

# Fine structure parametric analysis of the $f^3ds^2 + f^3d^2s$ configurations in U I

A. Petit<sup>a</sup>

CE Saclay, DCC/DPE/SPEA/SPS, 91191 Gif-sur-Yvette Cedex, France

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**Abstract.** The aim of the present work is a reanalysis of the fine structure (fs) of the lower levels up to  $24000 \text{ cm}^{-1}$  on the basis of the two lowest configurations of uranium without a truncation of the core in the case of the second configuration. This interpretation has been performed using Cowan's code which can manage such configurations without restriction. The average deviation of  $53 \text{ cm}^{-1}$  for 155 experimental values demonstrates a good quality of the fs fit. All fs parameters are in good agreement with theoretical predictions and existing empirical values and are obtained with a good precision ( $< 10\%$ ).

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31.15.Ar Ab initio calculations

## 1 Introduction

A lot of experimental data on uranium have been accumulated since 1975 for the project of laser isotope separation (Atomic Vapour Laser Isotope Separation, "AVLIS"). Unfortunately, only a few data have been allowed to be published. Nevertheless, recently a parametric interpretation of the hyperfine structure (hfs) constants has been made [1] on the basis of the fine structure analysis of Guyon [2]. The conclusion of [1] was that the interpretation of hfs constants A and B, obtained on a limited basis of the only  $5f^36d7s^2$  configuration, was reasonably satisfying for low lying levels ( $< 15000 \text{ cm}^{-1}$ ), considering the proximity of the neglected configuration ( $5f^36d^27s$ ) which perturbs a number of levels.

Guyon [2] obtained a parametric Condon-Slater-Racah representation of the fine structure (fs) of the lower levels up to  $15000 \text{ cm}^{-1}$  on the basis of the two lowest configurations in interaction ( $f^3ds^2 + f^3(^4I)d^2s$ ). The core  $f^3$  of  $f^3d^2s$  was restricted to the only term  ${}^4I$ , due to the limits of the computer facilities available in 1974.

Unfortunately, the matrices of the structure coefficients (calculated in LS coupling for the interacting configurations constructed by Guyon [2]) have not been maintained; for this reason, a representation on the basis of the only  $f^3ds^2$  configuration has been used in [1] with the corresponding set of fs parameters given in [2]. If we want to take into account both configurations, the truncation of the core is not satisfying, at least for the lower level  $J$  values.

The aim of the present work is a reanalysis of the fine structure of the lower levels up to  $24000 \text{ cm}^{-1}$  on the basis of the two lowest configurations of uranium without

a truncation of the core in the case of the second configuration. This interpretation has been performed using Cowan's code [3] which can manage such configurations without restriction.

## 2 Parametric interpretation of the energy levels in the odd configurations $5f^36d7s^2 + 5f^36d^27s$

Cowan's code package (RCN, RCN2, RCG and RCE) has been used for the analysis. No details on these codes are given in the present paper; but they can be found in [3]. All calculations have been performed on an IBM Risk (IBM RS-6000-590) computer. Calculations have been done in LS representation.

### 2.1 Parameters

There are 8 radial parameters [ $F^2(f, f); F^4(f, f); F^6(f, f); F^2(f, d); F^4(f, d); G^1(f, d); G^3(f, d)$  and  $G^5(f, d)$ ] for the electrostatic interaction in the configuration  $5f^36d7s^2$ , 12 [ $F^2(f, f); F^4(f, f); F^6(f, f); F^2(d, d); F^4(d, d); F^2(f, d); F^4(f, d); G^1(f, d); G^3(f, d); G^5(f, d); G^3(f, s); G^2(d, s)$ ] in the  $5f^36d^27s$  and 2 parameters for average energy (eav ( $f^3ds^2$ ) and eav ( $f^3d^2s$ )) of the 2 configurations. Two spin orbit parameters ( $\zeta_f, \zeta_d$ ) of the  $f$  and  $d$  electrons for each configuration. Three electrostatic interactions between the two configurations  $R^2(fs, fd)$ ,  $R^3(fs, df)$  and  $R^2(ds, dd)$ . The total number of parameters for the two complete configurations is 29. Effective parameters as  $\alpha, \beta, \gamma$  for  $f$  electrons and  $\alpha, \beta, T2(d)$  for  $d$  electrons have been introduced in the present optimization.

