROBLEM \_\_\_\_\_ A \_\_\_\_\_

PROGRAM SUPPRESS	STEP	OPERATION	STORAGE UNIT		COUNTER B							R	SELECTORS			
			IL	IR	A1	A2	DIVIDEND				A1			A2	6	
					1	2	3	4	5	6	7	8	9	10	11	12
13	1	READ 1 SKIP 2 PUNCH CYCLE 5 T O	RO													
14	2	X 5	RO	RO	+9	RO			+B1							
25	3	SKIP TO 5 IF -							-A2							
26	4								-25	+5						
27	5	X 5	RO	RO		RO			-A2							
39	6															
51	7				+10	+10			-75	+5						
55	8															
63	9	SKIP TO 10 IF +	RO		RO	+7	TEST		+A1	-1						
30	10															
31	11															
32	12															
42	13	"	RO		-4	RO	TEST		+A2	-1						
43	14	"	RO													
44	15	"	RO		RO	-4	TEST		+A1	-1						
45	16	"	RO													
46	17															
47	18															
48	19															
49	20															
50	21															
51	22															
52	23															
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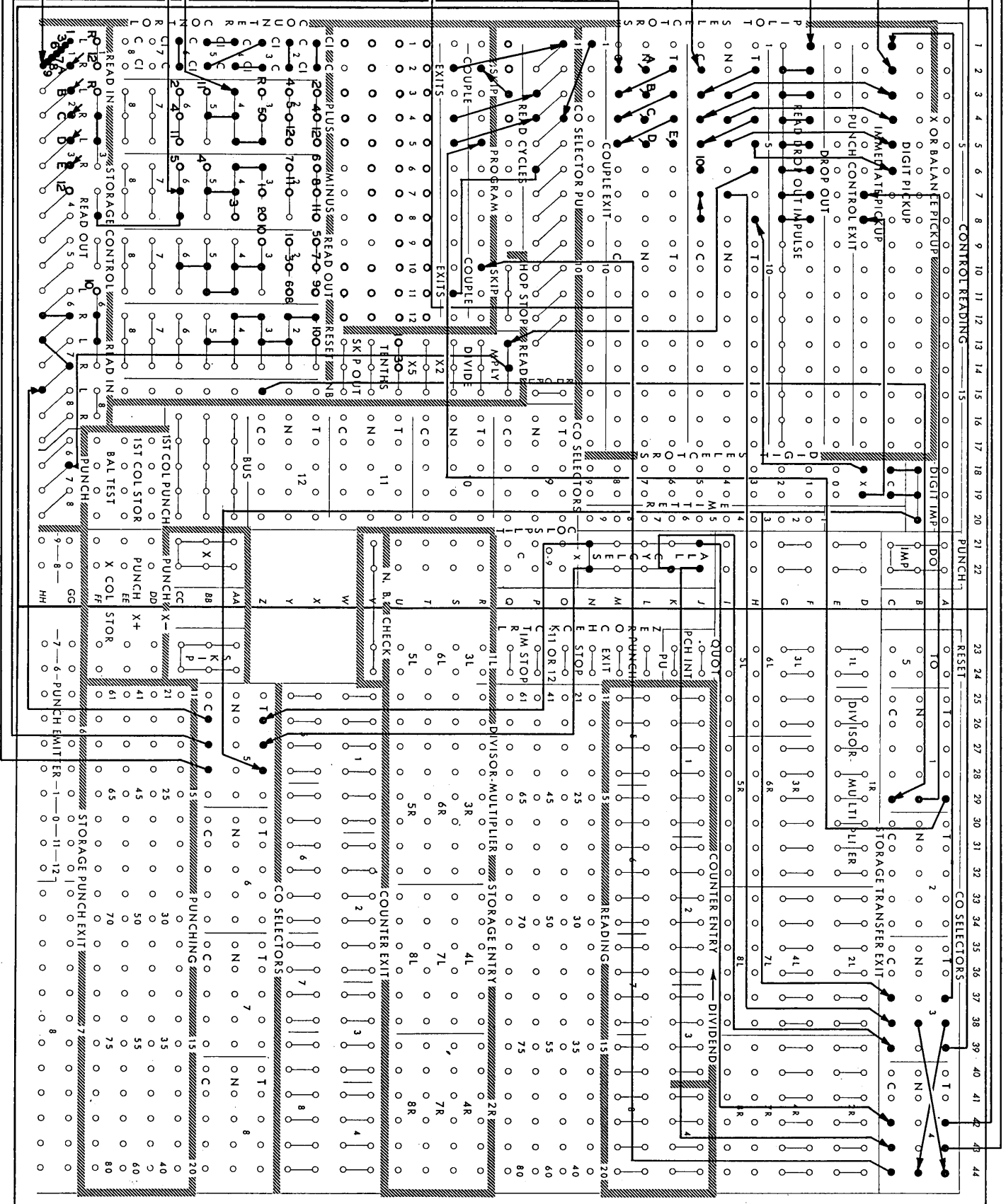
INTERNATIONAL BUSINESS MACHINES CORPORATION

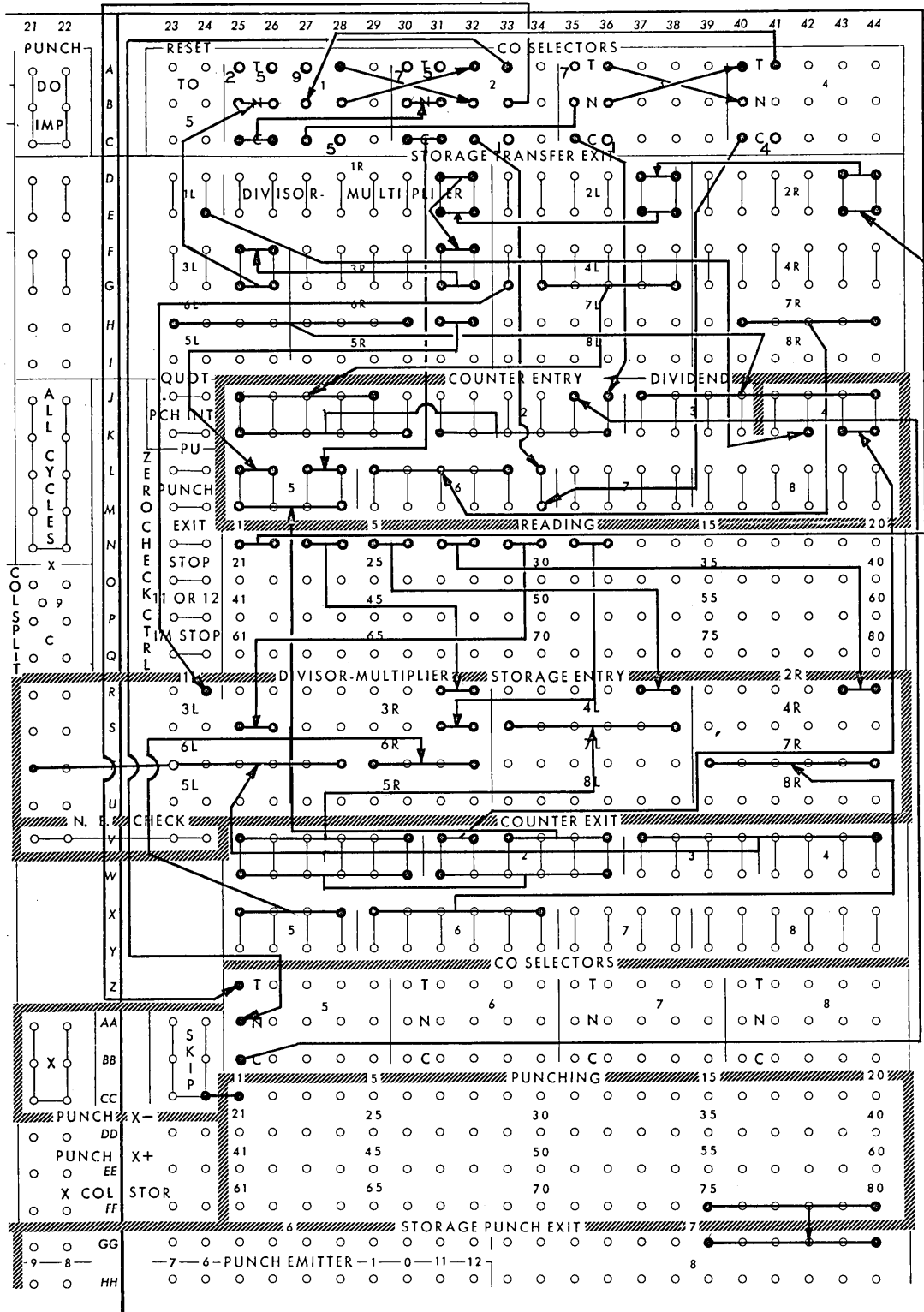


CALCULATING PUNCH  
TYPE 602 A CONTROL PANEL

FORM 22-9323-1

PRINTED IN U.S.A.







**Part 3**

**Uses of the IBM Card-Programmed Electronic Calculator**

FLOATING DECIMAL MATRIX INVERSION ON THE  
 IBM CARD-PROGRAMMED ELECTRONIC CALCULATOR  
 MODEL 402-417 BB, 604-3

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 International Business Machines Corporation

INTRODUCTION

“Floating decimal” notation is a means of representing any number by eight significant digits and an exponent, the high order digit not being zero. The decimal is affixed by considering the decimal to lie always after the first digit, and then placing after the eighth digit fifty plus some exponent of ten. This exponent is of such value that ten raised to this exponent multiplied by the eight digit term would place the decimal in the correct position. For example in “floating decimal” notation, the number 1.2345678 would be written as 1234567850, 12.345678 as 1234567851, 123.45678 as 1234567852, 0.12345678 as 1234567849, 0.0012345678 as 1234567847, and so on.

