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Fine Structure Analysis of the Configuration System of V II. Part I: Even-Parity Levels

Safa Bouazza[1], Richard A. Holt[2], David S. Rosner[2], Nathan M. R. Armstrong[3]

[1]LISM, Université de Champagne-Ardenne, Reims, France
[2]Department of Physics and Astronomy, University of Western Ontario, London, Canada
[3]Department of Physics and Astronomy, Mc Master University, Hamilton, Canada
Email: safa.bouazza@univ-reims.fr

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Abstract

Using a linked-parameter technique of level-fitting calculations in a multi configuration basis, a parametric analysis of fine structure (fs) for even-parity levels of V II, involving six configurations, has been performed. This led us to exchange the assignments of two triplets, $3d^3(^2F)4s$ c ^{3}F and $3d^4$ d ^{3}F, reported in earlier analyses as being located at 30,300 cm^{-1} and 30,600 cm^{-1}, respectively. This is confirmed by experimental hyperfine structure (hfs) A constants, used as fingerprints. Moreover, the current singlet $3d^24s^2$ ^{1}D$_2$ position is likely too high. The fs parameters, magnetic Landé g-factors, and the percentage of leading eigenvectors of levels are calculated. We present also predicted singlet, triplet and quintet positions for missing experimental levels up to 100,000 cm^{-1}. The single-electron hfs parameters are determined in their entirety for ^{51}V II for the model space $(3d + 4s)^4$ with good accuracy. For the model space $(3d + 4s)^4$ of ^{51}V II the single-electron hfs parameters are computed; furthermore, our achieved theoretical evaluations of the single-electron hfs parameters, thanks to the use of *ab initio* calculations, reinforce the validity of these hfs parameter values, deduced from experimental data.

Keywords

Fine Structure, Hyperfine Structure, Energy Levels, *Ab-Initio* Calculations, V II Spectrum

1. Introduction

The early successful fs analysis of the V II spectrum was due to Meggers and Moore [1]. According to their classification, all except two of the terms were known in the configurations $3d^34s$ and $3d^4$, but $3d^24s^2$ was altogether unknown. Later, Sugar and Corliss compiled the energy levels of vanadium in its 23 stages of ionization, which were analysed from atomic spectra [2]. Iglesias [3] added 30 new levels to those already published for the

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$3d^34d$ configuration, using 149 lines, classified as $3d^34p$ - $3d^34d$ transitions. Up to now, no parametric analysis of hfs exists for any even or odd configurations of V II. We propose to fill this absence, as we did previously for many singly ionized atoms: Hf II, Zr II, Ta II, Ti II and Nb II [4]-[8] in an aim to complete previous works and to eliminate erroneous level assignments. The background and motivation of this work should present high interest for astrophysical investigations, very useful in the study of the history of nucleosynthesis, chemically peculiar stars and the sun.

2. Accurate Fine and Hyperfine Structure Analysis

As only a few lowest energy configuration even-parity levels were available from experimental data, in our previous works regarding the fs of transition metal elements much of our analyses of model spaces were restricted to $(3d + 4s)^4$, $(4d + 5s)^4$ and $(5d + 6s)^4$. Fortunately, the energy levels of the five lowest configurations for V II are determined experimentally [1] [3]. We also know that there is poor isolation of the configurations $(3d + 4s)^4$ from other configurations in the 3*d*-elements since some of their levels are located above the levels belonging to other even-parity configurations whose centers of gravity positions are higher.

Therefore, we use a configuration basis set, called the extended model space, which consists of the following six configurations: $(3d + 4s)^4 + 3d^35s + 3d^34d + 3d^35d$. The interactions between particular states are determined quantitatively by this analysis. The complete details of fs analysis were already given in our previous papers: see for instance [8].

The fs least squares fitting procedure has been carried out for over 170 energy levels attributed to the extended model space. **Table 1** lists the observed energy levels, calculated eigenvalues, and percentages of the largest and next largest wave function components with the corresponding LS term designations. A set of 37 parameters selected among a total of 157, requisite for fs analysis, treated as free, concern only configurations with known experimental levels, *i.e.* $3d^24s^2$, $3d^34s$, $3d^4$, $3d^34d$ and $3d^35s$ in this work.

The fitted values of these parameters are given in **Table 2** and **Table 3** with their uncertainties in parentheses; the agreement was improved by taking into account the interactions between all known configuration energy levels. For comparison we have inserted also *ab initio* calculations using the Cowan code [9]. A fit with a standard deviation of 55 cm^{-1} has been achieved. This fit may be considered as good, considering the large number of degrees of freedom: 132 = 169 − 37. The other parameters with significant values are fixed to their weighted *ab initio* values while those expected to be small, although predicted by theory, are fixed to zero and then are not listed in these two tables. We confirm on the whole the attributions to term designations given previously [1]-[3] except in two cases: two triplet positions, $3d^3(^2F)4s$ c ^{3}F and $3d^4$d^{3}F, located at 30,300 cm^{-1} and 30600 cm^{-1}. We propose to invert these two triplet positions as we did in **Table 1**. It has been brought immediately to our attention by experimental hfs data given in **Table 1** of Ref. [10] since when comparing A values for J = 2 and J = 3 one can notice A values for $3d^3(^2F)4s$ c ^{3}F are smaller than those of $3d^4$ d ^{3}F and $3d^4$ b ^{3}F which means broadly that the magnetic contribution of an s-contact-electron is less important than that of a d-electron. We propose moreover to correct the wrong position of the singlet $3d^24s^2$ $^1D_2$ which must be rather lower than $3d^34s$ ^{2}D; ^{3}D, *i.e.* 44,104 (40) cm^{-1} instead of 44,657 cm^{-1}.

