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Spectral classification using pattern-recognition techniques. II. Application to curium energy levels

K. L. Peterson, D. L. Anderson, and M. L. Parsons
Department of Chemistry, Arizona State University, Tempe, Arizona 85281
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Curium energy levels have been classified according to configuration using pattern-recognition techniques. Four features—energy level, Landé g, J, and isotope shift—have been used to describe each level. Forty levels have been assigned with high probability based on consistent results obtained by various pattern recognition techniques. This represents an increase of 9% for even levels and 19% for odd levels. In addition, 14 levels have been assigned to one of two possible configurations. Pattern recognition in general, as applied to atomic energy-level classification, is discussed.

I. INTRODUCTION

In the preceding paper the utility of pattern recognition as a tool in classifying atomic transitions was demonstrated.[1] On the basis of the positive results obtained, we were encouraged to apply similar techniques to the classification of curium energy levels.

A relatively complete line list for Cm I contains more than 1700 transitions, 87% of which are classified.[2] The total number of observed lines is greater than 13 000, and this could conceivably be doubled by observing more intense spectra.[3] Most of these lines can be identified along with respective energy levels using search programs and other methods, described elsewhere.[3] It is important to classify the energy levels according to configuration. At present, there are 335 odd-parity levels and 348 even-parity levels known; of these, 76 odd and 170 even levels have been identified according to to configurations.

In this paper, pattern-recognition techniques are applied to known energy levels, and the training thus achieved is used to predict the configurations of 54 additional levels: 12 odd and 42 even. This represents an increase of 16% for odd levels and 27% for even levels.

We have used the computer package of pattern-recognition techniques obtained from Kowalski.[4] For a short discussion of pattern recognition and the different techniques available in the computer package, the reader is referred to the previous paper.[1] For a more detailed discussion several excellent reviews are available.[5-8]

II. PROCEDURE

The Cm I data of Worden and Conway were used.[3] Table I lists all unknown levels which have been classified by Worden and Conway.[3] Table II shows the possible configurations and their properties. The training data (levels which have been assigned a configuration) were split into two sets, one consisting of odd levels and the other, even levels. This separation presents no problems since the parity of all unclassified levels is known. Each configuration represents a category. For example, there are six categories in the even-level data set, each of the configurations $5f^87s^2$, $5f^77s^27p$, $5f^76d7s7p$, $5f^86d7s$, $5f^76d^27p$, and $5f^87s8s$ representing one category. In order to attempt to classify as many unknown levels as possible, we first used three parameters (which will be referred to as features): energy level (cm^{-1}), Landé g (Lorentz units), and the J, since these are known for almost all levels. (The energy levels and Landé g factors may be expressed in any convenient units. If the possible units of a feature are related by a proportionality constant, the feature expressed in one unit will be identical to the same feature expressed in another unit, after the feature has been autoscaled.) This resulted in relatively poor training (classification) of known data, and a fourth feature, the isotope shift (IS, cm^{-1}), was incorporated. Isotope-shift data have not been measured for the odd configurations $5f^76d7s8s$ and $5f^77s^28s$, or for the even configuration $5f^87s8s$. Thus these configurations have not been represented in the classification procedure. The training results using four features were much improved and are given in Table III. The large improvement is to be expected since the IS is configuration dependent.

Pattern-recognition methods were applied to all the unknown levels for which the four training features were available. Predictions of unknown levels are given in Table IV.

In addition to the various pattern-recognition techniques, we have made predictions solely on the basis of information provided by isotope-shift and configuration data. The isotope shift exhibits

TABLE I. Unknown Cm I levels and data used for classification in this study.