Zero matrix elements are entered as 1000000010 which is equal to  $1 \times 10^{-40}$ .

The method described below for inversion of a matrix is identical to that presented in the paper given on this subject at the 1950 seminar<sup>1</sup>. However, the difficulty caused by the presence of non-dominant diagonal elements is reduced by use of the floating decimal technique.

EXAMPLE

Given a matrix of coefficients in floating decimal notation:

$$\begin{vmatrix} 1000000050 & 2000000050 & 1000000050 \\ 6000000050 & 8000000050 & 9000000050 \\ 1000000050 & 5000000050 & 6000000050 \end{vmatrix}$$

Augment this matrix, forming:

$$\begin{vmatrix} 1000000050 & 2000000050 & 1000000050 & 1000000050 & -5000000050 \\ 6000000050 & 8000000050 & 9000000050 & 1000000010 & 1000000050 & -2400000051 \\ 1000000050 & 5000000050 & 6000000050 & 1000000010 & 1000000010 & 1000000050 & -1300000051 \end{vmatrix}$$

Apply  $\frac{a_i - \sum b_{i,j} b_{j,k}}{b_{i,i}}$  to all terms to the right of the principal diagonal and

$a_{i,k} - \sum b_{i,j} b_{j,k}$  to all other terms, where the “a” terms are originals and the “b”

terms are those previously operated on.

The resultant matrix is called the forward solution:

$$\begin{vmatrix} 1000000050 & 2000000050 & 1000000050 & 1000000050 & & & -5000000050 \\ 6000000050 & -4000000050 & -7500000049 & 1500000050 & -2500000049 & & -1500000050 \\ 1000000050 & 3000000050 & 7250000050 & -7586206949 & 1034482849 & 1379310349 & -4827586249 \end{vmatrix}.$$

Invert the order of each sub-matrix, keeping only applicable terms. Thus:

$$\begin{vmatrix} & & & 1379310349 & 1034482849 & -7586206949 & -4827586249 \\ -7500000049 & & & 1000000010 & -2500000049 & 1500000050 & -1500000050 \\ 1000000050 & 2000000050 & & 1000000010 & 1000000010 & 1000000050 & -5000000050 \end{vmatrix}.$$

Apply  $b_{i,k} - \sum c_{i,j} c_{j,k}$  to all terms, where the "b" terms are of the forward solution and the "c" terms are those which have already been operated upon in the back solution.

$$\begin{vmatrix} & & & 1379310349 & 1034482849 & -7586206949 & -4827586249 \\ -7500000049 & & & 1034482849 & -1724137949 & 9310344849 & -1862069050 \\ 1000000050 & 2000000050 & & -3448275949 & 2413793049 & 1034482849 & -7931034549 \end{vmatrix}.$$

The second sub-matrix, which is shown in inverted order, is the inversion of the original matrix of coefficients.

#### METHOD

To apply this process to the IBM Card-Programmed Electronic Calculator, two basic requirements are necessary. First, the 604 calculator must be wired to perform the necessary arithmetic operations in floating decimal notation. Secondly, a means of organization of data, instructions, and results is desired which facilitates ease in handling and is nearly automatic.

To suit the first requirement a 604 control panel has been designed which will perform the operations described in Table 1. By use of programming cards in addition to the cards containing the matrix elements, these operations are sufficient.

The second requirement is satisfied by means of 402 and 521 control panels which summary punch results with all instruction and identification necessary for continuation of the reduction process.

TABLE 1

604 Operations

<u>Operation Code</u>	<u>Calculation</u>	<u>Result Available</u>
blank	$C - A \times B$	A and C
4	$C/A$	“
3 and 8	transfer	“
3	$-A \times B$	“
2	$A + C$	“

Consider “a” elements as those of the original augmented matrix, “b” elements as the resultant elements from the forward solution, and “c” elements as the resultant elements from the back solution. There will be a division and a check sum program card associated with the “a” cards in the forward solution. Similarly, there will be a check sum program card associated with the “b” cards in the back solution. Breaking down the main classes of cards functionally, there are:

I. Matrix Element Cards (program 1)

1. Either:

- a) transfer element to storage
- b) negatively multiply element  $b_{i,j}$  or  $c_{i,j}$  by corresponding  $b_{j,k}$  or  $c_{j,k}$  term called from storage
- c) negatively multiply element  $b_{i,j}$  or  $c_{i,j}$  by corresponding  $b_{j,k}$  or  $c_{j,k}$  term called from storage and add the result to previous accumulated product
- d) add element to previous accumulated product and add row, column, and division identification to counter group 1

2. Cause summary punching (back solution divisions 2, 3 only)

3. Special Instructions (applicable to back solution only)

II. Division Cards (program 2, used only on forward solution)

1. Divide  $a_{i,k} - \sum b_{i,j} b_{j,k}$  by corresponding  $b_{i,i}$
2. Cause summary punching
3. Special Instructions

III. Check Sum Cards (program 3 on forward solution; 2 on back solution)

1. Add resultant element to the sum of previous resultant elements to the right of the principal diagonal.

REDUCTION CALCULATIONS

The basic computing scheme for the reduction of a given element  $b_{i,k}$  located to the right of the principal diagonal is as follows:

<u>Card</u>	<u>Program Number</u>	<u>Channel A</u> (from card)	<u>Channel B</u> (from storage)	<u>Operation</u>	<u>Result</u>	<u>Store</u>
1	1	$b_{1,k}$	$b_{1,1}$	$-A \times B$	$-\sum_{j=1}^1 b_{1,j} b_{j,k}$	C
2	1	$b_{2,k}$	$b_{1,2}$	$C - A \times B$	$-\sum_{j=1}^2 b_{1,j} b_{j,k}$	C
3	1	$b_{3,k}$	$b_{1,3}$	$C - A \times B$	$-\sum_{j=1}^3 b_{1,j} b_{j,k}$	C
.	.	.	.	.	.	.
.	.	.	.	.	.	.
(i-1)	1	$b_{(i-1),k}$	$b_{1,(i-1)}$	$C - A \times B$	$-\sum_{j=1}^{(i-1)} b_{1,j} b_{j,k}$	C
i	1	$a_{1,k}$		$A + C$	$a_{1,k} - \sum b_{1,j} b_{j,k}$	C
(i+1)	2	$b_{i,1}$ (from storage)		$C/A$	$b_{i,k}$	C (S. P.)
(i+2)	3	$\sum_{m=i+1}^{k-1} b_{i,m}$ (from ctr. grp. 7)		$A + C$	$\sum_{m=i+1}^k b_{i,m}$	C, ctr. grp. 7
(i+3)	1	$b_{1,(k+1)}$	$b_{1,1}$	$-A \times B$	$-\sum_{j=1}^1 b_{1,j} b_{j,(k+1)}$	C
(i+4)	1	$b_{2,(k+1)}$	$b_{1,2}$	$C - A \times B$	$\sum_{j=1}^2 b_{1,j} b_{j,(k+1)}$	C

To facilitate easy access to factors, row and column numbers are used which correspond with CPC storage in the following manner:

<u>Row or Column</u>	<u>Numbered</u>
1	11
2	12
3	13
4	14
5	15
6	16
7	17
8	18
9	21
10	22
11	23
12	24
13	25
14	26
15	27

<u>Row or Column</u>	<u>Numbered</u>
16	28
17	72
18	73
19	74
20	75
21	76

Using this numbering system, the  $b_{i,j}$  factors are entered into storage by column number. Then they are called out by the row number of the  $b_{j,k}$  cards.

#### CHECK SUM

Division 3 of the original augmented matrix is made up of elements which are the negative sum of the elements of their respective rows. This division is reduced just as Division 2. It is apparent that the sum of the resultant elements on a given row lying to the right of the principal diagonal is always  $-1$ . By adding these elements, a check on the computation is obtained row by row.

#### SUMMARY PUNCHING TO THE LEFT OF PRINCIPAL DIAGONAL

Occasionally it may be desirable to punch  $b_{i,k}$  terms on and to the left of the principal diagonal. This is accomplished by coupling nines which are punched in column 38 with the operation code through Co-selector 4 which is controlled by Setup Switch 3. Special Instruction 1 is used to cause an X to punch in column 34, identifying the elements on and to the left of the principal diagonal.

#### FORWARD SOLUTION

The description of the computation of  $b_{i,k}$  is duplicated for all values of  $b$  lying to the right of the principal diagonal except for the first row. As there is no product to be accumulated on the first row reduction,  $a_{i,k}$  is merely transferred and divided by  $a_{11,11}$ .

For values of  $b_{i,k}$  on or to the left of the principal diagonal there are no programming cards.  $b_{i,k}$  is not summary punched but is stored by column number. It will then be called out later by the row number of the  $b_{k,j}$  term. There is no check sum program card since these values should not enter the sum.

#### BACK SOLUTION

The back solution is similar to the forward with the principal difference being the absence of division programming cards. Therefore, summary punching must occur on the presence of the  $b_{i,k}$  card, where the "b" cards are to be added and the "c" cards form the accumulated product.

#### CARD FORM

The card form is as shown in Figure 1.\* Further identification and control punches are:

\*Figure 1 and all following figures will be found at the end of the article.

