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A CONVENIENT TABLE FOR DETERMINING METASTABLE TRANSITIONS IN MASS SPECTRA

BY R. A. MEYER AND D. G. EARNSHAW

United States Department of the Interior — April 1957

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UNITED STATES DEPARTMENT OF THE INTERIOR
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Marling J. Ankeny, Director

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A CONVENIENT TABLE FOR DETERMINING METASTABLE TRANSITIONS IN MASS SPECTRA

by

R. A. Meyer[1] and D. G. Earnshaw[2]

A table that greatly simplifies determination of metastable transitions in mass spectra has been prepared. All the mathematically possible metastable transitions of any compound whose molecular weight lies between 26 and 150 can be determined from the table without calculation. The method of utilizing the table is described, using selected peaks from the spectrum of normal butane for illustration.

In the mass spectrometer, ions are formed in the isatron and accelerated through a series of slits. Most of these ions reach the collector without further change, but a few dissociate in transit to form new ions. These ions appear in the mass spectrum at neither the mass-to-charge ratio (m/e) of the original ion nor that of the new ion. A formula that relates the appearance of these new ions to the ion from which they were formed is:

$$\underset{\text{(new ion)}}{\text{apparent m/e}} = \left[\frac{\text{actual m/e (new ion)}}{\text{m/e (original ion)}}\right]^2 .$$

A large number of trial-and-error calculations are required to select the peaks involved in the metastable transitions in a given spectrum. To reduce the time necessary for finding these transitions and to insure that all mathematically possible transitions are considered, the table presented in this paper was prepared.

The numbers on the left of the table are the mass-to-charge ratios of the ions before the transitions take place. These range from 26 to 150. The numbers across the top are the mass-to-charge ratios of the ions formed by the transitions. These range from 25 to 149. The numbers in the body of the table represent the apparent mass-to-charge ratios of the metastable peaks. To condense the body of this table, only the tenths and the first unit of each number have been included, and lines between decades have been inserted. For example, at the intersection of row 58 and column 43 the number 19 may be found. As it is within the space marked 30, as divided by the decade lines, the apparent mass-to-charge ratio resulting from this transition should be read as 31.9.

1/ Applications engineer, Consolidated Electrodynamics Corp., Pasadena, Calif.
2/ Physicist, Bureau of Mines, Region III, Laramie, Wyo.

To demonstrate the use of this table, consider 5 metastable peaks occurring at mass-to-charge ratios of 30.4, 31.9, 35.1, 37.1, and 39.1 in the spectrum of normal butane. To be noticeable, metastable peaks usually involve the dissociation of ions that are relatively abundant in the normal spectrum. In the normal butane spectrum these are the mass-to-charge ratios 58, 57, 43, 42, 41, and 39. Therefore, a straightedge is moved from row to row of original mass-to-charge ratios whose abundance warrants their consideration, and each transition whose apparent mass-to-charge ratio is within ± 0.1 unit of the metastable peaks under consideration is noted. Thus in figure 1 a straightedge is indicated along row 58, the first abundant peak in the spectrum of normal butane. The numbers along the straightedge represent mathematically possible apparent mass-to-charge ratios of metastable peaks. Two of these, 30.4 and 31.9, lie within ± 0.1 m/e of the metastable peaks selected for demonstration and would be noted. Moving the straightedge to row 57, the next large peak in the normal butane spectrum, the only transition that corresponds to one of the selected peaks is 37.1. A similar examination of rows 43, 42, 41, and 39, which are the other large peaks in the spectrum, gives the following 10 mathematically possible transitions for the 5 selected metastable peaks:

(1) 30.4 $(58^+) \rightarrow (42^+) + 16$

(2) 31.8 $(43^+) \rightarrow (37^+) + 6$

(3) 31.9 $(58^+) \rightarrow (43^+) + 15$

(4) 35.0 $(39^+) \rightarrow (37^+) + 2$

(5) 37.0 $(39^+) \rightarrow (38^+) + 1$

(6) 37.1 $(41^+) \rightarrow (39^+) + 2$

(7) 37.1 $(57^+) \rightarrow (46^+) + 11$

(8) 37.2 $(43^+) \rightarrow (40^+) + 3$

(9) 39.0 $(41^+) \rightarrow (40^+) + 1$

(10) 39.0 $(43^+) \rightarrow (41^+) + 2$

Several transitions result in similar apparent mass-to-charge ratios; however, 2, 7, and 8 can be eliminated because they require the formation of improbable neutral fragments. Transitions 5 and 9 can also be eliminated, as data from the literature[3] show that in instances where a metastable peak can be derived from a transition with a neutral remnant of either 1 or 2, the latter is far more probable. Thus the best sources of the five selected metastable peaks are the remaining transitions that are underlined. They are 1, 3, 4, 6, and 10.

ACKNOWLEDGMENT

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3/ Bloom, Evelyn G., Mohler, Fred L., Wise, C. Edward, Wells, Edmund J., Metastable Transitions in Mass Spectra of Hydrocarbons: Jour. Res. Nat. Bureau of Standards, vol. 43, No. 1, 1949, p. 65.

