Spectral classification of *U* II energy levels using pattern-recognition techniques

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(Received 30 October 1987; revised manuscript received 31 March 1988)

Twenty-four unknown U II energy levels are classified according to configuration using pattern-recognition methods. The energy level, Landé g factor, quantum number J, and ^{234}U isotope shift are used to describe each level. Preliminary results of the prediction of the extent of configuration mixing for low-energy odd levels are presented.

Pattern-recognition methods have been used successfully in classifying unknown U I energy levels.[1] In this paper we apply similar techniques in classifying U II energy levels. A uranium line list from high-resolution grating measurements between 3100 and 9000 Å contains 92 000 U I and U II lines.[2] The U II data of Ref. 3 contains 316 odd levels and 692 even levels; the lowest levels (consisting of 91 odd and 65 even levels) have been identified according to configuration, and have been assigned configuration percentages.[4]

As in previous works,[1,5,6] we apply pattern-recognition techniques to known energy levels, and use the resulting training to classify according to configuration 7 odd-parity and 17 even-parity levels. This is an increase of 8% for odd and 26% for even levels. As an extension of previous work evaluation and prediction of configuration percentage (i.e., mixing) is discussed for low levels. The computer package of pattern-recognition techniques ARTHUR is used.[7] The reader is referred to Refs. 1, 5, and 6, and references therein, for discussions of relevant pattern recognition methodology.

Observed energy levels of U II are described in Table I. The U II data of Refs. 3 and 4, and isotope shift (IS) data of Ref. 3 are used. Table II lists unknown odd-parity levels with the four-features energy level (cm^{-1}), quantum number J, ^{234}U IS (10^{-3} cm^{-1}), and Landé g factor. Table III lists unknown even-parity levels with the same four features.[3] As in U I energy-level classification,[1] these tables do not list all unclassified levels of U II because (1) not all unknowns have experimental values for all four features, and (2) many unknowns are at relatively high energy. There are few classified levels at these high energies, and configurations that lie in these regions are not well represented. The high-energy unknown levels included in this study lie close in energy to classified levels. For further discussion of this point, see Refs. 1 and 5.

Assigning configurations to levels is accomplished by training and testing classified levels and using the training to classify unknown levels with the features in Tables II and III. The configurations $5f^37s^2$, $5f^36d^2$, $5f^36d7s$, and $5f^47p$ are used as odd-level categories. For even levels, the configurations $5f^47s$, $5f^46d$, $5f^26d^27s$, $5f^26d^3$, $5f^37s7p$, and $5f^36d7p$ are used. Good training and testing is accomplished for odd and even levels (Table IV). Based on these positive results, pattern-recognition methods are applied to unknown levels; predictions are given in Tables V and VI. See Ref. 1 for details of this procedure.

TABLE I. Even and odd configurations of U II.

Index No.	Configurations	Lowest level (cm^{-1})	Number of levels in interval
Odd			
1	$5f^37s^2$	0.0000	1
2	$5f^36d^2$	289.0355	6
3	$5f^36d7s$	4706.2771	209
4	$5f^47p$	30 301.0377	100
Even			
1	$5f^47s$	4663.8027	8
2	$5f^46d$	12 513.8830	6
3	$5f^26d^27s$	13 783.0293	68
4	$5f^26d^3$	21 975.5898	23
5	$5f^37s7p$	23 315.0898	70
6	$5f^36d7p$	26 191.3066	517

TABLE II. Unknown odd-parity U II levels and data used for classification in this study.

Index No.	Level (cm^{-1})	J	Isotope shift 234U (10^{-3} cm^{-1})	Landé g factor
1	17 922.7699	5.5	−1526.5	0.985
2	19 473.3764	5.5	−1560.4	0.990
3	32 272.3845	3.5	−1704.2	1.080
4	33 037.9210	3.5	−1577.4	1.075
5	33 411.9316	3.5	−1674.6	1.000
6	34 070.7928	5.5	−1367.8	1.040
7	34 634.5781	5.5	−1692.2	1.090
8	34 845.5881	4.5	−1510.6	1.070
9	35 523.0917	4.5	−1655.9	1.045
10	36 433.3383	2.5	−1706.0	0.765
11	36 464.7286	2.5	−1607.8	1.060
12	36 956.0515	5.5	−1686.5	1.050
13	37 635.8867	3.5	−1841.7	1.040
14	40 344.2572	5.5	−1588.7	1.080

TABLE III. Unknown even-parity U II levels and data used for classification in this study.