- X21 original matrix elements
- X36 back summaries
- X33 forward summaries
- X34 summaries on and to the left of principal diagonal
- X70 unit matrix right of diagonal
- X78 clear identification on forward solution
- X80 clear identification on back solution

### COLLATING

The reduction calculations during either the forward or back solutions are processed one row at a time. After completion of a given row of reductions, the summary cards are merged with the element cards for the next row. Then, on a second collator run, the summaries and the element cards for the next row along with their associated programming cards are inserted; at the same time, the old element cards along with their associated programming cards are removed. As an example, suppose that row ten has just been processed. The  $b_{10,1}$  would be taken and merged before the  $a_{11,1}$  cards. Then, on a second run, the  $b_{10,1}$  will be placed after the  $b_{9,1}$  cards and the  $a_{10,1}$  element and program cards will be replaced by the  $a_{11,1}$  element and program cards. Thus, the deck is prepared for processing the eleventh row.

The control panel wiring for the forward solution and back solution are shown in Figures 2 and 3, respectively.

Because the back solution requires inverted element order within each division, a back division number is punched to replace 1 with 3 and 3 with 1. The program number is similarly treated for the back solution.

### 402 ACCOUNTING MACHINE

Different instructions as necessary for the forward and back solutions are punched into the "b" cards automatically. The instructions CH A, CH B, CH C, and Oper. apply to the forward solution and the instructions CH A, CH B\*, CH C\*, and Oper.\* apply to the back solution. The instructions to be effective are controlled through Co-selectors 1, 2 and 5 which are transferred by Setup Switch 2. This switch is turned "on" during the back solution.

Listing is obtained ordinarily by an X punch in the operation field. Listing of all cards is obtained by turning Setup Switch 1 on.

Identification (matrix no., division no., row no., column no.) is added to Counter group 1 with an X in column 21 on the forward solution and an X in 33 on the back. Counter group 1 is cleared on X33 or X78 on the forward solution and X36 or X80 on the back solution.

All counters are cleared on a minor control break. This break in control is obtained as follows: division number and program number are compared with digits 3 and 3 or 2 respectively depending on which solution is being processed. Unless there is an equal condition, Co-selector 11 is transferred, this co-selector having an emitted X wired to

common and the normal wired to minor program start. Therefore, the control break is obtained only on an equal condition. The card with Division 3 and Program 3 (2 on back solution) represents the last card concerned with the reduction of a given row and, therefore is where clearing is desired.

Figure 4 shows the 402 wiring diagram.

#### 521 SUMMARY PUNCH

The 521 will punch instructions in the following manner:

- A. During the forward solution
  - 1. CH A
    - a) punch 00
  - 2. OPER.
    - a) if Special Instruction 3, punch 3
    - b) otherwise, blank
  - 3. OPER.\*
    - a) if division 3, overpunch with an X
    - b) if Special Instruction 3, punch 3 and 8
    - c) if Division 1, punch 3 and 8
    - d) if not Division 1, underpunch with a 9
    - e) if not Special Instruction 3 or Division 1, punch 2.
  - 4. CH B
    - a) punch row number
  - 5. CH B\*
    - a) blank
  - 6. CH C
    - a) blank
  - 7. CH C\*
    - a) if Division 1 or Special Instruction 3, punch column number
    - b) if Division 2 or 3 and no Special Instruction 3, punch 00
- B. During the back solution
  - 1. CH A
    - a) punch 00
  - 2. OPER.
    - a) blank
  - 3. OPER.\*
    - a) if Special Instruction 3, punch 3
    - b) otherwise, blank
  - 4. CH B
    - a) blank
  - 5. CH B\*
    - a) punch with row number
  - 6. CH C
    - a) blank



7. CH C\*

a) blank

The wiring diagram for the 521 is shown in Figure 5.

604 CALCULATOR

Some explanation of the planning chart (Figure 6) and the selector diagram (Figure 7) is necessary. The notation 012, 025, 252 is used in the remarks and on the selector diagram to fix hub locations. The first two digits identify the program number and the last digit identifies the exit hub. For example 053 refers to the fifth program step and its third exit hub.

The suppression code is as follows:

1. Group Suppress Unit 1
2. Group Suppress Unit 2
3. Group Suppress Unit 3
4. Group Suppress Unit 4
5. + Balance
6. - Balance
7. Zero
8. Non-zero
- 10 to 18. Suppress on division
- 20 to 28. No suppression on division
32. No suppression when Selector 3 is transferred

REFERENCES

1. Justus Chancellor, John W. Sheldon, G. Liston Tatum. "The Solution of Simultaneous Linear Equations using the IBM Card-Programmed Electronic Calculator". Proceedings, Industrial Computation Seminar, September 1950 --- IBM Corporation.

FLLOATING DECIMAL MATRIX INVERSION

AMERICAN U.S.A.