Let us point out that all parameters except spin-orbit ζ_{nd} and energies of configuration centers of gravity E_{av} are weighted by a factor $0.7696 = \dfrac{F^2(3d,3d)(fs)}{F^2(3d,3d)(ab-initio)} =$, *i.e.* the ratio between Slater integrals $F^2(3d, 3d)$ for the $3d^34s$ configuration obtained thanks to the fs study and *ab initio* calculations, as we did previously [4]-[8]. In **Table 4** we give up to 100,000 cm^{-1} our predicted data for missing experimental energies for these five configurations, analysed in [1]-[3]. This will surely help further experimental V II work to complete this ion study.

Concerning the hfs analysis we follow the many-body parametrisation method [11] which allows us to take advantage of similarities between configuration interaction effects observed independently in spin-orbit and hyperfine splitting. The radial parameters $a_{nl}^{\kappa k}$, $b_{nl}^{\kappa k}$, a_i and b_i have been evaluated by fitting them to experimentally determined hfs constants A and B using the theoretical expressions (Equations (4) and (5) of [12] for instance).

In 2011, Armstrong, Rosner and Holt applied fast-ion-beam laser-fluorescence spectroscopy to measure with good accuracy the magnetic dipole hfs A constants of 24 even levels and 31 odd levels of ^{51}V II [10] which are the first published data for hfs of this ion.

Table 1. Comparison between the observed and calculated energy levels (in·cm^{-1}) and g$_J$-factors. For each state the parent terms are given immediately after the configuration label in columns 3 & 4.

Obs. energy level [2]	Calc. eigenvalue	Largest eigenvector component (%)	Next largest eigenvector component	Calc. g$_J$	Obs g$_J$ [1]
J = 0					
0.00	−37.25	99.60 C ^{5}D	0.29 M ^{4}F, ^{5}D	0.00	
11295.513	11366.99	53.92 C ^{3}P	37.54 C ^{3}P	0.00	
19161.422	19128.46	95.13 B ^{2}P; ^{3}P	2.39 B ^{4}P; ^{3}P	0.00	
19902.608	19803.77	63.38 C ^{1}S	18.80 C ^{1}S	0.00	
20156.670	20101.10	75.22 B ^{4}P ; ^{3}P	12.45 C ^{1}S	0.00	
32420.050	32464.18	52.32 C ^{3}P	41.44 C ^{3}P	0.00	
48898.010	48892.84	96.44 A ^{3}P	2.91 C ^{3}P	0.00	
74949.580	74965.42	94.88 M ^{4}F, ^{3}P	1.82 M ^{2}P; ^{3}P	0.00	
76281.366	76278.52	91.57 M ^{4}F, ^{5}D	5.34 M ^{4}P; ^{5}D	0.00	
81669.529	81693.78	98.90 K ^{4}P; ^{3}P	0.58 K ^{2}P; ^{3}P	0.00	
87230.300	87236.45	76.93 M ^{4}P; ^{3}P	13.06 M ^{2}P; ^{3}P	0.00	
J = 1					
36.102	−0.56	99.62 C ^{5}D	0.29 M ^{4}F, ^{5}D	1.501	
2604.040	2585.86	99.95 B ^{4}F; ^{5}F	0.03 B ^{2}D; ^{3}D	0.000	
11514.784	11571.95	54.07 C ^{3}P	37.42 C ^{3}P	1.501	1.48
13511.799	13545.15	99.75 B ^{4}P; ^{5}P	0.13 B ^{2}P; ^{3}P	2.502	2.39
18269.514	18268.86	61.04 C ^{3}D	29.43B ^{2}D; ^{3}D	0.509	0.49
19166.314	19144.69	89.70 B ^{2}P; ^{3}P	6.51 B ^{4}P; ^{3}P	1.484	1.40
20089.650	20095.10	81.72 B ^{4}P; ^{3}P	5.27 C ^{3}P	1.438	1.35
20522.147	20534.46	44.22 B ^{2}D; ^{3}D	33.39 C ^{3}D	0.571	0.58
22273.636	22272.534	96.87 B ^{2}P; ^{1}P	1.29 B ^{4}P; ^{3}P	0.999	0.97
32299.257	32369.00	52.38 C ^{3}P	41.43 C ^{3}P	1.501	1.48
44201.640	44200.00	76.60 B ^{2}D; ^{3}D	23.13 B ^{2}D; ^{3}D	0.499	0.50?
48975.700	48981.81	96.55 A ^{3}P	2.85 C ^{3}P	1.501	
69146.385	69130.36	99.91 K ^{4}F; ^{5}F	0.04 M ^{2}D; ^{3}D	0.000	
72518.626	72485.99	99.20 M ^{4}F; ^{5}P	0.38 N ^{4}F; ^{5}P	2.500	
72839.345	72852.27	89.92 M ^{4}F; ^{5}F	9.65 M ^{4}F; ^{3}D	0.059	
73181.639	73195.11	87.78 M ^{4}F; ^{3}D	9.96 M ^{4}F; ^{5}F	0.443	
75080.541	75097.44	94.40 M ^{4}F; ^{3}P	1.82 M ^{2}P; ^{3}P	1.499	
76322.694	76320.27	91.47 M ^{4}P; ^{5}D	5.38 M ^{4}P; ^{5}D	1.501	
80542.337	80549.73	99.36 K ^{4}F; ^{5}P	0.31 K ^{2}P; ^{3}P	2.500	
81735.141	81751.39	98.55 K ^{4}P; ^{3}P	0.68 K ^{2}P; ^{1}P	1.498	
84359.490	84352.76	39.36 M ^{4}P; ^{3}D	37.06 M ^{4}P; ^{5}F	0.318	
85096.450	85089.15	77.90 M ^{4}P; ^{5}P	18.81 M ^{4}P; ^{5}D	2.452	
87184.950	87180.72	72.36 M ^{4}P; ^{3}P	12.14 M ^{2}P; ^{3}P	1.468	