Mass-to-charge ratios of ions after dissociation

Mass to charge ratios of ions before dissociation	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49
(39)	96	14	32	51	70											
(40)	89	06	24	42	61	80										
(41)	82	99	16	34	52	71	90									
(42)	75	92	09	26	44	62	81	00								
(43)	69	85	01	18	36	54	72	91	10							
(44)	63	78	94	11	28	46	64	82	01	20						
(45)	57	72	88	04	21	38	56	74	92	11	30					
(46)	51	66	82	98	14	31	48	65	83	02	21	40				
(47)	46	61	76	91	07	24	40	58	75	93	12	31	50			
(48)	41	55	70	85	01	17	33	50	68	85	03	22	41	60		
(49)	36	50	64	79	95	10	27	43	60	77	95	13	32	51	70	
(50)	31	45	59	74	89	04	20	36	53	70	87	05	23	42	61	80
(51)	27	40	54	68	83	98	14	30	46	63	80	97	15	33	52	71
(52)	22	36	49	63	78	93	08	23	39	56	72	89	07	25	43	62
(53)	18	31	45	58	72	87	02	17	33	49	65	82	99	17	35	53
(54)	14	27	40	54	67	82	96	11	27	42	59	75	92	09	27	45
(55)	10	23	36	49	63	77	91	06	21	36	52	68	85	02	19	37
(56)	06	19	31	44	58	72	86	00	15	30	46	62	78	94	11	29
(57)	03	15	27	40	53	67	81	95	09	24	40	55	71	88	04	21
(58)	99	11	23	36	49	62	76	90	04	19	34	49	65	81	97	14

10 20 30 40

Figure 1. - Portion of metastable table.

APPARENT MASS-TO-CHARGE RATIOS OF METASTABLE TRANSITIONS

BY

R.A. MEYER & D.G. EARNSHAW
PETROLEUM & OIL-SHALE EXPERIMENT STATION
BUREAU OF MINES, U.S. DEPARTMENT OF THE INTERIOR
LARAMIE, WYO.

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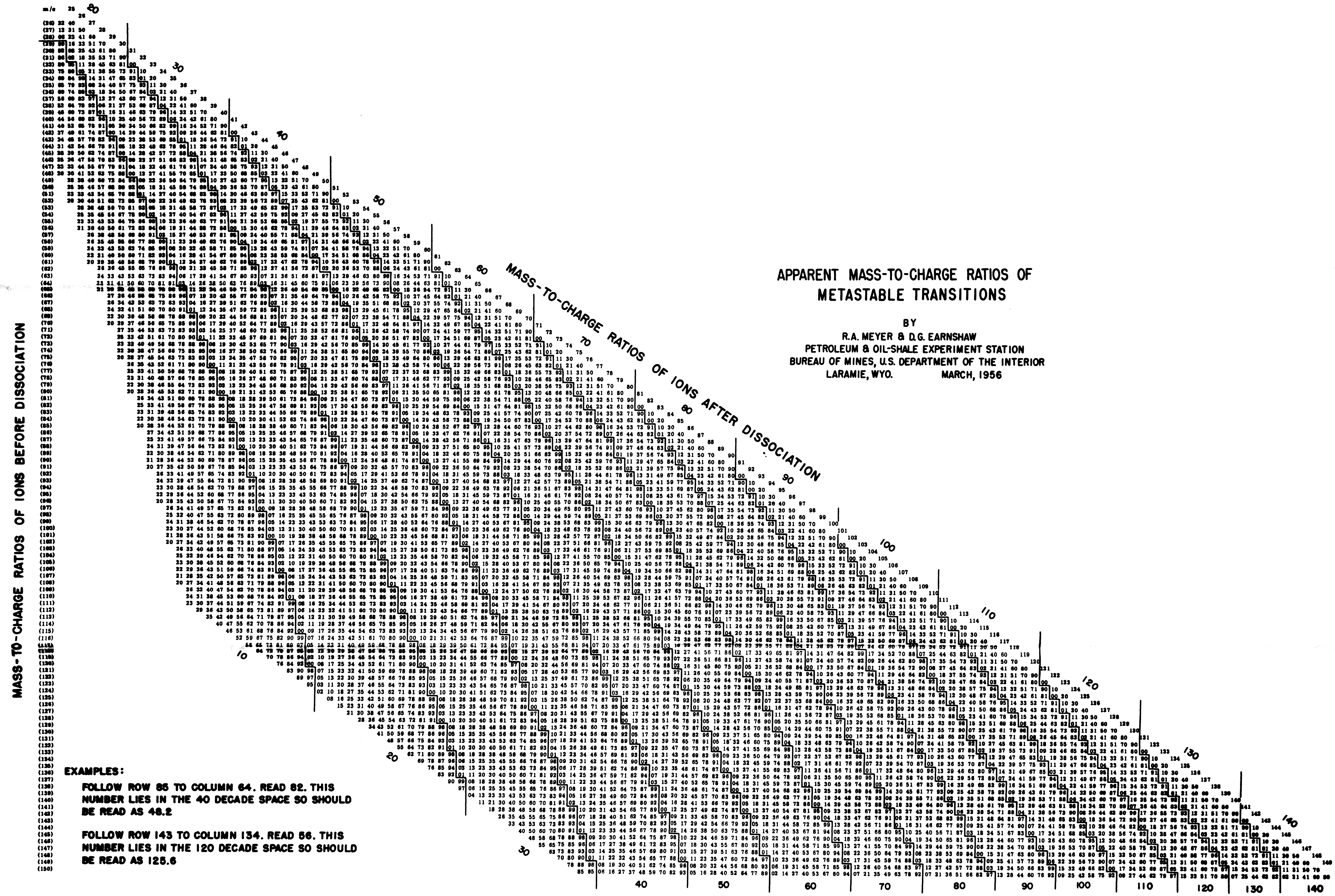

EXAMPLES:

FOLLOW ROW 85 TO COLUMN 64. READ 82. THIS NUMBER LIES IN THE 40 DECADE SPACE SO SHOULD BE READ AS 48.2

FOLLOW ROW 143 TO COLUMN 134. READ 56. THIS NUMBER LIES IN THE 120 DECADE SPACE SO SHOULD BE READ AS 125.6