<sup>a</sup> e-mail: apetit@cea.fr

## 2.2 Optimization of the fine structure parameters

Only main results are given here to show the procedure used in the present work for the optimization of all parameters. Results have been obtained using the RCE program. We have worked in 5 steps:

a) Only levels for which assignments have been given by Blaise [4] have been taken into account. This represents 69 levels. A few levels have been excluded from the fit just because of large deviations ( $> 120 \text{ cm}^{-1}$ ) in the difference between calculated and observed values for energy levels. These levels are

$$\begin{aligned} J = 0 : & 5988; & J = 3 : & 10819; \\ J = 4 : & 4453, 11558; & J = 5 : & 11633; \\ J = 6 : & 13402; & J = 7 : & 13567; \\ J = 8 : & 14501, 14842, 16244, 17428; \\ J = 9 : & 13535, 18511, 19297, 19509; \\ J = 11 : & 23673. \end{aligned}$$

Then ratios between parameters for the  $f^3d^2s$  configuration have been fixed in order to reduce the number of free parameters:

$$\begin{aligned} F^4(f, f)/F^2(f, f) &= 0.786 \text{ (close to the value recommended by [5])}, \\ F^4(d, d)/F^2(d, d) &= 0.641 \text{ (close to the calculated value given in [5])}, \\ F^4(f, d)/F^2(f, d) &= 0.583 \text{ (close to the calculated value given in [5])}, \\ G^3(f, d)/G^1(f, d) &= 0.584 \text{ (arbitrary fixed)} \end{aligned}$$

ratios  $R^2(fs, fd)/R^3(ds, dd)$  and  $R^2(ds, dd)/R^3(ds, df)$  have been fixed according to the values given in [5].

Results are given in column [a] of Table 1.

b) Progressively, more levels have been included into the least square fitting process up to 116, but with the same fixed ratios. Results for this fit are given in column [b] of Table 1, the average deviation in  $55 \text{ cm}^{-1}$ .

c) Using the same set of levels, all the 27 parameters have been let free. In this case the average deviation is  $54 \text{ cm}^{-1}$  and results are presented in column [c] of Table 1. But ratios of configuration interaction integrals have been kept fixed.

d) Then progressively, more levels have been introduced up to 155. Results are given in column [d] of Table 1. The average deviation is  $53 \text{ cm}^{-1}$ , and all parameters have been determined with a precision better than 10%. As in c), ratios of configuration interaction integrals have been kept constant.

e) Configuration interaction parameters have been let free and effective parameters like  $\alpha$ ,  $\beta$ ,  $\gamma$  have been introduced;  $\gamma(f)$  for  $f^3ds^2$ ;  $\gamma(f)$  and  $T2(d)$  for  $f^3d^2s$  have been held fixed to zero. Results are given in column [e] of Table 1. The average deviation is  $46 \text{ cm}^{-1}$  for 183 levels. Of course, standard average deviation is a little better than other cases. But parameter values are not significantly different. All parameters have been determined

with a precision better than 10% excepted for  $F^4(d, d)$  and  $R^3(fs, df)$  parameters and effective parameters, no significative values have been obtained for  $\beta$  parameters. Only  $\alpha(f, f)$  for the configuration  $f^3ds^2$  ( $12 \pm 3 \text{ cm}^{-1}$ ) and  $\alpha(d, d)$  for the configuration  $f^3d^2s$  ( $34 \pm 9 \text{ cm}^{-1}$ ) are well determined.

## 3 Discussion

Since results with the introduction of effective parameters are not significantly different, we have taken the column [d] of Table 1 as final results for the discussion.