MULTIPLE LAYOUT FORM  
FOR ELECTRIC ACCOUNTING MACHINE CARDS

BRANCH OFFICE NO. \_\_\_\_\_

DATE \_\_\_\_\_

FORM 12-4833-3ENCO

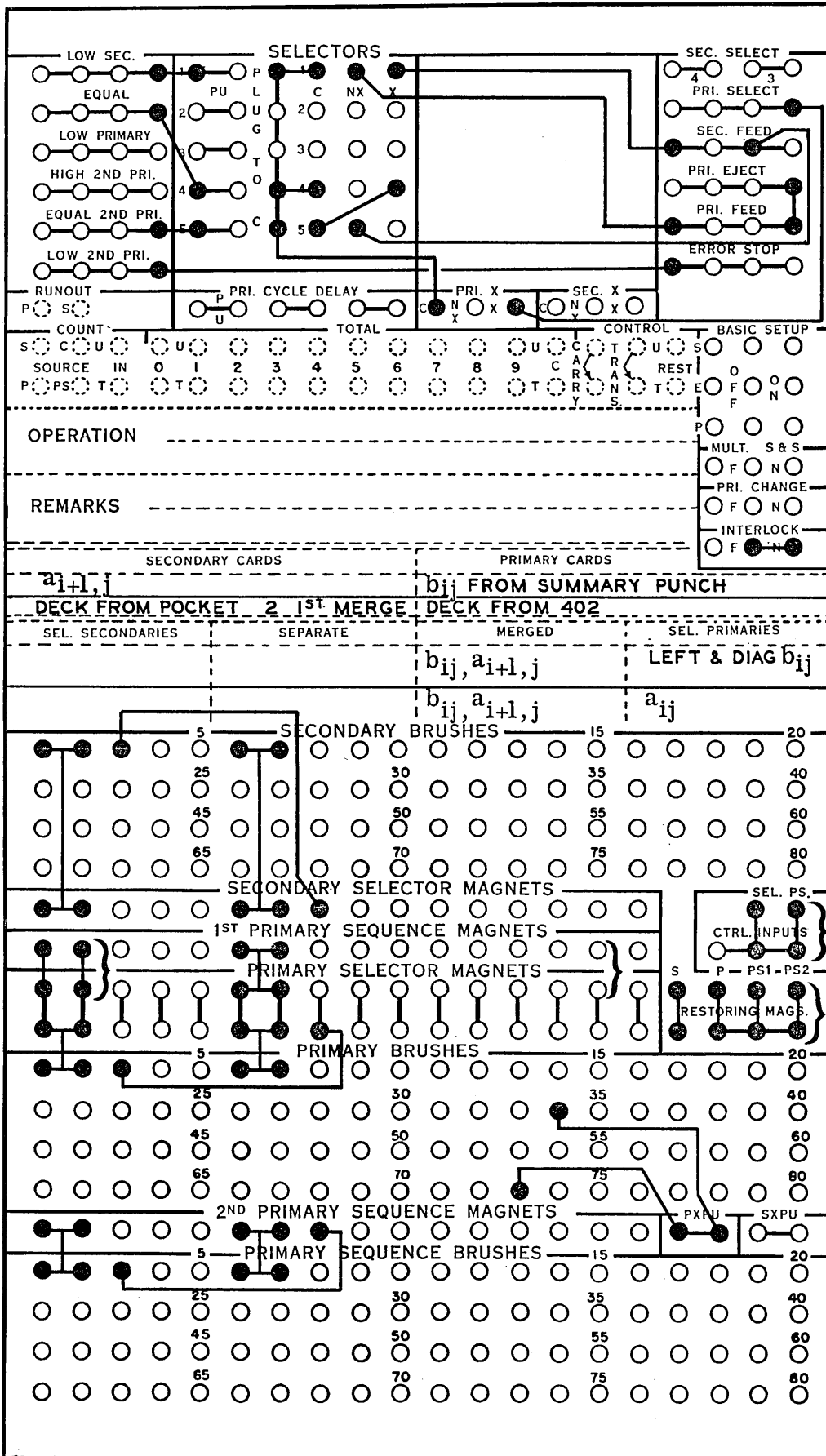
FIGURE 1

1.		2.		3.		4.		5.		6.	
ELECTRO NUMBER		ELECTRO NUMBER		ELECTRO NUMBER		ELECTRO NUMBER		ELECTRO NUMBER		ELECTRO NUMBER	
1	2	1	2	1	2	1	2	1	2	1	2
3	4	3	4	3	4	3	4	3	4	3	4
5	6	5	6	5	6	5	6	5	6	5	6
7	8	7	8	7	8	7	8	7	8	7	8
9	10	9	10	9	10	9	10	9	10	9	10
11	12	11	12	11	12	11	12	11	12	11	12
13	14	13	14	13	14	13	14	13	14	13	14
15	16	15	16	15	16	15	16	15	16	15	16
17	18	17	18	17	18	17	18	17	18	17	18
19	20	19	20	19	20	19	20	19	20	19	20
21	22	21	22	21	22	21	22	21	22	21	22
23	24	23	24	23	24	23	24	23	24	23	24
25	26	25	26	25	26	25	26	25	26	25	26
27	28	27	28	27	28	27	28	27	28	27	28
29	30	29	30	29	30	29	30	29	30	29	30
31	32	31	32	31	32	31	32	31	32	31	32
33	34	33	34	33	34	33	34	33	34	33	34
35	36	35	36	35	36	35	36	35	36	35	36
37	38	37	38	37	38	37	38	37	38	37	38
39	40	39	40	39	40	39	40	39	40	39	40
41	42	41	42	41	42	41	42	41	42	41	42
43	44	43	44	43	44	43	44	43	44	43	44
45	46	45	46	45	46	45	46	45	46	45	46
47	48	47	48	47	48	47	48	47	48	47	48
49	50	49	50	49	50	49	50	49	50	49	50
51	52	51	52	51	52	51	52	51	52	51	52
53	54	53	54	53	54	53	54	53	54	53	54
55	56	55	56	55	56	55	56	55	56	55	56
57	58	57	58	57	58	57	58	57	58	57	58
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71	72	71	72	71	72	71	72	71	72	71	72
73	74	73	74	73	74	73	74	73	74	73	74
75	76	75	76	75	76	75	76	75	76	75	76
77	78	77	78	77	78	77	78	77	78	77	78
79	80	79	80	79	80	79	80	79	80	79	80