Index No.	Level (cm^{-1})	J	Isotope shift ^{234}U (10^{-3} cm^{-1})	Landé g factor	Index No.	Level (cm^{-1})	J	Isotope shift ^{234}U (10^{-3} cm^{-1})	Landé g factor
1	19 395.1719	2.5	0.0	0.510	29	23 107.5664	6.5	−1182.0	1.060
2	19 517.7285	3.5	−1141.5	0.815	30	23 234.8223	6.5	−1141.0	1.090
3	19 977.0957	6.5	−585.0	0.960	31	23 241.0332	4.5	−434.1	1.050
4	20 345.9883	5.5	−730.3	1.015	32	23 241.3672	5.5	−437.9	0.95
5	20 571.6816	3.5	−1073.4	0.935	33	23 553.9746	5.5	−1664.0	1.040
6	20 635.2637	4.5	−914.1	0.945	34	23 635.9160	6.5	−1173.2	0.920
7	20 961.7246	3.5	−896.7	0.855	35	23 778.1699	5.5	−1032.4	0.865
8	21 021.3652	3.5	−894.3	0.896	36	23 817.5059	4.5	−970.8	0.885
9	21 154.5586	4.5	0.0	1.010	37	23 911.6309	4.5	−1398.5	1.060
10	21 207.7383	3.5	−995.8	1.145	38	24 010.4609	5.5	−1252.2	0.970
11	21 320.2012	3.5	−1187.0	0.835	39	24 152.8086	5.5	−1246.6	0.910
12	21 555.2754	4.5	−1281.1	1.025	40	24 159.6934	6.5	−1265.9	0.965
13	21 691.5117	5.5	−871.2	0.975	41	24 293.0937	6.5	−1378.2	1.030
14	21 710.7695	6.5	−959.0	0.915	42	24 305.6250	4.5	−785.4	0.980
15	21 831.0410	4.5	−1194.8	0.890	43	24 453.4258	4.5	−1443.6	1.100
16	21 860.0527	3.5	−1134.5	0.67	44	24 537.5625	3.5	−1161.8	1.020
17	21 975.5898	6.5	−1592.0	1.03	45	24 923.6230	6.5	−1315.0	1.090
18	22 101.3320	4.5	−1152.1	0.89	46	25 047.8379	5.5	−1272.3	1.030
19	22 165.1758	4.5	−1013.2	0.89	47	25 130.7168	3.5	0.0	0.990
20	22 250.4004	3.5	−1196.7	0.885	48	25 163.9043	6.5	−1141.8	1.035
21	22 389.5723	5.5	−1084.6	1.040	49	25 200.7773	5.5	−795.5	1.045
22	22 429.8594	4.5	−662.7	0.935	50	25 213.7949	3.5	0.0	1.035
23	22 615.3164	6.5	−1365.4	0.995	51	25 317.6934	4.5	−608.1	0.995
24	22 642.4727	4.5	−1143.1	0.875	52	25 356.9746	5.5	−1620.0	1.020
25	22 764.9062	5.5	−496.3	0.980	53	25 437.5664	4.5	−993.1	0.930
26	22 868.0332	4.5	−1605.4	0.985	54	25 492.9180	5.5	−959.4	0.990
27	22 917.4531	5.5	−1245.8	0.860	55	25 495.4941	3.5	−1150.9	0.945
28	22 960.6641	3.5	0.0	0.950	56	25 713.6328	4.5	−987.6	0.915

TABLE IV. Training and test results for even- and odd-level four-feature training.

Method[a]	Odd Levels Training data % correct	Test data % correct	Method[a]	Even Levels Training data % correct	Test data % correct
KNN	100	100	KNN	81	100
PNN	100	100	PNN	88	100
SICLASS	100	100	SICLASS	94	100
LEAST	80	80	LEAST	92	80
BACLASS	100	98	BACLASS	97	100

[a]See Ref. 1 for explanations of classification methods.

TABLE V. Classification results for odd levels based on four-feature training.

Index No.	Classification methods[a] KNN	PNN	SICLASS	LEAST	BACLASS
1	2	2	3	3	4
2	2	2	2	3	4
3	4	4	4	4	4
4	4	4	4	4	4
5	4	4	4	4	4
6	4	4	4	4	2
7	4	4	4	4	2
8	4	4	4	4	4
9	4	4	4	4	4
10	4	4	4	4	4
11	4	4	4	4	3
12	4	4	4	4	2
13	4	4	4	4	4
14	4	4	4	4	2

[a]See Ref. 1 for explanations of classification methods. Integers refer to the odd-parity electron configurations of Table I.

TABLE VI. Classification results for even levels based on four-feature training.

Index No.	KNN	PNN	SICLASS	LEAST	BACLASS	Index No.	KNN	PNN	SICLASS	LEAST	BACLASS
	Classification methods[a]						Classification methods[a]				
1	3	3	5	5	3	29	5	5	5	3	5
2	3	3	6	3	5	30	5	5	5	3	5
3	3	3	3	3	3	31	5	5	5	3	5
4	3	3	5	3	5	32	5	5	5	3	5
5	5	5	5	3	5	33	5	5	5	5	5
6	5	5	5	3	3	34	2	2	5	3	5
7	5	5	5	3	3	35	5	5	6	5	5
8	5	5	5	3	5	36	5	5	6	5	5
9	3	3	3	3	3	37	5	5	5	5	5
10	5	5	5	3	5	38	5	5	5	3	5
11	5	5	6	3	5	39	5	5	5	5	5
12	5	5	5	3	5	40	5	5	6	5	5
13	5	5	5	3	5	41	5	5	5	5	5
14	5	5	5	3	5	42	5	5	5	5	5
15	5	5	6	3	5	43	5	5	5	5	5
16	5	5	6	3	2	44	5	5	5	3	6
17	2	2	5	3	2	45	5	5	5	3	5
18	5	5	6	3	5	46	5	5	5	5	1
19	5	5	5	3	5	47	5	5	5	5	5
20	5	5	5	3	5	48	5	5	5	5	5
21	5	5	5	3	5	49	5	5	5	5	5
22	5	5	5	3	5	50	5	5	5	5	5
23	5	5	5	3	5	51	5	5	5	5	5
24	5	5	6	3	5	52	6	6	5	5	6
25	5	5	5	5	2	53	5	5	5	5	5
26	2	2	5	3	5	54	5	5	5	5	5
27	5	5	6	6	5	55	5	5	5	5	5
28	3	3	5	5	5	56	5	5	5	5	5