Continued

J = 2					
106.643	70.89	99.64 C ^{5}D	0.29 M ^{4}F; ^{5}D	1.501	
2687.208	2665.31	99.95 B ^{4}F; ^{5}F	0.02 B ^{2}D; ^{3}D	1.000	0.97
8640.362	8668.69	94.36 B ^{4}F; ^{3}F	4.45 C ^{3}F	0.666	0.65
11908.261	11977.54	54.12 C ^{3}P	37.09 C ^{3}P	1.501	1.49
13490.883	13467.88	69.00 C ^{3}F	23.80 C ^{3}F	0.666	0.59
13594.723	13623.51	99.58 B ^{4}P; ^{5}P	0.22 B ^{2}P; ^{3}P	1.834	1.78
18293.871	18294.96	63.00 C ^{3}D	27.31 B ^{2}D; ^{3}D	1.172	1.13
19132.791	19122.80	80.94 B ^{2}P; ^{3}P	13.70 B ^{4}P; ^{3}P	1.486	1.38
20343.046	20335.14	68.38 B ^{4}P; ^{3}P	9.95 B ^{2}D; ^{3}D	1.439	1.36
20617.073	20627.27	36.11 B ^{2}D; ^{3}D	20.10 C ^{3}D	1.213	1.25
20980.927	20993.21	37.78 B ^{2}D; ^{1}D	32.50 C ^{1}D	1.027	1.02
25191.035	25150.22	36.51 C ^{1}D	33.78 B ^{2}D; ^{1}D	1.000	0.99
30267.511	30257.99	38.55 C ^{3}F	22.71 B ^{2}F; ^{3}F	0.666	0.67
30673.088	30669.40	76.09 B ^{2}F; ^{3}F	15.57 C ^{3}F	0.666	0.67
32040.635	32115.49	52.52 C ^{3}P	41.26 C ^{3}P	1.501	1.38
37937.694	37933.75	76.22 A ^{3}F	18.91 C ^{3}F	0.666	
44657.941*	44105.45	60.81 A ^{1}D	22.76 C ^{1}D	1.001	
44159.460	44185.34	76.77 B ^{2}D; ^{3}D	22.67 B ^{2}D; ^{3}D	1.167	1.14
47324.288	47302.16	70.03 B ^{2}D; ^{1}D	22.38 B ^{2}D; ^{1}D	1.001	
49204.650	49190.71	95.74 A ^{3}P	2.60 C ^{3}P	1.496	
50951.660	50930.31	48.61 C ^{1}D	32.62 C ^{1}D	1.003	
69228.318	69214.03	99.55 K ^{4}F; ^{5}F	0.38 K ^{4}F; ^{3}F	0.999	
70415.542	70397.31	99.16 K ^{4}F; ^{3}F	0.38 K ^{4}F; ^{5}F	0.667	
72674.924	72643.66	98.63 M ^{4}F; ^{5}P	0.49 M ^{4}F; ^{3}D	1.831	
72878.056	72868.91	59.43 M ^{4}F; ^{5}G	36.08 M ^{4}F; ^{5}F	0.604	
73027.311	73026.02	55.47 M ^{4}F; ^{5}F	38.44 M ^{4}F; ^{5}G	0.738	
73310.069	73294.71	90.74 M ^{4}F; ^{3}D	4.04 M ^{4}F; ^{5}F	1.162	
75335.879	75355.16	94.09 M ^{4}F; ^{3}P	1.72 M ^{2}P; ^{3}P	1.500	
75813.489	75805.22	92.33 M ^{4}F; ^{3}F	2.96 M ^{2}G; ^{3}F	0.668	
76403.674	76403.25	91.33 M ^{4}F; ^{5}D	4.73 M ^{4}P; ^{5}D	1.501	
80623.249	80633.56	98.95 K ^{4}P; ^{5}P	0.60 K ^{2}P; ^{3}P	1.833	
81914.328	81918.43	99.16 K ^{4}P; ^{3}P	0.21 L ^{4}P; ^{3}P	1.501	
84406.210	84451.41	43.57 M ^{4}P; ^{3} D	26.93 M ^{2}G; ^{3}D	1.126	
85045.572	85043.16	83.87 M ^{4}P; ^{5}P	13.43 M ^{4}P; ^{5}D	1.812	
86001.530	86003.05	29.26 M ^{4}P; ^{3}F	26.59 M ^{2}G; ^{3}F	0.787	
87215.750	87224.76	74.09 M ^{4}P; ^{3}P	11.65 M ^{2}P; ^{3}P	1.490	