CUSTOMER'S NAME & NO. \_\_\_\_\_  
ADDRESS \_\_\_\_\_

INTERNATIONAL BUSINESS MACHINES CORPORATION  
 TYPE 077 COLLATOR CONTROL PANEL

FLOATING DECIMAL  
 MATRIX INVERSION

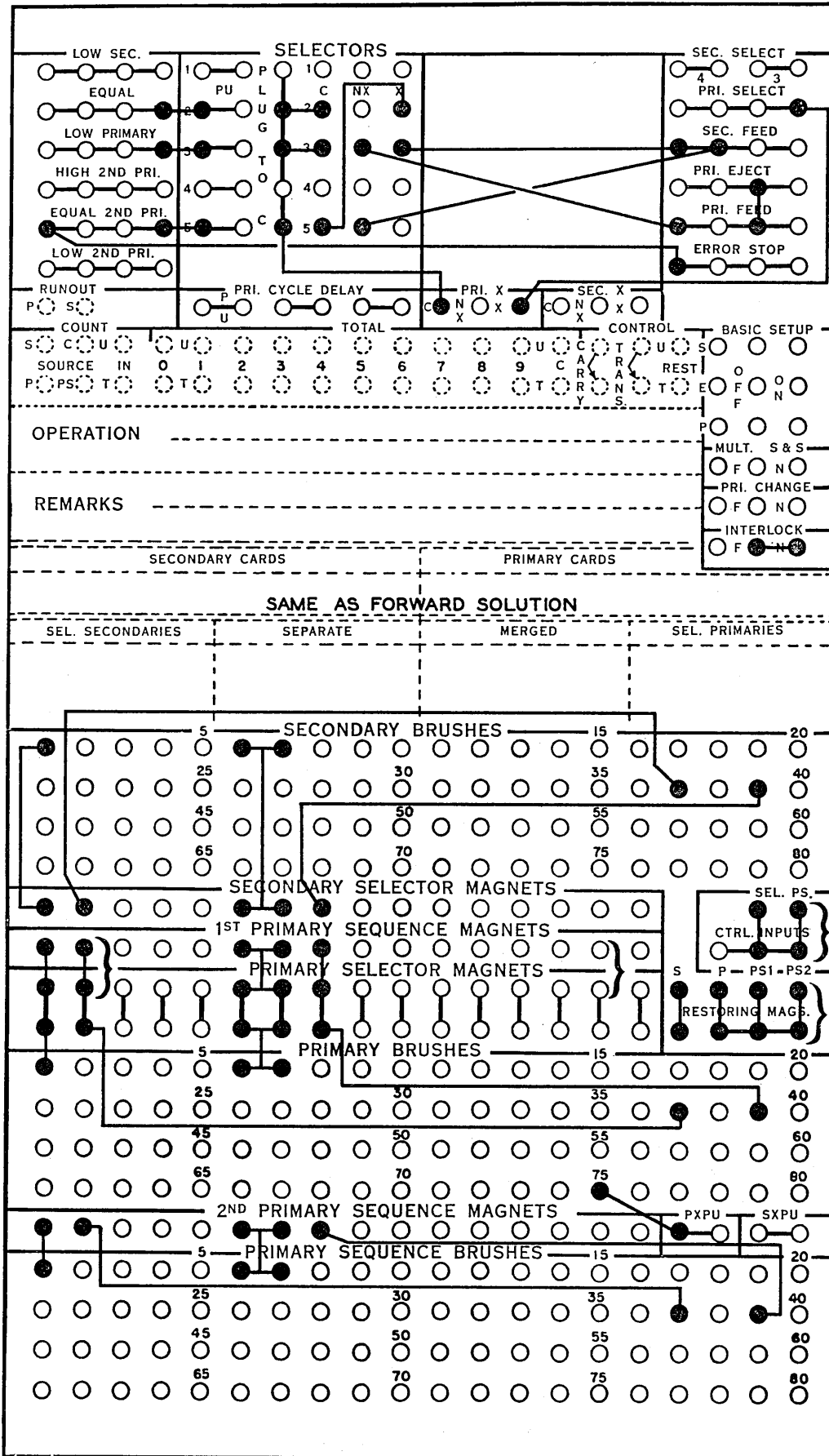


FORWARD  
 SOLUTION

FIGURE 2

INTERNATIONAL BUSINESS MACHINES CORPORATION  
 TYPE 077 COLLATOR CONTROL PANEL

FLOATING DECIMAL  
 MATRIX INVERSION

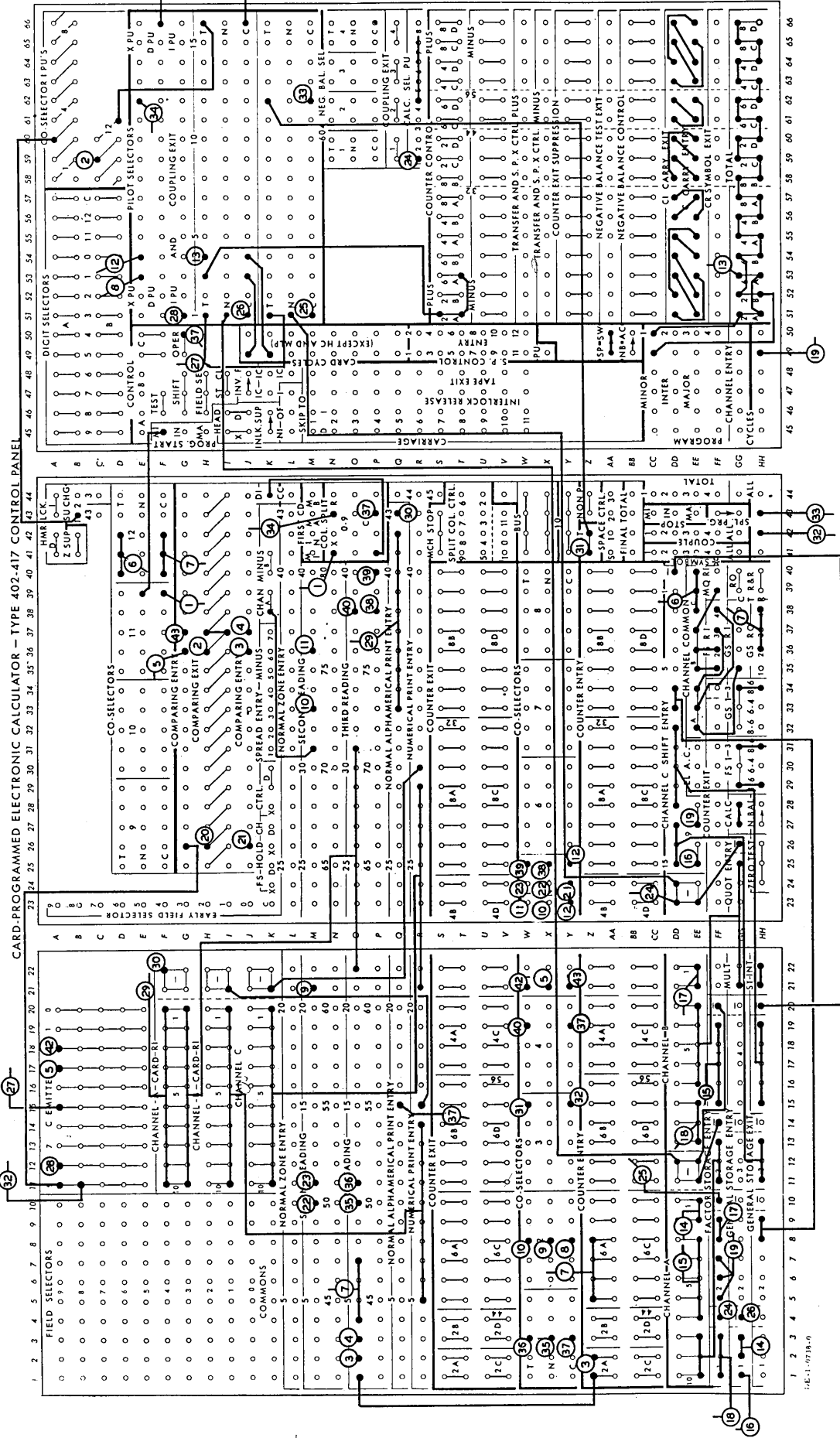


BACK  
 SOLUTION

FIGURE 3

# FLOATING DECIMAL MATRIX INVERSION

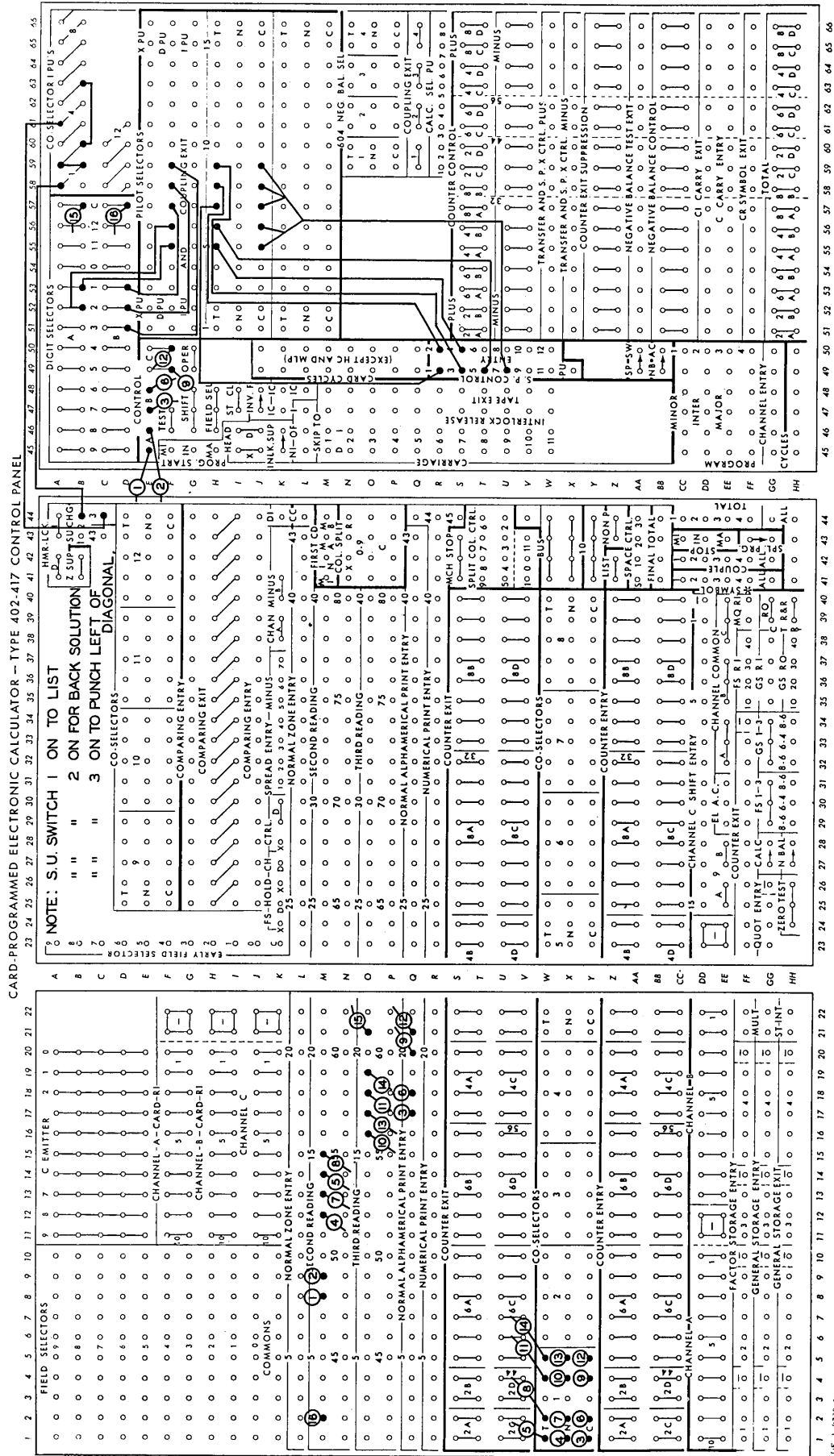
## FIGURE 4A



402-1-0719-0

FIGURE 4B

FLOATING DECIMAL MATRIX INVERSION



# FLOATING DECIMAL MATRIX INVERSION

## FIGURE 5

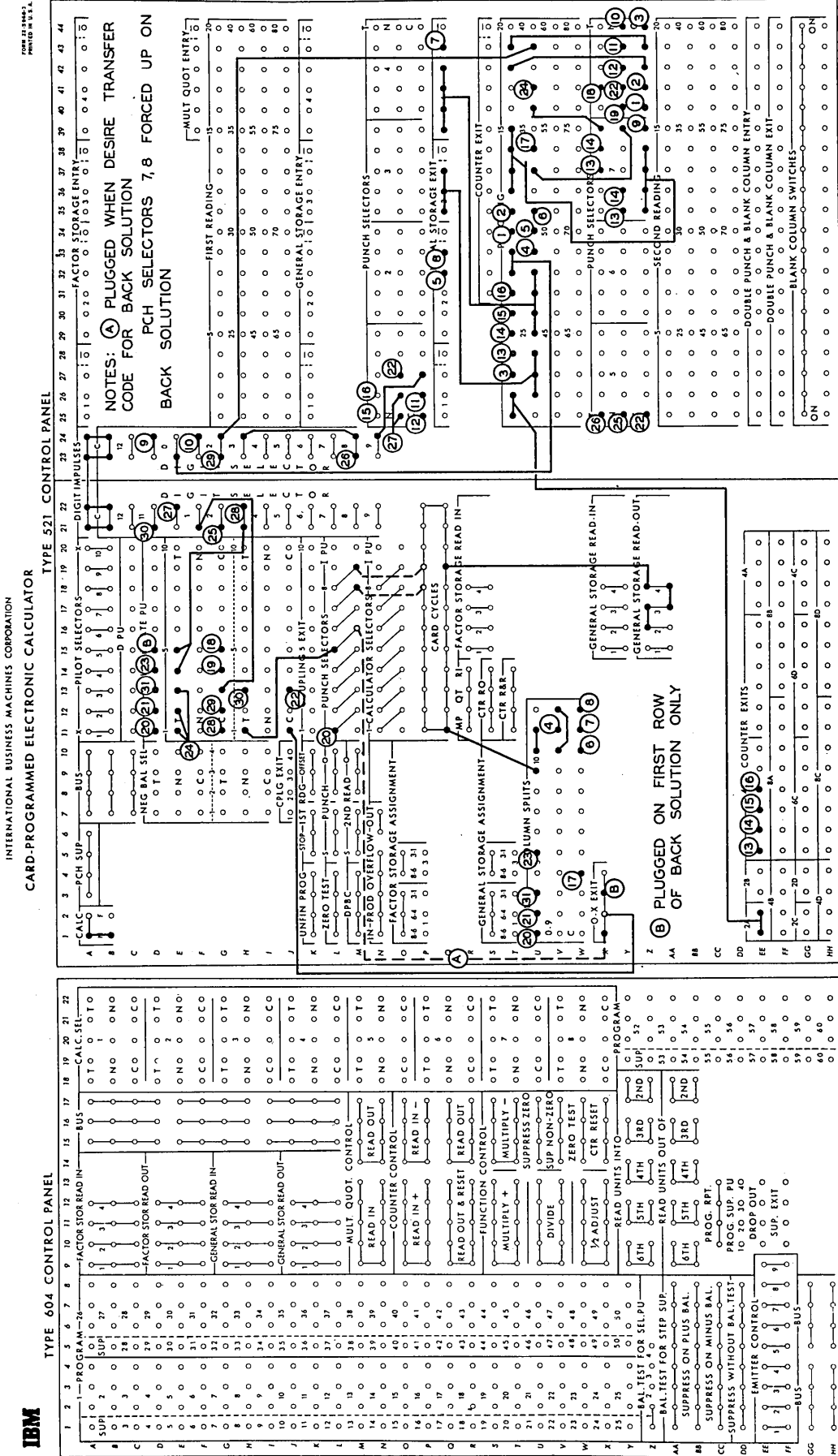


Figure 6

PROG	SUPP	READ OUT	READ IN	SHIFT	
		EXIT 1	EXIT 2	EXIT 3	
1	4	Reset	*	*	012 RIGS2 if sel 8 up.
2	1	GS1	*EC+	*BTSS	013 RIGS3&4 if sel 8 up.
3	14	FS2	*EC+	GSU#1PU	022 EC- if sel 5 up.
4	21	GS2	*EC-	BTSS	023 GSU#4PU if sel 8 or sel 2 up.
5	4	Emit 5	*EC+	Into 2	032 EC- if sel 5 up
6	20	Emit 1	EC+	BTSS	042 EC+ if sel 5 up.
7	4	RR	GS1	GSU#1DO	052 EC- if sel 5 up.
8	1	Reset	GSU#2DO	Zero Test	
9	14	FS1	EC+		
10	6	GS1	EC+		
11	6	GS2	GS1	GSU#3DO	
12	6	RR	GS2		
13	26	GS3&4	EC+	*	133 Into 5 if sel 6 up.
14	26	FS3&4	*GS3&4		142 RI FS1 & 2 if sel 6 up.
15	20	FS1	$\frac{\cdot}{\cdot}$	ROFS2	
16	26	RR	FS3 & 4		
17	7	*GS3&4	EC+		171 RO FS3&4 if sel 3 up.
18	7	$\frac{1}{2}$ Adj.			
19	27	*RO	GS3 & 4	*Out of 2*	191 RO MQ if sel 6 up.
20	14	RR	FS1 & 2	Out of 6	193 Into 2 if sel 7 up.
21	4	FS3&4	*X-*	*Prog RPT*	212 EC+ if sel 7 up.