### 3.1 Spin orbit coupling constants

As predicted by [5],  $\zeta_f$  spin orbit coupling constants are almost the same for both configurations. HFR values from [5] are quite close to empirical values; a subtractive correction of  $50-70 \text{ cm}^{-1}$  is consistent with the prediction of [5]. For both configurations  $f^3ds^2$  and  $f^3d^2s$ , present empirical values ( $1734 \pm 6 \text{ cm}^{-1}$  and  $1740 \pm 8 \text{ cm}^{-1}$ ) are comparable to Guyon's values ( $1759 \pm 14 \text{ cm}^{-1}$  and  $1781 \pm 40 \text{ cm}^{-1}$ ).

The  $\zeta_d$  spin orbit coupling constants are much more sensitive than  $\zeta_f$  to the nature of other electrons in the configuration. For the configuration  $f^3ds^2$ , our empirical value ( $1303 \pm 17 \text{ cm}^{-1}$ ) is different from HFR value given in [5]:  $1519 \text{ cm}^{-1}$ , but in agreement with the experimental value of [2]:  $1213 \pm 39 \text{ cm}^{-1}$ . For the other configuration  $f^3d^2s$ , our empirical value ( $1169 \pm 16 \text{ cm}^{-1}$ ) is different from Guyon's value ( $1464 \pm 70 \text{ cm}^{-1}$ ), but consistent with a subtractive correction of  $\#200 \text{ cm}^{-1}$  between HFR and empirical values as observed in the other configuration. In fact, the high value given by Guyon [2] is only due to the truncation of the core  $f^3$  restricted to the multiplet  ${}^4I$  and there is no need to take into account pseudo configuration interaction operators as suggested in [5].

### 3.2 Slater integrals

$-F^k$  integrals

Values of  $F^k$  ratios are given in Table 2 for comparison with HFR values [5] and empirical values from Guyon [2].

The ratio of  $F^4(f, f)/F^2(f, f)$  ( $= 0.76$ ) fit both configurations corresponds to the value recommended by Rajnak (0.74-0.78) [5]. The ratio of  $F^6(f, f)/F^2(f, f)$  for the  $f^3d^2s$  configuration ( $0.82 \pm 0.1$ ) is different from Rajnak prediction: 0.55-0.56, but this is certainly due to the determination of  $F^6(f, f)$  which is less precise in this case. These ratios are comparable to the values obtained by Carnall *et al.* [6] in the case of  $\text{Bk}^{3+}$  ( $5f^9$ ):  $F^4/F^2 = 0.737$ ;  $F^6/F^2 = 0.559$  and of  $\text{Cf}^{3+}$  ( $5f^{10}$ ):  $F^4/F^2 = 0.741$ ;  $F^6/F^2 = 0.557$  and by Conway [7] for the configuration  $f^8s^2$  of  $\text{CmI}$ :  $F^4/F^2 = 0.762$ ;  $F^6/F^2 = 0.551$ .

All predicted values of  $F^4(f, d)/F^2(f, d)$  are nearly constant and close to the HFR values. Our value of

**Table 1.** Fine structure parameter values in  $\text{cm}^{-1}$ . Guyon's experimental results and Rajnak's *ab initio* results are also given for comparison; columns indicated as [a], [b], [c], [d] and [e] correspond to the different optimizations given in Section 2.2.