Index No.	Level (cm^{-1})	J	Landé g	Isotope shift
	(a) Odd levels			
1	22 640.04	5	0.98	0.0
2	23 282.58	4	1.176	0.0
3	23 299.44	5	0.968	0.0
4	24 900.55	3	1.54	−0.40
5	25 518.80	6	1.51	−0.39
6	25 878.11	5	1.49	−0.35
7	28 487.41	4	1.328	−0.18
8	28 634.99	4	1.731	−0.08
9	28 880.03	5	1.46	−0.58
10	28 989.06	4	1.648	−0.25
11	31 104.82	4	1.485	−0.41
12	31 167.95	4	1.759	−0.12
	(b) Even levels			
1	25 237.89	4	1.38	−0.565
2	26 730.23	4	0.886	−0.28
3	27 263.19	2	1.280	−0.280
4	28 629.20	3	1.006	−0.270
5	31 185.81	3	1.321	−0.412
6	31 413.22	2	1.255	−0.474
7	31 574.14	2	1.161	−0.487
8	31 655.78	3	1.310	−0.198
9	31 721.56	4	1.411	−0.449
10	31 730.96	4	1.194	−0.472
11	31 750.19	2	1.358	−0.523
12	31 954.42	4	1.51	−0.427
13	31 975.65	1	1.539	−0.509
14	31 982.85	2	1.44	−0.280
15	32 441.09	4	1.297	−0.485
16	32 787.87	4	1.28	−0.568
17	33 391.14	3	1.474	−0.462
18	33 433.15	7	1.54	−0.374
19	33 439.28	2	1.762	−0.491
20	33 518.27	4	1.491	−0.366
21	33 860.10	3	1.40	−0.393
22	34 290.51	5	1.467	−0.511
23	34 317.25	5	1.412	−0.553
24	34 520.33	4	1.573	−0.318
25	34 526.19	5	1.498	−0.285
26	34 858.38	5	1.38	−0.313
27	35 139.55	5	1.230	−0.483
28	35 335.36	7	1.525	−0.368
29	35 459.79	6	1.56	−0.380
30	35 461.45	4	1.33	−0.229
31	35 838.78	6	1.422	−0.540
32	35 943.30	6	1.342	−0.490
33	36 390.78	4	1.58	−0.371
34	36 842.85	3	1.577	−0.277
35	38 373.25	4	1.401	−0.501
36	38 563.03	5	1.336	−0.422
37	38 599.35	3	1.385	−0.382
38	38 676.40	5	1.345	−0.500
39	39 071.51	8	1.531	−0.358
40	39 288.89	4	1.505	−0.524
41	40 263.76	3	1.314	−0.331
42	40 603.67	4	1.57	−0.497

values characteristic of a given configuration. Further, because the lowest possible energy level for each configuration is known, we can eliminate some unknown levels from certain configurations. This consideration is important because there are three configurations which are not represented in the training sets because isotope-shift data were not available. On this basis alone we can conclude that no odd unknown level should belong to a configuration not represented in the training set. The situation is not as clear cut for even levels. Unknowns 17–42 (Table I) may belong to the unrepresented $5f^87s8s$ configuration. Further discussion of the possibility that these levels belong to this configuration will be given later.

III. RESULTS AND DISCUSSION

Overall final predictions are given in Table V. Unknown levels for which only one configuration is given are considered to be high probability predictions because the various methods show consistent agreement for these levels. Some inconsistency has been found for certain levels, which is indicated in Table V. Several of the levels have two predictions indicated with an "or." These are thought to be equally likely configurations based on the various techniques.

In arriving at these predictions, different confidence levels are ascribed to different methods. We have relied more heavily on those methods which trained to the highest levels. The value of the isotope shift was considered to be important and was used along with the multihyperplane-separation technique and the K-nearest-neighbor observation (where K is 1, 3, 4, 5, 6, 7, 8, 9, and 10) as the most reliable classifiers. When further information became necessary the least-squares multilinear regression and the minimal-spanning tree techniques were used.

Strictly speaking, the minimal-spanning tree technique is not a supervised learning technique as are the other methods. It is, therefore, difficult to ascribe a level of training to it. The minimal-spanning tree was mainly used to determine which unknowns were clustered with which knowns. For example, if an unknown was clustered with knowns of a given configuration, this was evidence for the level belonging to that configuration. Predictions which are uncertain (i.e., more that one predicted configuration) have been clustered with roughly equal confidence to two different configurations. For unknown levels which constitute an entire cluster, no prediction is made. The minimal-spanning tree technique may be looked on as supplying useful information, but it cannot be considered to be as reliable as methods such as multi-

TABLE II. Even and odd configurations of Cm I.