Continued

J = 3					
208.790	176.03	99.65 C ^{5}D	0.29 M ^{4}F; ^{5}D	1.501	
2808.959	2784.06	99.95 B ^{4}F; ^{5}F	0.02 B ^{4}F; ^{3}F	1.251	1.20
8842.050	8860.61	94.04 B ^{4}F; ^{3}F	4.72 C ^{3}F	1.083	1.04
13542.645	13515.81	67.97 C ^{3}F	23.09 C ^{3}F	1.079	1.06
13741.640	13753.15	99.89 B ^{4}F; ^{5}P	0.03 M ^{4}F; ^{5}P	1.668	1.62
14461.748	14501.41	60.98 C ^{3}G	36.44 B ^{2}G; ^{3}G	0.754	0.74
16340.981	16372.76	62.73 B ^{2}G; ^{3}G	36.14 C ^{3}G	0.750	0.76
18353.827	18330.97	68.46 C ^{3}D	24.53 B ^{2}D; ^{3}D	1.334	1.30
20622.983	20668.95	52.95 B ^{2}D; ^{3}D	30.24 C ^{3}D	1.334	1.26
26839.749	26638.09	90.37 C ^{1}F	8.13 B ^{2}F; ^{1}F	1.000	0.97
30306.389	30299.56	33.57 C ^{3}F	32.42 B ^{2}F; ^{3}F	1.083	1.06
30641.767	30647.98	65.93 B ^{2}F; ^{3}F	21.59 C ^{3}F	1.083	1.05
34228.852	34216.02	91.47 B ^{2}F; ^{1}F	8.11 C ^{1}F	1.000	1.00
38193.021	38185.64	77.69 A ^{3}F	17.89 C ^{3}F	1.084	
44098.473	44121.78	77.37 B ^{2}D; ^{3}D	22.33 B ^{2}D; ^{3}D	1.334	
69352.530	69341.00	99.36 K ^{4}F; ^{5}F	0.59 K ^{4}F; ^{3}F	1.250	
70629.831	70616.64	98.96 K ^{4}F; ^{3}F	0.59 K ^{4}F; ^{5}F	1.084	1.06
72448.600	72439.34	98.32 M ^{4}F; ^{5}H	0.75 M ^{4}F; ^{5}G	0.503	
72908.997	72881.92	97.83 M ^{4}F; ^{5}P	1.39 M ^{4}F; ^{3}D	1.663	
72951.558	72937.71	77.16 M ^{4}F; ^{5}G	44.68 M ^{4}F; ^{5}F	1.118	
73146.343	73128.86	76.27 M ^{4}F; ^{5}F	45.04 M ^{4}F; ^{5}G	1.046	
73530.712	73517.55	94.14 M ^{4}F; ^{3}D	1.82 M ^{4}P; ^{3}D	1.337	
75422.910	75412.58	92.32 M ^{4}F; ^{3}G	2.20 M ^{2}G; ^{3}G	0.757	
75966.119	75963.84	90.07 M ^{4}F;^{3}F	3.05 M ^{2}G; ^{3}F	1.077	
76521.357	76522.23	91.27 M ^{4}F; ^{5}D	4.84 M ^{4}P; ^{5}D	1.501	
80782.426	80783.98	99.62 K ^{4}F; ^{5}P	0.23 M ^{4}P; ^{5}P	1.668	
81263.626	81321.39	99.91 K ^{2}G; ^{3}G	0.02 L ^{2}G; ^{3}G	0.750	
84459.916	84504.10	53.04 M ^{4}P; ^{3}D	27.87 M ^{2}G; ^{3}D	1.307	
84643.381	84670.91	86.67 M ^{2}G; ^{1}F	7.33 M ^{2}G; ^{3}G	0.983	
84999.355	85012.56	89.91 M ^{4}P; ^{5}P	6.53 M ^{4}P; ^{5}D	1.655	
85076.720	85088.67	82.85 M ^{2}G; ^{3}G	8.16 M ^{2}G; ^{1}F	0.772	
86113.793	86098.83	46.73 M ^{2}G; ^{3}F	35.01 M ^{4}P;^{3}F	1.096	
90381.370	90328.91	54.69 M ^{2}H; ^{1}F	26.04 M ^{2}D; ^{1}F	0.998	
93806.100	93703.86	37.36 M ^{2}H; ^{1}F	24.29 M ^{2}D; ^{1}F	1.001	