22	14	FS2	MQ	GSU#1PU	213 Into 6 if sel 7 up.
23	14	RR	FS1 & 2	Out of 6	No oper. if sel 3 up.
24	14	FS3&4	*X-	GSU#2PU	242 x+ if sel 1 up.
25					
26					
27	4	FS1	*EC+	ROFS2	272 $\div$ if sel 6 up.
28	28	Reset	Zero Test	Into 2	
29	17	*Prog RPT	GSU#2PU	GSU#3PU	291 No oper. if sel 3 up.
30	12	FS3&4	EC+	*Into 3	303 Into 4 if sel 8 up.
31	2	GS3&4	EC+	*Into 3	313 Into 6 if sel 6 up.
32	20	MQ	EC+	Into 2	
33	4	$\frac{1}{2}$ Adj.		Into 2	
34	3	RO	FS3 & 4	Out of 3	
35	3	$\frac{1}{2}$ Adj.	BTSS	Into 3	
36	3	RR	FS1 & 2	Out of 4	
37	6	FS1	EC+	ROFS2	
38	5	FS1	EC-	ROFS2	
39	18		GSU#1PU	GSU#2DO	
40	11	Reset			
41	None	Emit 1	MQ	Into 3	

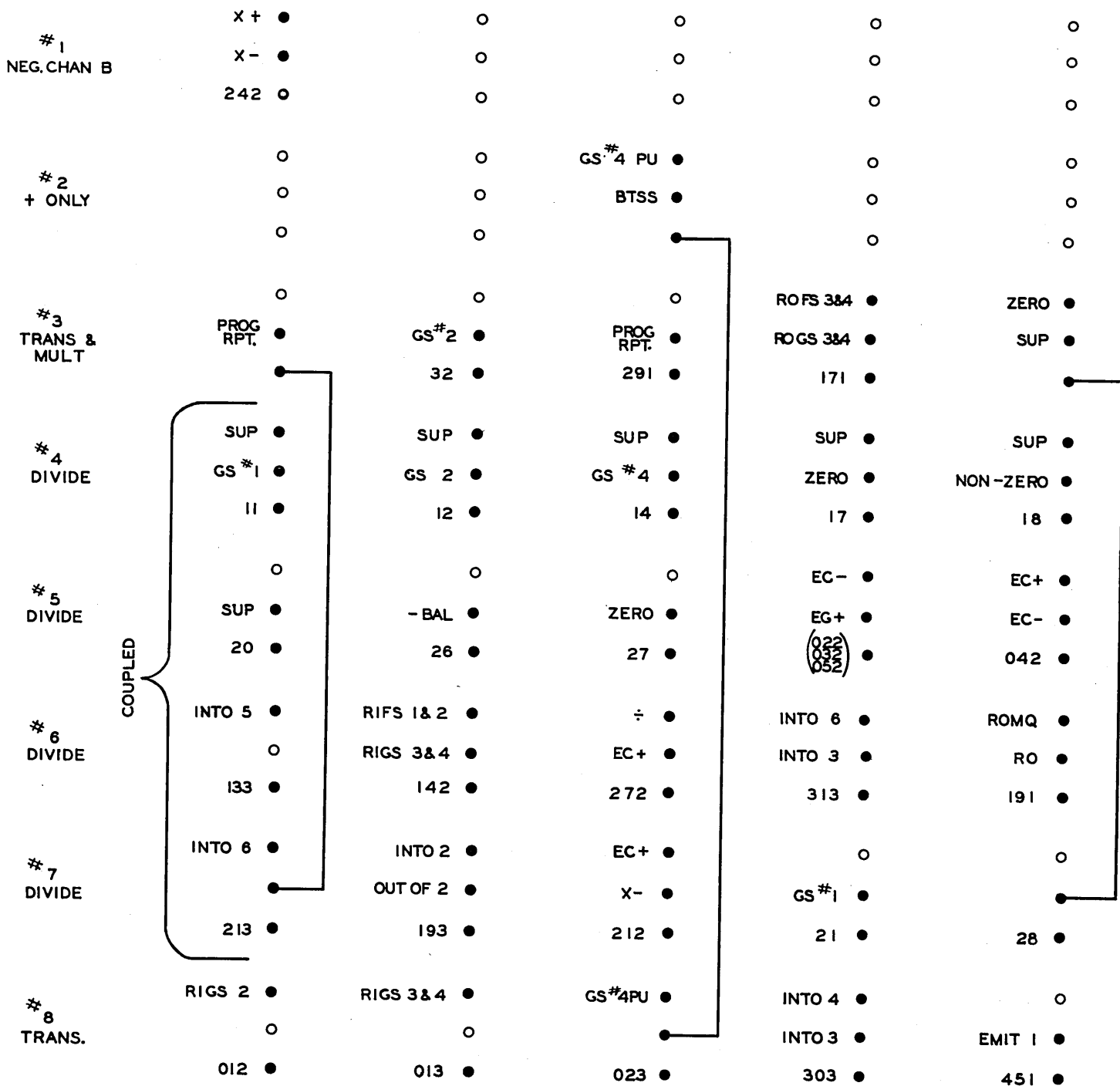


Figure 6 (cont.)

42	None	MQ	EC-	Into 6
43	None	Reset		BTSS
44	6	FS1	FS3 & 4	ROFS2
45	6	*Emit 1	EC-	GSU#2PU 451 No oper. if sel 8 up.
46	4			GSU#2PU
47	2	Emit 1	EC+	Prog. RPT.
48	11	Emit 1	EC-	
49	3	GS1	EC+	
50	11	GS2	EC+	
51	3	RR	GS1	
52	11	RR	GS2	
53	26		GSU#2DO	GSU#3PU
54	14		GSU#1DO	GSU#2PU
55	14		GSU#3PU	GSU#4PU
56	3		GSU#4DO	GSU#2PU
57	32	FS3 & 4	GS3 & 4	
58	32	GS1	GS2	
59	14	FS3 & 4	EC+	Into 4
60	14	MQ	EC+	GSU#4PU

# MATRIX INVERSION 604 SELECTION

FIGURE 7



## SPECIAL METHODS FOR IBM COMPUTATIONS

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### INTRODUCTION

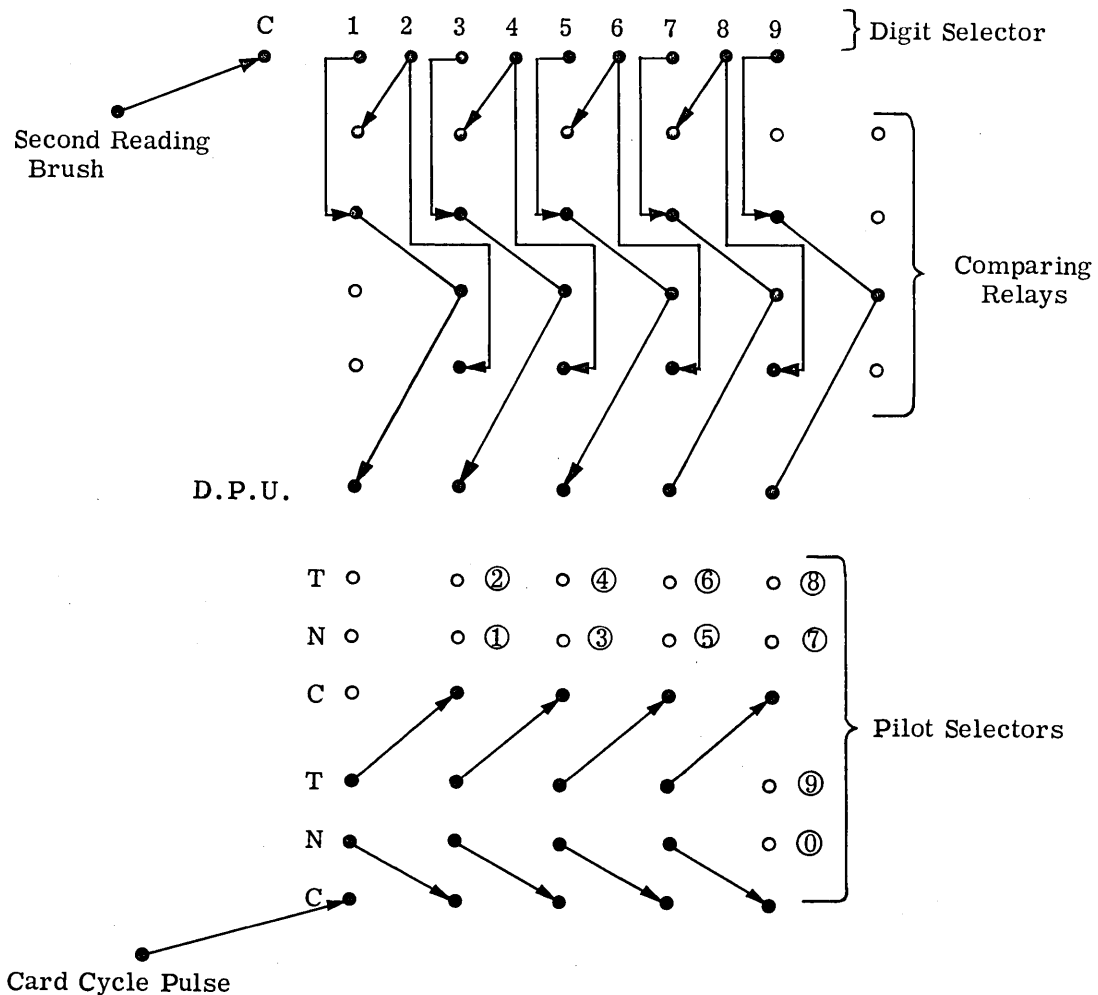
This article contains a group of six sub-articles showing various wiring diagrams and methods of computing on the IBM Type 417 or 402 Accounting Machine, the IBM Type 604 Electronic Calculating Punch, and the IBM Card-Programmed Electronic Calculator.