Index no.	Configurations	Lowest level (cm^{-1})	Number of levels Expected	Found
Odd				
I	$5f^7 6d 7s^2$	0.00	10	10
II	$5f^7 6d^2 7s$	10 144.93	86	36
III	$5f^8 7s 7p$	17 656.63	74	13
IV	$5f^7 6d^3$	(26 103.06) [a]	100	5
V	$5f^7 6d 7s 8s$ [b]	34 255.16	40	12
VI	$5f^7 7s^2 8s$ [b]	~31 000 [c]	2	0
Even				
VII	$5f^8 7s^2$	1 214.18	12	10
VIII	$5f^7 7s^2 7p$	9 263.37	6 [d]	6
IX	$5f^7 6d 7s 7p$	15 252.70	118 [d]	77
X	$5f^8 6d 7s$	16 932.72	114	62
XI	$5f^7 6d^2 7p$	(36 128.79) [a]	252 [d]	10
XII	$5f^8 7s 8s$ [b]	33 013.09	26	5

[a] Lowest level found. The predicted lowest level has not been found.
[b] Not represented in training set because no isotope-shift data are available.
[c] Estimated prediction. No levels belonging to this configuration have been found.
[d] Based on $^8S^o$ only.

hyperplane separation, K nearest neighbor, or percentage nearest neighbor.

It will be noted that occasionally the multihyperplane-separation method predicts two different configurations. This can be explained by observing Fig. 1, which consists of two-dimensional Karhunen-Loeve transformation plots of the even- and odd-level data sets. Although we are dealing with four-dimensional space, the first two Karhunen-Loeve transformation dimensions provide 73.6% and 14.6% of the total information or variance of the even and odd data sets, respectively. To illustrate this, consider a line separating categories 1 and 2 (i.e., $5f^8 6d 7s$ and $5f^7 6d^2 7p$ configurations, Fig. 2). It is seen that an infinite number of lines may be drawn which effect 100% separation of these categories. Depending upon where the line is drawn, different unknowns (category 0) may be classified differently. This reasoning, best seen in two dimensions, holds equally for n dimensions. For example, in four dimensions a three-dimensional hyperplane will be the separating surface.

In cases where the multihyperplane-separation technique was ambiguous, K-nearest-neighbor observations and the isotope shift were utilized. The high training level of K nearest neighbors indicates that the "quality" of the clusters (i.e., the levels representing a particular configuration) is good; that is, the clusters are tight and well separated. Because of this, it was felt that K-nearest-neighbor observation was a good method for resolving ambiguities.

As was mentioned earlier, there is the possibility that certain of the even levels belong to the configuration $5f^8 7s 8s$ which was not represented in the training set. In an attempt to determine which of these levels might actually belong to this configuration, Karhunen-Loeve transformation plots of a three-feature (energy level, g, J) data set were obtained. The $5f^8 7s 8s$ configuration was then represented. From inspection of the plot of the first two Karhunen-Loeve transformation dimensions of this data set (containing 78.3% of the total information) an estimate can be made of suspect unknowns (see Table VI). These data were also studied using K-nearest-neighbor observations to determine unknowns were closest to the $5f^8 7s 8s$ configuration. These unknowns are also listed in Table VI.

The above discussion indicates several ways in which pattern-recognition techniques may lead to erroneous classifications even where all methods

TABLE III. Training results for even- and odd-level training sets: energy level, J, g, and IS.