Continued

J = 4					
339.125	310.43	99.63 C ^{5}D	0.29 M ^{4}F; ^{5}D	1.501	
2968.389	2941.09	99.96 B ^{4}F; ^{5}F	0.02 B ^{4}F; ^{3}F	1.351	1.30?
9097.889	9106.94	93.55 B ^{4}F; ^{3}F	5.12 C ^{3}F	1.250	1.22
12545.100	12622.67	97.95 C ^{3}H	0.68 B ^{2}H; ^{3}H	0.801	0.83?
13608.939	13583.18	67.66 C ^{3}F	22.40 C ^{3}F	1.246	1.19
14556.068	14595.48	60.41 C ^{3}G	36.44 B ^{2}G; ^{3}G	1.052	1.00
16421.528	16456.92	62.28 B ^{2}G; ^{3}G	35.98 C ^{3}G	1.050	1.03
17910.913	17867.69	50.71 C ^{1}G	24.10 C ^{1}G	1.000	0.95
19112.929	19115.38	73.06 B ^{2}G; ^{1}G	11.99 C ^{1}G	0.995	0.98
20242.382	20227.53	96.35 B ^{2}H; ^{3}H	2.52 B ^{2}G; ^{1}G	0.806	0.82
30318.528	30322.35	35.04 C ^{3}F	32.06 B ^{2}F; ^{3}F	1.251	1.25
30613.910	30628.55	52.07 B ^{2}F; ^{3}F	30.39 C ^{3}F	1.251	1.23
36424.870	36385.28	58.77 C ^{1}G	35.58 C ^{1}G	1.000	0.96
38517.080	38512.88	79.22 A ^{3}F	16.63 C ^{3}F	1.250	
53607.200	53615.63	96.56 A ^{1}G	2.86 C ^{1}G	1.000	
69518.528	69513.26	99.47 K ^{4}F; ^{5}F	0.47 K ^{4}F; ^{3}F	1.350	
70898.570	70896.31	99.04 K ^{4}F; ^{3}F	0.47 K ^{4}F; ^{5}F	1.251	1.23
72551.297	72541.81	97.53 M ^{4}F; ^{5}H	1.39 M ^{4}F; ^{5}G	0.904	
73063.719	73048.13	50.08 M ^{4}F; ^{5}G	49.00 M ^{4}F; ^{5}F	1.249	
73279.343	73269.52	51.31 M ^{4}F; ^{5}F	48.49 M ^{4}F; ^{5}G	1.249	
75140.638	75161.09	93.03 M ^{4}F; ^{3}H	1.98 M ^{4}F; ^{3}G	0.805	
75615.397	75611.13	89.92 M ^{4}F; ^{3}G	2.54 M ^{4}F; ^{3}F	1.051	
76143.052	76148.98	89.63 M ^{4}F; ^{3}F	3.25 M ^{2}G; ^{3}F	1.245	
76673.101	76776.57	91.15 M ^{4}F; ^{5}D	4.96 M ^{4}P; ^{5}D	1.501	
81343.015	81401.08	97.12 K ^{2}G; ^{3}G	2.73 K ^{2}G ; ^{1}G	1.049	
82025.721	82075.24	96.61 K ^{2}G; ^{1}G	2.76 K ^{2}G; ^{3}G	1.001	
85060.717	85083.03	85.44 M ^{2}G; ^{3}G	3.43 M ^{2}H; ^{3}G	1.041	
85159.641	85168.02	90.41 M ^{2}G; ^{3}H	5.61 M ^{2}H; ^{3}H	0.805	
86028.099	85974.94	99.40 K ^{2}H; ^{3}H	0.29 K ^{2}G; ^{1}G	0.801	
86211.050	86215.96	49.90 M ^{2}G; ^{3}F	34.78 M ^{4}P; ^{3}F	1.249	
87457.980	87494.83	69.77 M ^{2}G; ^{1}G	19.46 M ^{2}D; ^{1}G	1.003	
90543.971	90500.11	51.57 M ^{2}H; ^{1}G	23.57 M ^{2}D; ^{1}G	1.005	

Continued

J = 5					
3162.966	3129.47	99.95 B ^{4}F; ^{5}F	0.04 B ^{2}G; ^{3}G	1.401	1.28?
12621.485	12702.6	98.13 C ^{3}H	0.68 B ^{2}H; ^{3}H	1.034	1.02
14655.607	14690.69	62.29 C ^{3}G	36.07 B ^{2}G; ^{3}G	1.200	1.17
16532.983	16569.48	62.99 B ^{2}G; ^{3}G	35.75 C ^{3}G	1.200	1.16
20280.251	20274.02	98.99 B ^{2}H; ^{3}H	0.68 C ^{3}H	1.034	1.01
23391.150	23410.26	99.71 B ^{2}H; ^{1}H	0.12 K ^{2}H; ^{1}H	1.000	1.04
69724.236	69729.28	99.91 K ^{4}F; ^{5}F	0.05 K ^{2}G; ^{3}G	1.401	1.39
72680.856	72672.75	97.24 M ^{4}F; ^{5}H	1.65 M ^{4}F; ^{5}G	1.104	
73223.351	73206.48	53.20 M ^{4}F; ^{5}G	44.80 M ^{4}F; ^{5}F	1.326	
73417.330	73417.60	53.98 M ^{4}F; ^{5}F	44.70 M ^{4}F; ^{5}G	1.339	
75346.306	75383.89	93.06 M ^{4}F; ^{3}H	1.92 M ^{4}F; ^{3}G	1.037	
75854.219	75861.13	92.60 M ^{4}F; ^{3}G	2.03 M ^{2}G; ^{3}G	1.197	
81483.278	81541.61	99.50 K ^{2}G; ^{3}G	0.22 K ^{2}H; ^{3}H	1.200	
84742.170	84771.02	97.89 M ^{2}G; ^{3}I	1.43 M ^{2}H; ^{3}I	0.833	
84896.899	84927.93	90.38 M ^{2}G; ^{1}H	6.46 M ^{2}G; ^{3}G	1.004	
85140.362	85162.11	84.54 M ^{2}G; ^{3}G	3.85 M ^{2}H; ^{3}G	1.192	
85301.938	85308.03	82.79 M ^{2}G; ^{3}H	7.49 M ^{2}G; ^{1}H	1.035	
86091.728	86039.72	97.94 K ^{2}H; ^{3}H	1.74 K ^{2}H; ^{1}H	1.033	
86766.880	86695.84	96.71 K ^{2}H; ^{1}H	1.82 K ^{2}H; ^{3}H	1.001	
88939.995	88915.30	97.24 M ^{2}H; ^{3}I	1.52 M ^{2}G; ^{3}I	0.834	
89053.341	89027.95	92.39 M ^{2}H; ^{1}H	2.50 M ^{2}D; ^{3}G	1.008	
J = 6					
12706.078	12789.28	99.04 C ^{3}H	0.69 B ^{2}H; ^{3}H	1.167	1.27?
19191.326	19194.69	99.15 C ^{1}I	0.45 M ^{2}H; ^{1}I	1.000	0.96?
20363.335	20362.12	99.21 B ^{2}H; ^{3}H	0.69 C ^{3}H	1.167	1.14
72837.581	72833.32	97.72 M ^{4}F; ^{5}H	1.25 M ^{4}F; ^{5}G	1.216	
73499.773	73440.60	98.00 M ^{4}F; ^{5}G	1.26 M ^{4}F; ^{5}H	1.332	
75592.481	75643.20	94.82 M ^{4}F; ^{3}H	1.89 M ^{2}H; ^{3}H	1.167	
84859.580	84883.73	97.83 M ^{2}G; ^{3}I	1.23 M ^{2}H; ^{3}I	1.024	
85415.904	85440.02	91.53 M ^{2}G; ^{3}H	5.15 M ^{2}H; ^{3}H	1.166	
86191.750	86143.63	99.86 K ^{2}H; ^{3}H	0.05 M ^{2}G; ^{3}H	1.167	
86453.764	86471.68	87.34 M ^{2}G; ^{1}I	10.63 M ^{2}H; ^{1}I	1.000	
89005.580	89013.81	97.89 M ^{2}H; ^{3}I	1.26 M ^{2}G; ^{3}I	1.024	
94371.80	94306.91	80.48 M ^{2}H; ^{1}I	8.89 M ^{2}G; ^{1}I	1.000	
J = 7					
73021.143	73024.65	99.28 M ^{4}F; ^{5}H	0.61 N ^{4}F; ^{5}H	1.286	
85004.880	85002.77	98.25 M ^{2}G; ^{3}I	1.01 M ^{2}H; ^{3}I	1.143	
89082.769	89094.38	98.38 M ^{2}H; ^{3}I	0.99 M ^{2}G; ^{3}I	1.143	
J = 8					
	90180.86	99.57 M ^{2}H; ^{3}K	0.43 N ^{2}H; ^{3}K	1.125	