	F. Guyon [2]	K. Rajnak [5]	This work [a]	This work [b]	This work [c]	This work [d]	This work [e]
eav $f^3ds^2$			26213 (126)	26160 (64)	26053 (121)	26025 (98)	26342 (99)
$F^2(f, f)$	44501	68573	42688 (782)	42554 (478)	42526 (496)	42613 (381)	43891 (344)
$F^4(f, f)$	29898	44317	32889 (1449)	32545 (681)	32436 (708)	32181 (567)	32431 (608)
$F^6(f, f)$	32896	32357	25084 (1705)	24597 (1003)	24823 (1065)	24720 (794)	23128 (664)
$\alpha$						12 (3)	
$\beta$						-73 (111)	
$\gamma$						0	
$\zeta_f$	1759 (14)	1808	1736 (10)	1735 (7)	1735 (7)	1734 (6)	1723 (6)
$\zeta_d$	1219 (39)	1519	1283 (26)	1299 (18)	1292 (20)	1303 (17)	1270 (15)
$F^2(f, d)$	14595 (630)	25079	16860 (412)	16692 (238)	16412 (366)	16381 (313)	16600 (284)
$F^4(f, d)$	7761 (1039)	13350	9488 (679)	9658 (448)	9586 (464)	9748 (408)	10938 (328)
$G^1(f, d)$	7455 (210)	16192	8010 (132)	8057 (91)	8019 (101)	8031 (88)	8201 (75)
$G^3(f, d)$	9009 (504)	11494	9242 (323)	9337 (224)	9258 (238)	9100 (212)	9193 (202)
$G^5(f, d)$	3354 (914)	8484	4991 (602)	5397 (418)	5286 (442)	5493 (374)	5903 (298)
eav $f^3d^2s$			41639 (644)	41470 (170)	41581 (222)	41930 (233)	41420 (184)
$F^2(f, f)$	44501	67649	46465 (2092)	45592 (836)	46165 (2425)	48706 (1982)	46912 (1454)
$F^4(f, f)$	29898	43658	36527 (1645)	35842 (657)	36367 (4118)	37103 (2178)	32517 (2165)
$F^6(f, f)$	32896	31938	36619 (9437)	34364 (2036)	35781 (3688)	40032 (3296)	37210 (2461)
$\alpha$						-19 (12)	
$\beta$						447 (377)	
$\gamma$						0	
$F^2(d, d)$	22540	29240	16344 (1022)	17090 (361)	16611 (945)	15979 (411)	16896 (671)
$F^4(d, d)$	13009	18899	10489 (656)	10968 (231)	9938 (2105)	8760 (838)	7750 (1437)
$\alpha$						34 (9)	
$\beta$						-184 (326)	
$T2(d)$						0	
$\zeta_f$	1781 (40)	1787	1738 (21)	1739 (10)	1742 (10)	1740 (8)	1750 (11)
$\zeta_d$	1464 (70)	1343	1167 (42)	1165 (19)	1161 (20)	1169 (16)	1144 (15)
$F^2(f, d)$	14595*	23184	15291 (1789)	14775 (603)	14936 (776)	14181 (436)	13203 (399)
$F^4(f, d)$	5682*	12235	8235 (963)	7956 (325)	7724 (873)	7102 (428)	6922 (362)
$G^1(f, d)$	7420 (200)	15165	8812 (314)	8856 (144)	8638 (252)	8572 (112)	8440 (102)
$G^3(f, d)$	5953*	10614	5151 (184)	5060 (84)	5169 (418)	4938 (323)	4871 (285)
$G^5(f, d)$	2744*	7792	6438 (830)	5832 (425)	5778 (892)	5794 (379)	5837 (340)
$G^3(f, s)$	2100*	3354	2236 (561)	1942 (163)	1919 (247)	1948 (143)	2106 (137)
$G^2(d, s)$	11390 (500)	19432	11522 (1000)	11920 (243)	12040 (374)	11969 (198)	11649 (195)
$R^2(fs, fd)$	-2000*	-9048	-4883 (220)	-4792 (88)	-4477 (322)	-4337 (275)	-5178 (402)
$R^3(fs, df)$	-500*	-2060	-1094 (49)	-1073 (20)	-1073 (72)	-972 (62)	-1343 (309)
$R^2(ds, dd)$	-5087 (1384)	-22396	-12194 (549)	11965 (219)	-11179 (800)	-10830 (688)	-11639 (671)
Levels	68 levels		69	116	116	155	183
Parameters	17		22	22	27	27	35
Standard Dev.	124 $\text{cm}^{-1}$		62 $\text{cm}^{-1}$	55 $\text{cm}^{-1}$	54 $\text{cm}^{-1}$	53 $\text{cm}^{-1}$	46 $\text{cm}^{-1}$

\* Values held fixed.