\* Valuable contributions were also provided by Mr. A. O. Jones, Customer Engineer, International Business Machines Corporation

Using n Pilot Selectors of the 417 or 402 for 2n Selections - James H. Alexander

The diagram below uses a digit selector, five sets of comparing relays, and five pilot selectors. With these components, a card cycle pulse may be obtained from one of ten indicated positions (circled) of the pilot selectors when a card is at the third reading station by reading that position from a designated column of the card at the second reading station. A "1" punched in the designated column will cause the card cycle pulse to be emitted at the "1-position" of the group of pilot selectors; a "2" punched in the designated column will cause the card cycle pulse to be emitted at the "2-position" of the group of pilot selectors; etc. Nothing punched in the designated column will cause the card cycle pulse to be emitted at the "0-position" of the group of pilot selectors.

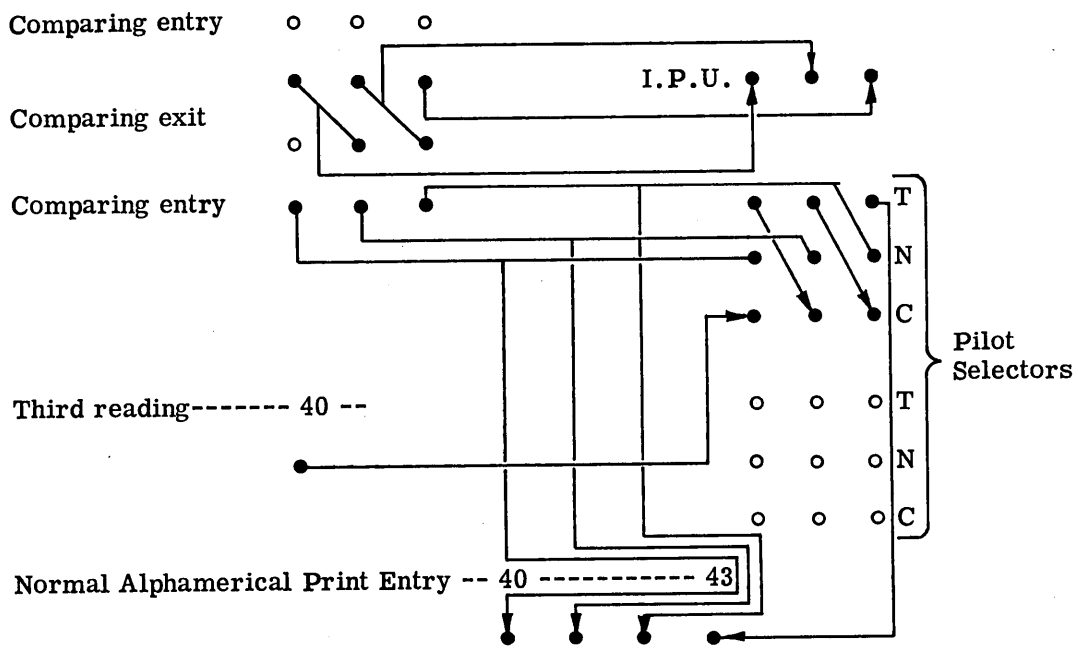
For each group of five pilot selectors used, this process requires an additional instruction column of the card, an additional digit selector, and five additional comparing relays. Finally, it should be noted that the instruction columns cannot be double punched to give two card cycle pulses from any one group of five pilot selectors.



Separating Digits Without A Digit Selector On The 402 - A. O. Jones, IBM Customer Engineer

In the diagram which follows, three pilot selectors and three comparing relays are used to separate four digits picked up from a third reading brush. These digits, then, are listed separately. The number of digits to be separated may be increased by increasing the number of pilot selectors and comparing relays. In the example shown, four digits punched in column 40 of a card are read by that third reading brush and are listed at the normal alphanumerical print positions 40 through 43. The largest number is listed at position 40, the next largest at 41, etc.

Figure 2



Basic Instruction of the CPC from the 417- James H. Alexander, Elwin L. Dershem,  
Janet L. Sukup, George W. Evans II.

The "417 Programmed Electronic Calculator" is very useful in problems in which more than one card per calculation would be needed under the normal card-programmed arrangement.

The 417 programming of the CPC saves on quantity of cards, collating time, and sometimes also on CPC time.

417 programming also keeps most of the flexibility available in the card programming, and for some problems actually adds to the flexibility of CPC control. This is demonstrated in the following articles: "Instructing the CPC from 417 Counters", outlining the more usual means of obtaining flexibility; and "417 Programming of the CPC by Co-Selectors", describing the optional elimination of "in-between" programs. We shall deal with only the basic control in this introductory article.

The basic CPC control with 417 programming requires the digit emitter at all program levels for channel instructions, operation instructions unless calculate selector pickup is used, and shift instructions other than zero. At card cycles, instructions can be received from the digit selector or the card in preference to the digit emitter.

The digit selector (or the card) therefore, may provide instructions for the information which will pass through channels and the shift unit at minor program (if there is a program start), but provides operation instructions for the 604 calculations following card cycles.

When more than one calculate selector must be transferred for an operation, calculate selector pickup may be preferable to operation, to avoid connecting digit emitters which are being used elsewhere at the same time.

Any instructions from the digit emitter must pass through common and transfer hubs of a selector transferred at the proper program level. Usually, co-selectors need not be used if the field selector is available. The use of the field selector is described in a following article: "Increased Selector Capacity for 417 Programming of the CPC".

Instructing the CPC from 417 Counters - A. O. Jones, IBM Customer Engineer  
 James H. Alexander, Elwin L. Dershem

Wide use of the instruction of the CPC from 417 counters is possible. Two examples of such use are given below.

One application of this method is instruction of the CPC based on the results of computations within the 417. An example of this is the computation of

$$e^{-(k-x)}$$

where  $0 \leq k-x < g$  and  $k > x$

and where  $k - x$  is formed in the 417,  $x$  varying from point to point, and  $k$  being constant for a group of points. Then let

$$e^{-(k-x)} = e^{-y_1} \times e^{-y_2}$$

where  $y_1$  is the integral portion of  $k - x$  and  $y_2$  is the decimal portion of  $k - x$ .

Values of  $1 - e^{-y_1}$  are kept in one bank of the auxiliary storage ( $1 - e^{-1}$  in storage 11,  $1 - e^{-2}$  in storage 12, etc.).

When the 417 counter containing  $y_1 + y_2$  is totalled,  $y_2$  travels via channel to the 604 and  $y_1$  pulses the units position of channel A (or B) control. At the same time a 1 (which may be digit emitted) pulses the tens position of the channel control.

The 604 then calculates

$$e^{-y_2} = \sum_{n=0}^{\infty} \left( \frac{y_2}{n} \right) \left( \frac{-1}{n!} \right)^n .$$

$1 - e^{-y_1}$  next enters the 604, and  $e^{-y_1} \times e^{-y_2}$  is formed, giving  $e^{-(k-x)}$ .

If  $y_1$  is zero, "storage 10" is pulsed and the channel reads in zero. This is excellent because

$$1 - e^{-0} = 0.$$

This is the reason  $1 - e^{-y_1}$  instead of  $e^{-y_1}$  is kept in auxiliary storage.

A second application of the instruction of the CPC from 417 counters is one which can frequently be of advantage when using 417 programs with the CPC.

When it is desired at some 417 program level to pulse channel control with a number punched on a card (instead of with ordinary digit emission), this number may be stored in a 417 counter until needed. This application is widely useful where card identification may be correlated with storage (or counter) location.

Certain wiring is required to enable the 417 counter to signal CPC control properly. The selection principle is shown in a previous article entitled "Separating Digits Without

a Digit Selector on the 402''. In the examples in this article only one pilot selector and one set of comparing relays are needed.

The selector and set of comparing relays are required because the 417 counter must not always be connected with channel control. The number desired from the 417 counter is the first one sent out as the counter begins to roll on reading out, but channel control accepts all digits it receives, the last (lower) digit always cancelling the higher digits.