Method	Training data classified correctly (%) Even levels	Odd levels
Multihyperplane separation	96.5	98.1
K nearest neighbors	86.0	92.5
Least-squares multilinear regression	91.2	80.7
Percentage nearest neighbors	80.7	87.6

TABLE IV. Curium unknowns by configuration.[a]

Index no.	A	B	C	D	E	F
			Classification type[b]			
			Odd levels			
1	II	I	II	I	II	I
2	II	I	II	I	II	I
3	II	I	II	I	II	I
4	II	II	II	III	III	II
5	II	II	II	II	II	II
6	II	II	II	II	II	II
7	II	II	II	II	II	I
8	II	I	II	II	II	I
9	III	IV	IV	III	IV	IV
10	II	II	II	II	II	II
11	IV	IV	II	III	II	III
12	II	II	II	II	II	I
			Even levels			
1	X	X	X	X	X	X, XI
2	VII	VII	IX	IX	IX	IX
3	IX	VII	IX	IX	IX	IX, VII
4	VII	VII	VII, XI	IX	IX	IX
5	IX	IX	X	IX	X	IX, X
6	X	X	X	IX	X	IX, X
7	X	X	X	IX	X	IX, X
8	IX	IX	VII, IX	IX	VII, IX	VII, IX
9	IX	IX	X, IX	X	IX	IX, X
10	X	X	X	X	X	IX, X
11	X	X	X	X	X	X, XI
12	IX	IX	IX	X	IX	IX, X
13	X	X	IX	X	IX	X, XI
14	IX	IX	IX	IX	IX	IX
15	X	X	X	X	X	IX, X
16	X	X	X	X	X	X, XI
17	IX	XI	IX, X	X	IX, X	IX, X
18	IX	IX	IX	X	IX	IX
19	X	X	IX	X	IX	IX, X, XI
20	IX	IX	IX	IX	IX	IX
21	IX	IX	IX	IX	IX	IX
22	X	XI	X	X	X	X, XI
23	X	XI	X	X	X	X, XI
24	IX	IX	IX	IX	X	IX
25	IX	IX	IX	IX	IX	IX
26	IX	IX	IX	IX	IX	IX
27	X	XI	X	X	X	IX, X
28	IX	IX	IX	X	IX	IX
29	IX	IX	IX	X	IX	IX
30	IX	IX	IX	IX	IX	IX
31	X	XI	XI	X	XI	X, XI
32	IX	XI	XI	X	X, XI	IX, X
33	IX	IX	IX	X, IX	IX	IX
34	IX	IX	IX	IX	IX	IX
35	XI	XI	XI, IX, X	X	X	X, XI
36	IX	XI	XI, IX	X	X	IX, X
37	IX	IX	IX	IX	IX	IX
38	XI	XI	XI	X	XI	X, XI, IX
39	IX	IX	IX	X	IX, X	IX
40	XI	XI	XI	X	XI	X, XI
41	IX	X	IX	IX	IX	IX
42	XI	XI	XI	X	XI	X, IX

[a]See Table II for key to configuration.

[b]The key to methods used for classification is as follows: (A) Data are autoscaled and then the multihyperplane-separation technique is applied. (B) The Karhunen-Loeve transformation is performed followed by the multihyperplane-separation technique. (C) K-nearest-neighbor observations are made where K is 1, 3, 4, 5, 6, 7, 8, 9, or 10. (D) Least-squares multilinear-regression analysis is performed. (E) Percentage of nearest-neighbor observations are made. (F) Isotope-shift data are used.

employed give consistent predictions. These possible disadvantages, as well as some unique advantages of pattern recognition in classifying atomic energy levels, merit further comment.

A high level of training implies that predictions based on this training may be regarded with high confidence. However, this will be true only when all of the categories in the training set are well represented. Therefore, each category should contain as much known data as possible. For atomic energy levels this number is clearly limited as can be seen in Table II, where the number of expected levels for each configuration is given. The number of levels are in most cases based on an $^8S^o$ parent term only. They are probably not exact values, but in any case should serve to be good approximations. It is seen that these estimates vary greatly. A category can be considered well represented if it contains a relatively large fraction of the expected number of levels. The configuration $5f^76d7s7p$ and $5f^86d7s$ are well represented while the $5f^76d^27p$ configuration is not. We will refer to this idea as "training quality." The term should not be confused with what we have called the level of training.