A: 3$d^2$4s^2 configuration; B: 3$d^3$4s configuration; C: 3d^4 configuration; K: 3$d^3$5s configuration; L: 3$d^3$6s configuration; M: 3$d^3$4d configuration; N: 3$d^3$5d configuration; *See text.

Table 2. Fine structure fitted parameters values (in·cm^{-1}) for the even-parity levels of V II (Fit) with their uncertainties in parentheses and for comparison their corresponding *ab initio* values computed by means of the Cowan code (C.C.). See also text.

Config.	$3d^24s^2$		$3d^34s$		$3d^35s$	
	Fit	C.C.	Fit	C.C.	Fit	C.C.
E_{av}	43,799 (94)	43,799^a	19,730 (30)	18,489	84,820 (42)	78,881
F^2 (3d, 3d)	62,037 (199)	60,288	54,057 (66)	54,104	57,330 (90)	55,519
F^4 (3d, 3d)	38,140 (271)	37,703	31,693 (236)	33,596	34,978 (92)	34,544
G^2 (3d, ns)			8144 (43)	8207	1339 (35)	1523
ζ_{3d}	200 (17)	184	156 (10)	157	171 (10)	161
α	50 (1)		50 (1)			
β	−130 (19)		−130 (19)			
T_s			4 (11)			
T_2			−45 (11)			
T_3			−239 (13)			

Config.	$3d^4$		$3d^34d$		$3d^35d$	
	Fit	C.C.	Fit	C.C.	Fit	C.C.
E_{av}	18,687 (13)	17,691	89,766 (32)	83,105	103,174 (351)	100,986
F^2 (3d, 3d)	48,480 (56)	47,503	56,710 (118)	55,559	57,837 (360)	55,725
F^4 (3d, 3d)	28,317 (72)	29,249	33,302 (178)	34,573	32,727 (330)	34,682
ζ_{3d}	138 (9)	131	166 (9)	161	166 (9)	161
ζ_{nd}			11 (6)	9	5 (3)	4
α	50 (1)		7 (1)			
β	−130 (19)		−83 (16)			
T_2	−45 (11)					
T_3	−239 (13)					
F^2 (3d, 4d)			4484 (98)	5238	1910 (82)	1847
F^4 (3d, 4d)			2196 (99)	2230	864 (39)	826
G^0 (3d,4d)			1923 (26)	2155	717 (10)	1247
G^2 (3d, 4d)			1551 (124)	1927	610 (50)	922
G^4 (3d, 4d)			1900 (86)	1449	758 (34)	637

[a] Fixed to the fitted value.

Table 3. Fine structure configuration interaction parameters and for comparison their corresponding *ab initio* values computed by means of the Cowan code (C.C.).