[a]Classification methods are explained in Ref. 1. Integers refer to the even-parity electron configuration of Table I.

In the U I classification work we used two isotope shifts, comparing classification results based on four-feature (one IS) and five-feature (two IS's) analyses. In this present work we used only the ^{234}U IS because (1) two IS's are unavailable for most odd levels, (2) although two IS's (^{235}U from Ref. 4 and ^{234}U from Ref. 3) for many even levels are available, absence of the ^{235}U IS for some levels would decrease training set size and number of unknowns, and (3) ^{234}U IS data is thought to be of better quality than ^{235}U IS data.[3] Our previous work failed to demonstrate superiority of five- over four-feature analyses, and we use the best available data that allows the largest training set.

Table I includes the even-parity configuration $5f^2 6d^3$ that was not included in the original training set as it contains one member. Several routines in ARTHUR require categories of two members or more (see Ref. 1 for further discussion). When this configuration was included, no unknown levels are assigned to it. This is strong evidence that no even levels belong to a classification not

TABLE VII. Comparison of Crosswhite's configuration percentages of certain odd-parity levels to those predicted by the continuous property algorithms STEP and LEAST.

Energy level (cm^{-1})	Configuration % $5f^3 7s^2$	Configuration % $5f^3 6d 7s$	Configuration % $5f^3 6d^2$	STEP $5f^3 7s^2$	STEP $5f^3 6d 7s$	STEP $5f^3 6d^2$	STEP $5f^4 7p$	LEAST $5f^3 7s^2$	LEAST $5f^3 6d 7s$	LEAST $5f^3 6d^2$	LEAST $5f^4 7p$
4585.434	0	45	55	0	42	58	0	0	35	65	0
6283.41	0	55	45	0	51	49	0	0	41	69	0
9626.113	0	88	12	0	69	31	0	0	63	27	0
10 198.312	0	89	11	0	72	28	0	0	51	49	0
10 444.432	2	69	29	0	74	26	0	0	98	0	2
11 544.674	1	31	68	0	80	20	0	0	16	84	0
11 787.318	0	62	38	0	81	29	0	0	80	20	0

TABLE VIII. Net configuration predictions for unknown levels.

Odd parity Index No.	Level (cm^{-1})	Configuration	Even parity Index No.	Level (cm^{-1})	Configuration
5	32 272.3845	$5f^47p$	3	19 977.0957	$5f^26d^27s$
6	33 037.9210	$5f^47p$	9	21 154.5586	$5f^26d^27s$
7	33 411.9316	$5f^47p$	33	23 553.9746	$5f^37s7p$
10	34 845.5881	$5f^47p$	37	23 911.6309	$5f^37s7p$
11	35 523.0917	$5f^47p$	39	24 152.8086	$5f^37s7p$
12	36 433.3383	$5f^47p$	41	24 293.0937	$5f^37s7p$
15	37 635.8867	$5f^47p$	42	24 305.6250	$5f^37s7p$
			43	24 453.4258	$5f^37s7p$
			47	25 130.7168	$5f^37s7p$
			48	25 163.9043	$5f^37s7p$
			49	25 200.7773	$5f^37s7p$
			50	25 213.7949	$5f^37s7p$
			51	25 317.6934	$5f^37s7p$
			53	25 437.5664	$5f^37s7p$
			54	25 492.9180	$5f^37s7p$
			55	25 495.4941	$5f^37s7p$
			56	25 713.6328	$5f^37s7p$

represented in the training set.

Low levels of Crosswhite's data have been assigned configuration percentages. Certain routines in ARTHUR are continuous property algorithms capable of calculating nondiscrete categories for each energy level. Table VII shows a comparison of some of Crosswhite's configuration percentages for low-lying odd levels and predictions of continuous property algorithms of ARTHUR. One sees a marked correlation of the percent configuration predicted by these algorithms as compared to Crosswhite's calculations. These preliminary results will be refined and extended by applying other continuous property classification algorithms to the levels in Table VII and to the other levels as well.

Seven unknown odd levels and 17 unknown even levels are classified with high certainty, meaning that each pattern-recognition method used predicted the same configuration. Table VIII summarizes the results. Predicted configurations cannot be checked for consistency with term data as this data is not available for listed levels.

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