Consider a two-category problem, one of which is well represented and the other of which is poorly represented. An unknown level actually belonging to a well represented configuration should have a higher confidence of being correctly assigned (to that category). A well represented category will have more levels near its boundaries as represented in four-dimensional space (coordinates being energy level, g, J, and IS) than will a poorly represented category. Therefore, separating hyperplanes will more likely classify this unknown correctly. Other techniques such as K nearest neighbors should perform similarly. However, an un-

TABLE V. Net configuration predictions for unknown levels.

Index no.	Level (cm^{-1})	Configuration
A. High-certainty predictions		
Odd		
4	24 900.55	$5f^7 6d^2 7s$
5	25 518.80	$5f^7 6d^2 7s$
6	25 878.11	$5f^7 6d^2 7s$
7	28 487.41	$5f^7 6d^2 7s$
9	28 880.03	$5f^7 6d^3$
10	28 989.06	$5f^7 6d^2 7s$
12	31 167.95	$5f^7 6d^2 7s$
Even		
1	25 237.89	$5f^8 6d 7s$
3	27 263.19	$5f^7 6d 7s 7p$
6	31 413.22	$5f^8 6d 7s$
7	31 574.14	$5f^8 6d 7s$
8	31 655.78	$5f^7 6d 7s 7p$
9	31 721.56	$5f^7 6d 7s 7p$
10	31 730.96	$5f^8 6d 7s$
11	31 750.19	$5f^8 6d 7s$
12	31 954.42	$5f^7 6d 7s 7p$
14	31 982.85	$5f^7 6d 7s 7p$
15	32 441.09	$5f^8 6d 7s$
16	32 787.87	$5f^8 6d 7s$
18	33 433.15	$5f^7 6d 7s 7p$
20	33 518.27	$5f^7 6d 7s 7p$
21	33 860.10	$5f^7 6d 7s 7p$
23	34 317.25	$5f^8 6d 7s$
24	34 520.33	$5f^7 6d 7s 7p$
25	34 526.19	$5f^7 6d 7s 7p$
26	34 858.38	$5f^7 6d 7s 7p$
27	35 139.55	$5f^8 6d 7s$
28	35 335.36	$5f^7 6d 7s 7p$
29	35 459.79	$5f^7 6d 7s 7p$
30	35 461.45	$5f^7 6d 7s 7p$
31	35 838.78	$5f^7 6d^2 7p$
32	35 943.30	$5f^7 6d^2 7p$
33	36 390.78	$5f^7 6d 7s 7p$
34	36 842.85	$5f^7 6d 7s 7p$
37	38 599.35	$5f^7 6d 7s 7p$
38	38 676.40	$5f^7 6d^2 7p$
39	39 071.51	$5f^7 6d 7s 7p$
40	39 288.89	$5f^7 6d^2 7p$
41	40 263.76	$5f^7 6d 7s 7p$
42	40 603.67	$5f^7 6d^2 7p$
B. Medium-certainty predictions		
Even		
4	28 629.20	$5f^8 7s^2$ $(5f^7 6d 7s 7p)$
22	34 290.51	$5f^8 6d 7s$ $(5f^7 6d^2 7p)$
35	38 373.25	$5f^7 6d^2 7p$ $(5f^8 6d 7s)$
36	38 563.03	$5f^7 6d^2 7p$ $(5f^8 6d 7s)$
C. Equally likely predictions		
Odd		
1	22 640.04	$5f^7 6d^2 7s$ or $5f^7 6d 7s^2$
2	23 282.58	$5f^7 6d^2 7s$ or $5f^7 6d 7s^2$
3	23 299.44	$5f^7 6d^2 7s$ or $5f^7 6d 7s^2$
8	28 634.99	$5f^7 6d^2 7s$ or $5f^7 6d 7s^2$
11	31 104.82	$5f^7 6d^3$ or $5f^7 6d^2 7s$
Even		
2	26 730.23	$5f^7 6d 7s 7p$ or $5f^8 7s^2$
5	31 185.81	$5f^8 6d 7s$ or $5f^7 6d 7s 7p$
13	31 975.65	$5f^8 6d 7s$ or $5f^7 6d 7s 7p$
17	33 391.14	$5f^7 6d 7s 7p$ or $5f^8 6d 7s$
19	33 439.28	$5f^7 6d 7s 7p$ or $5f^8 6d 7s$