Values of main configuration interaction parameters		Fit	C.C.
$3d^24s^2$ - $3d^34s$	R^2 ($3d3d$, $3d4s$)	−1960 (192)	−4679
$3d^24s^2$ - $3d^4$	R^2 ($4s4s$, $3d3d$)	11869 (82)	11839
$3d^34s$ - $3d^4$	R^2 ($3d4s$, $3d3d$)	−4741 (42)	−6813
$3d^34d$ - $3d^35d$	R^2 ($3d4d$, $3d5d$)	2205 (173)	2606
	R^4 ($3d4d$, $3d5d$)	1853 (253)	1288
$3d^34s$ - $3d^34d$	R^2 ($3d4s$, $3d4d$)	4564 (320)	4109
$3d^4$ - $3d^34d$	R^2 ($3d3d$, $3d4d$)	6185 (380)	8434
	R^4 ($3d3d$, $3d4d$)	3043 (583)	5580
$3d^35s$ - $3d^34d$	R^2 ($3d5s$, $3d4d$)	−320 (70)	−321
$3d^24s^2$ - $3d^34d$	R^2 ($4s4s$, $3d4d$)	−2303 (446)	−2946

Table 4. Predicted singlet, triplet and quintet positions for missing experimental energy levels of the configurations mentioned in **Table 2**.

Configuration	Designation	J value	Energy (cm^{-1})	Composition LS (%)
$3d^4$	^{1}S			
		0	60,212	65.7
$3d^24s^2$	^{1}S			
		0	77,196	89.6
$3d^34d$	(^{4}P) ^{5}F			
		1	84,407	63.7
		2	84,376	65.8
		3	84,427	76.7
		4	84,503	98.0
		5	84,599	98.6
	(^{4}P) ^{5}D			
		0	85,178	91.8
		1	85,221	89.1
		2	85,260	88.2
		3	85,291	89.3
		4	85,313	91.2
	(^{2}G) ^{3}D			
		1	86,241	52.5
		2	86,359	30.1
		3	86,346	36.9
	(^{4}P) ^{3}F			
		2	86,536 A.G.E.	28.8
		3	86,624	36.8
		4	86,806	44.3
	(^{2}P) ^{3}D			
		1	87,969	67.4
		2	88,102	69.5
		3	88,420	41.8
	(^{2}D) ^{3}G			
		3	88,968	47.3
		4	89,005	56.2
		5	89,166	57.2

Continued

(^{2}P) ^{3}F			
	2	89,031	40.4
	3	89,204	35.8
	4	89,386	42.1
(^{2}D) ^{3}F			
	2	89,966	32.8
	3	89,988	31.9
	4	90,015	35.8
(^{2}H) ^{3}K			
	6	89,998	99.2
	7	90,072	97.2
	8	90,180	99.6
(^{2}H) ^{3}G			
	3	90,608	70.3
	4	90,726	68.8
	5	90,813	71.5
(^{2}D) ^{3}P			
	0	90,707	59.6
	1	90,840	56.7
	2	91,075	48.3
(^{2}D) ^{3}D			
	1	91,494	42.8
	2	91,440	35.9
	3	91,354	44.5
(^{2}H) ^{3}H			
	4	91,203	85.1
	5	91,278	86.1
	6	91,351	87.2
(^{2}D) ^{1}S			
	0	94,473	71.6
(^{2}P) ^{1}P			
	1	87,655	51.5
(^{2}D) ^{1}P			
	1	89,006	49.4
(^{2}D) ^{1}D			
	2	90,040	67.8
(^{2}P) ^{1}D			

Continued

		2	92,624	59.6
	(^{2}P) ^{1}F	3	88,207	36.4
	(^{2}D) ^{1}G	4	93,122	31.1
	(^{2}H) ^{1}K	7	90,605	97.8
$3d^35s$				
	(^{2}P) ^{3}P	0	84,728	98.8
		1	84,741	94.9
		2	84,793	88.1
	(^{2}D) ^{3}D	1	85,873	49.8
		2	85,809	68.5
		3	85,888	76.6
	(^{2}F) ^{3}F	2	96,784	99.8
		3	96,740	99.0
		4	96,690	99.8
	(^{2}P) ^{1}P	1	85,233	68.0
	(^{2}F) ^{1}F	3	97,299	98.8

A.G.E.: already given experimentally.

A good fit, with a root mean square uncertainty of 6.2 MHz was obtained. The values of the model space hfs parameters, quoted with their uncertainties, are presented in **Table 5**. In order to check the validity of these fitted parameters we have compared some of them to those computed using values obtained by means of the Cowan code. For example one can use the well-established relation $a_{nl}^{\kappa k}(\text{MHz}) = 2\mu_0\mu_B\mu_I \left\langle r^{-3}\right\rangle_{nl}^{\kappa k} \big/ 4\pi I = 95.4128 g_I \left\langle r^{-3}\right\rangle_{nl}^{\kappa k}$. Using the values of line 2 of **Table 6**, knowing that the nuclear spin and magnetic dipole moment of ^{51}V are equal respectively to 7/2 and 5.1485 μ_{n} one gets the a_{3d}^{01} values of line 3 of **Table 6** which are on the whole close to the experimental ones, located in line 1 of the same Table. This confirms the well-founded basis of our work.

To check the value of the most influential hfs-deduced parameter, $a_{4s}^{10}\left(3d^34s\right)$, it is interesting to compare the ratio $\frac{a_{4s}^{10}\left(3d^44s\right)}{a_{4s}^{10}\left(3d^34s\right)} = \frac{2535}{4519.76} = 0.56$ relative to V I [13] and V II (this work) with $\frac{a_{4s}^{10}\left(3d^34s\right)}{a_{4s}^{10}\left(3d^24s\right)} = \frac{-487}{-836.27} = 0.58$ relative to Ti I [14] and Ti II [7]. Since these ratios are very close for these two neighbour elements in the Periodic Table, we can conclude that the deduced $a_{4s}^{10}\left(3d^34s\right)$ value for V II is really satisfactory. To extract magnetic dipole A-values from experimental hfs splitting the electric quadrupole hfs B factors preferably were fixed deliberately to zero in [12] because the electric quadrupole moment of ^{51}V is small: −0.05b. In this case it is not useful to compute $b_{nl}^{\kappa k}$ values since it is not possible to make comparisons between experimental and theoretical $b_{nl}^{\kappa k}$ values.