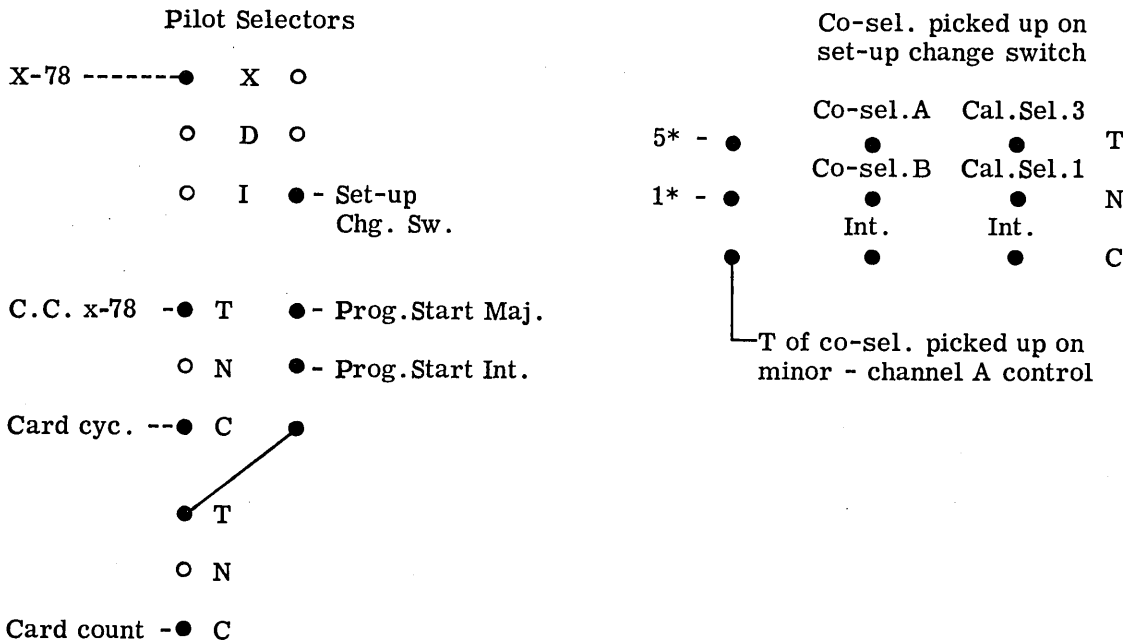


## 417 Programming of the CPC by Co-Selectors - J. L. Sukup

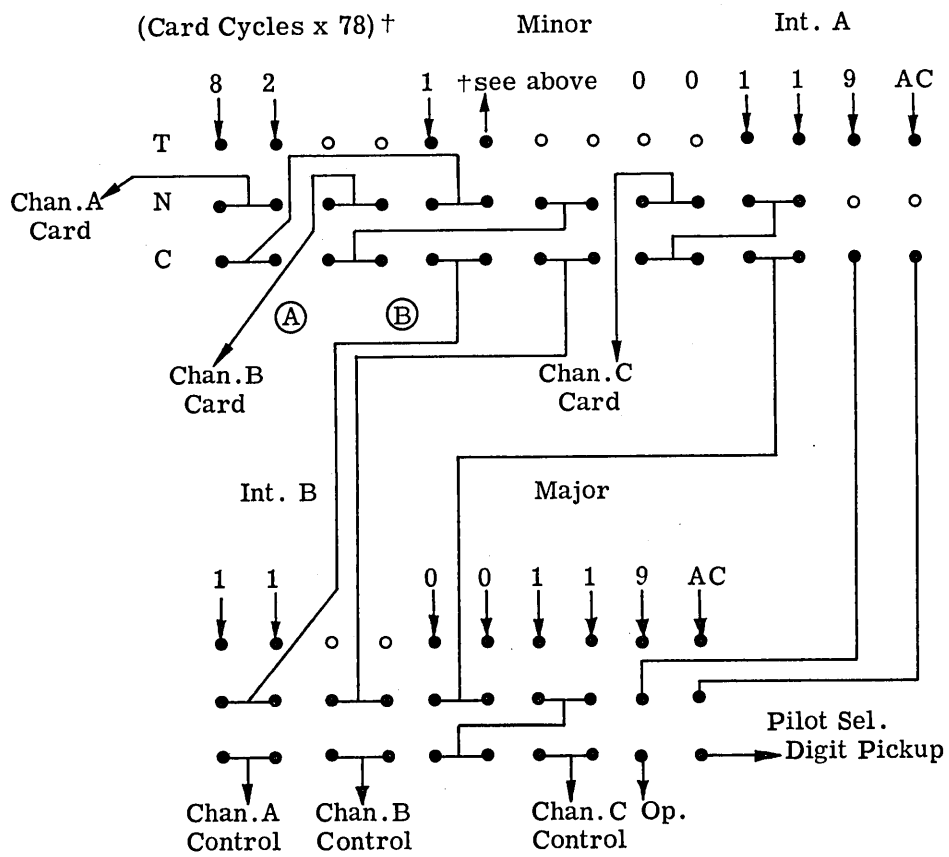
The diagrams of this note show the wiring of the 417 channel instructions and operations for program levels while it is a part of the CPC. The wiring scheme is one that is being used here with the actual instructions and operation coding. A unique feature is the use of the set-up change switch which signals the intermediate program start in the "off" position and major program start in the "on" position; both program starts are activated by an X in column 78 of a card. From the diagrams which follow, it may be seen that the read and minor programs are the same whether the set-up change switch is "on" or "off"; however, by changing the switch from "off" to "on", one changes the intermediate program and adds a major program. In practice, any combination of programs may be used, limited only by the set-up change switch, co- and pilot selector capacities of the machine.

It must be remembered that channels A and B are necessarily instructed one machine cycle before the numbers to be used are entered. This corresponds to taking channel A and B instructions from the second read brushes and the numbers on those channels from the third read brushes. Notice too, although there are no instructions on channel B, except from the card, those columns must be wired through co-selectors. Although there is a blank card behind the X-78 card, this wiring is necessary because the second read brushes (for channel B) would be resting on the roller during channel instruction time and would cause channel B to open.

	A	B	C	Op	
Read	x-78	Card			} → A. Set-up change switch "off" Int. Program start.
Min.	82	--	00	1	
Int.	11*	--	11	1, 9	
			Blank card		
Read	x-78	Card			} → B. Set-up change switch "on" Maj. Program start.
Min.	82	--	00	1	
Int.	15*	--	00	3	
Maj	11	--	11	1, 9	
			Blank card		



\*Note: This is the only difference between channel A and B control on intermediate program. It is handled by method shown - left hand hubs of this co-selector.

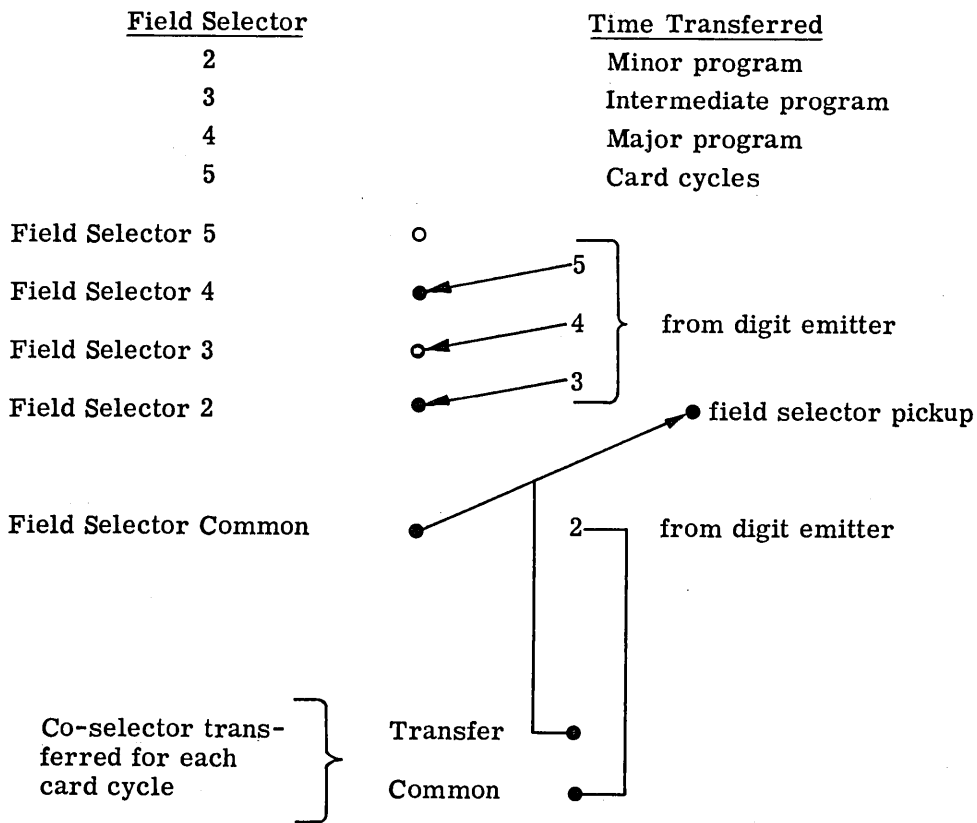


Increased Selector Capacity for 417 Programming of the CPC - Elwin L. Dershem

The field selector can handle most of the digit emitted channel and operations instructions for 417 programming of the CPC, and also be available for additional program level selection.

One of the ten columns of field selector hubs is used to control its own pickup, as shown by the diagram below. The remaining nine sets of hubs are available as selector positions at the respective programs.

The following example assumes major program start is used, and that the field selector is successively transferred to levels 2, 3, 4, and 5.





## ERRATA

The following addition should be made to the article by William P. Heising  
“An Eight-Digit General-Purpose Control Panel” in Technical Newsletter No. 3.

- p. 82     The symbol XII (Suppression Group XII) should be added to the line  
          joining the first common hub of Selector 6 to the first common hub  
          of Selector 7.

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