known belonging to a poorly represented configuration is more likely to be classified incorrectly. Ideally, the boundaries of each category will be well defined so that all unknowns will be located within them. For such a case, predicted configurations will have a confidence matching the level of training. To summarize, poorly represented categories should be weighted to reflect their true importance.

The previous discussion implies systems having experimentally accurate data are needed for pattern-recognition techniques to work best. Also, the levels in the training set must be correctly classified, and they must be truly representative.

The above factors must be considered when applying pattern recognition to atomic energy levels. However, these techniques have an inherent advantage over conventional classification techniques in that they are capable of looking at all the differentiating parameters of a level, simultaneously. Conventional techniques use all the parameters utilized in this study, but often consider only one or two at a time. The initial classification steps consider wavelengths to establish the position of the energy levels, and configurations are assigned largely on the basis of IS values alone. For curium many of the unclassified levels do not have IS data. (This would present a problem for both conventional and pattern-recognition techniques.) Furthermore, observed values of IS overlap for different configurations, making a classification on this basis alone clearly ambiguous. In these cases pattern recognition has the advantage of looking at all four parameters at once. Two-dimensional plots of these parameters show that they are all related in some way to configuration. Thus, it is clearly advantageous to use all features simultaneously in an attempt to resolve uncertainties arising from use of isotope shift alone. A further advantage would be gained by using a three-dimensional graphics terminal to observe the data. In the present case a three-dimensional Karhunen-