In **Table 7** we have listed the measured hfs constants A given in MHz, used in our fitting procedure. In this

Table 5. The fitted hfs many-body parameter values in MHz for the model space $(3d + 4s)^4$. The uncertainties given in parentheses are the standard deviations.

a_{3d}^{01}	498.71 (6.62)	a_1	177.04 (6.45)
a_{3d}^{12}	469.24 (23.02)	a_2	51.34 (1.87)
a_{3d}^{10}	−14.86 (9.33)	a_3	34.17 (1.24)
a_{4s}^{10}	4519.76 (130.78)	a_9	813.26 (36.93)
a_{IC}^{12}	44.50 (19.81)	a_{11}	−3617.15 (135.90)

$a_4 = a_5 = a_6 = a_7 = a_8 = a_{10} = 0.00$ (fixed).

Table 6. Comparison between fitted and calculated hfs many-body parameter a_{3d}^{01} in MHz. Radial integrals are computed by means of the pseudo-relativistic Cowan code.

Parameter	$3d^2 4s^2$	$3d^3 4s$	$3d^4$
a_{3d}^{01} (Fit) (MHz)	427.90	357.09	286.27
$<r^{-3}>_{3d}$ (a.u.)	3.018	2.615	2.233
a_{3d}^{01} (Cal) (MHz)	423.58	367.02	313.41

Table 7. Our computed hfs A-constants of V II (in MHz), compared with those obtained experimentally by Armstrong *et al.* [10].

Energy (cm^{-1})	Designation [1]		A_{exp} (MHz) [10]	A_{cal} (MHz) This work
J = 1				
18269.49	$3d^4$	a ^3D	−38.51	−36.48
32299.27	$3d^4$	d ^3P	−73.33	−69.03
J = 2				
13490.89	$3d^4$	b ^3F	481.96	480.84
13594.73	$3d^3 4s$	a ^5P	1096.69	1098.88
18293.88	$3d^4$	a ^3D	488.08	453.85
30267.47	$3d^4$	d $^3F^*$	397.31	424.89
30673.08	$3d^3 4s$	c $^3F^*$	−250.92	−269.78
32040.64	$3d^4$	d ^3P	0 (fixed)	−2.72
44657.94	$3d^2 4s^2$	c ^1D	365.79	379.22
J = 3				
13542.67	$3d^4$	b ^3F	250.91	255.18
13741.61	$3d^3 4s$	a ^5P	840.96	850.03
16340.97	$3d^3 4s$	b ^3G	138.66	148.39
18353.88	$3d^4$	a ^3D	502.93	494.22
26839.77	$3d^4$	a ^1F	301.10	293.02
30306.38	$3d^4$	d $^3F^*$	332.71	331.54
30641.76	$3d^3 4s$	c $^3F^*$	414.24	422.43
34228.82	$3d^3 4s$	b ^1F	355.08	352.80

Continued

J = 4				
13608.96	$3d^4$	b ^3F	171.4	174.57
16421.51	$3d^34s$	b ^3G	423.32	416.55
30318.55	$3d^4$	d $^3F^*$	434.52	394.42
30613.92	$3d^34s$	c $^3F^*$	591.70	623.83
38517.06	$3d^24s^2$	e ^3F	276.67	263.47
J = 5				
14655.63	$3d^4$	a ^3G	436.10	452.52
16533.00	$3d^34s$	b ^3G	498.41	495.91

*: See text.

Table we inserted also our computed values which confirm totally the Armstrong, Rosner and Holt experimental data [12] which are sometimes different from those of Arvidsson [15]. As regards the $3d^24s^2$ e $^3F_4$ (38517.06 cm^{-1}) hfs value we reject A= −351.28 and we keep A= 276.67 MHz since two values were proposed in [12] (owing to an unavoidable ambiguity in $\Delta J = 0$ transitions).

3. Conclusion

Parametric fs studies including configuration interactions have been carried out for five interacting configurations of V II. We furthermore propose predicted energy level values for missing experimental ones up to 100,000 cm^{-1} for further investigations. One can also note that calculated Landé g_J-factors were also in good agreement with the experimental ones. Unfortunately the latter are not as numerous as we might have expected and thus our work to check level assignments became more difficult. We give for the first time the hfs many-body parameter values with good accuracy for the model space $(3d + 4s)^4$, taking advantage of the accurate work done in [10]. This provides better predictions for still unknown levels. The conclusive comparison between the experimental and calculated hfs A-constants, given in **Table 7**, provides a good check on the quality of the wave functions obtained by the least squares fit of the fine structure, used to determine the expansions of hfs A-constants in intermediate coupling. Very recently the spectrum of V II has been recorded by FTS and thirty-nine of the additional eighty-five high levels published by Iglesias *et al.* [3] have been confirmed or revised, and four of their missing levels have been found [16] as regards even-parity levels. One can note in our **Table 1** a total agreement with the assignments of these four new levels given in this interesting work.

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