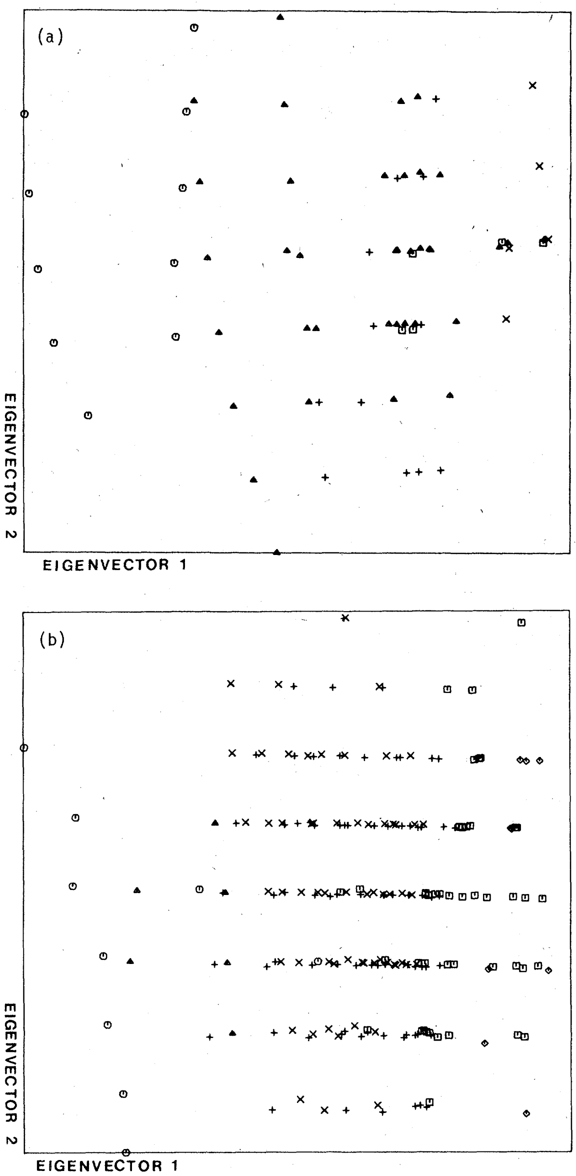

FIG. 1. (a) Plot of the first two eigenvectors from the Karhunen-Loeve transformation for odd levels. Category 1 (O) is the configuration $5f^7 6d7s^2$, 2 (Δ) is $5f^7 6d^2 7s$, 3 (+) is $5f^8 7s7p$, and 4 (×) is $5f^7 6d^3$. (b) Plot of the first two eigenvectors for even levels. Category 1 (O) is $5f^8 7s^2$, 2 (Δ) is $5f^7 7s^2 7p$, 3 (+) is $5f^7 6d7s7p$, 4 (×) is $5f^8 6d7s$, and ◇ is $5f^7 6d^2 7p$. □ represents an unknown level. For both plots, the original four features were energy level, J, g, and IS. The odd-level plot contains 19% of the total information, and the even plot contains 9%.

Loeve transformation projection from the original four parameters would provide 90% or more of the total information of the data set and therefore be an excellent approximation to it.

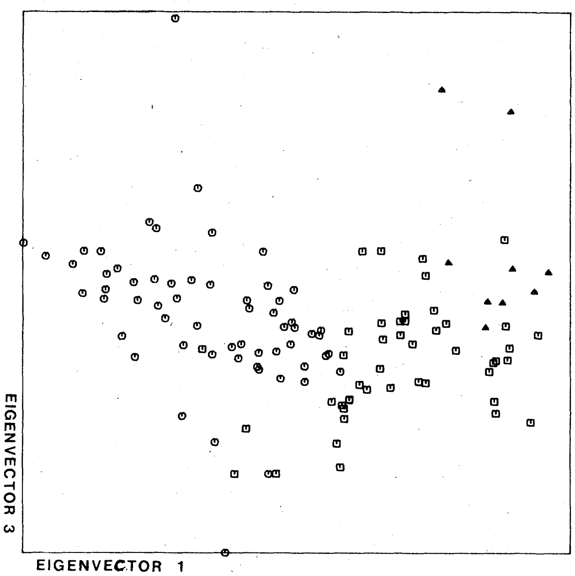

FIG. 2. Plot of the first and third eigenvectors from the Karhunen-Loeve transformation for even levels. The original three features were energy level, J, and g. The categories are the same as in Fig. 1.

IV. CONCLUSION

We have classified 40 levels of curium representing an increase of 9% for even levels and 19% for odd levels, over previously published results. On the basis of the consistent results obtained by

TABLE VI. Unknown even levels which may belong to the configuration $5f^8 7s8s$: (A) determined from Fig. 2; (B) determined from K-nearest-neighbor observation, three-feature data set.

Index no.	Level (cm^{-1}) A	B
18	33 433.15	33 433.15
22	34 290.51	
23	34 317.25	34 317.25
24	34 520.33	
25	34 526.19	
26	...	34 858.38
27	35 139.55	35 139.55
28	35 335.36	35 335.36
29	35 459.79	35 459.79
30	35 461.45	35 461.45
31	...	35 838.78
32	35 943.30	35 943.30
33	36 390.78	
35	38 373.25	
38	38 676.40	
39	39 071.51	39 071.51
42	40 603.67	

the pattern-recognition techniques, the assignments are thought to be highly certain. As discussed previously these certainties will vary with the training quality of the categories. Fourteen additional levels have been assigned to one of two configurations. Pattern-recognition techniques were not capable of resolving ambiguities in these cases. The newly classified levels should be of considerable help in assigning configurations to more levels of curium. Our techniques will also be useful as more isotope-shift and Zeeman-effect data become available.

Pattern recognition is most useful when a representative training set is available. Therefore, conventional methods of classification will always be important. Once this training set is available, however, pattern recognition offers unique advantages in looking at the entire data set, and as such, has the potential to be an extremely useful aid in the classification of atomic transitions and levels.

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