**Table 2.** Comparison between ratios of  $F^k(5f, 5f)$ ,  $F^k(5f, 6d)$  and  $F^k(6d, 6d)$  integrals.

	$f^3d^2s$	$f^3ds^2$	$f^3d^2s$	$f^3ds^2$	$f^3d^2s$	$f^3ds^2$	$f^3d^2s$	$f^3d^2s$
	$\frac{F^4(f, f)}{F^2(f, f)}$	$\frac{F^4(f, f)}{F^2(f, f)}$	$\frac{F^6(f, f)}{F^2(f, f)}$	$\frac{F^6(f, f)}{F^2(f, f)}$	$\frac{F^4(f, d)}{F^2(f, d)}$	$\frac{F^4(f, d)}{F^2(f, d)}$	$\frac{F^2(f, d)}{F^2(d, d)}$	$\frac{F^4(d, d)}{F^2(d, d)}$
Guyon [2]	0.67	0.67	0.74	0.74	0.53	0.53	0.64	0.58
Rajnak [5]	0.64	0.64	0.47	0.47	0.52	0.53	0.79	0.64
This work	$0.76 \pm 0.07$	$0.75 \pm 0.02$	$0.82 \pm 0.1$	$0.58 \pm 0.02$	$0.50 \pm 0.04$	$0.59 \pm 0.03$	$0.88 \pm 0.05$	$0.54 \pm 0.06$

**Table 3.** Comparison between ratios of  $F^k(5f, 6d)$  and  $G^k(5f, 6d)$  and  $\zeta_f(f, f)$  integrals for both configurations.

	$f^3d^2s$	$f^3ds^2$	$f^3d^2s$	$f^3ds^2$	$f^3d^2s$	$f^3ds^2$	$f^3d^2s$	$f^3ds^2$
	$\frac{G^1(f, d)}{F^2(f, d)}$	$\frac{G^1(f, d)}{F^2(f, d)}$	$\frac{G^3(f, d)}{G^1(f, d)}$	$\frac{G^3(f, d)}{G^1(f, d)}$	$\frac{G^5(f, d)}{G^1(f, d)}$	$\frac{G^5(f, d)}{G^1(f, d)}$	$\frac{\zeta_f}{F^2(f, f)}$	$\frac{\zeta_f}{F^2(f, f)}$
Guyon [2]	0.51	0.51	0.80	1.20	0.37	0.45	0.04	0.04
Rajnak [5]	0.65	0.64	0.70	0.70	0.51	0.52	0.026	0.026
This work	0.60	0.49	0.57	1.13	0.67	0.68	0.035	0.04

$F^2(f, d)/F^2(d, d) = 0.88$  is closer to the value of 0.9-1.0 given by Rajnak [5] in the case of the configuration  $f^2d^2s^2$  in UI than the value given by Guyon [2]: 0.64. Our ratio  $F^4(d, d)/F^2(d, d)$  is in excellent agreement with the value recommended by Guyon [2].

#### - $G^k$ integrals

Our empirical  $G^k$  integral ratios (Tab. 3) confirm the predicted results of [5], excepted the case of the  $G^3(f, d)/G^1(f, d)$  ratio for the configuration  $f^3ds^2$  for which we observe that  $G^3$  is greater than  $G^1$  as found by Guyon [2]; but for the other configuration  $G^1$  is smaller than  $G^3$  as predicted by HFR calculations and Guyon's result. The obtained value of  $G^3(f, s)$ :  $1948 \text{ cm}^{-1}$  is consistent with the value fixed by Guyon [2]:  $2100 \text{ cm}^{-1}$ .

### 3.3 Configuration interaction integrals

All configuration interaction integrals are well determined (better than 10%), when their ratios are held fixed. Our value of  $R^2(ds, d2)$ :  $10830 \pm 688 \text{ cm}^{-1}$  is different from the HFR value ( $22396 \text{ cm}^{-1}$ ) [5] and Guyon's value ( $5087 \pm 1384 \text{ cm}^{-1}$ ) [2]; but compares well to the value found for PaI [8]:  $-15500 \pm 974 \text{ cm}^{-1}$ . In this latter atom, for other integrals ( $R^2(fd, fs)$ ,  $R^3(fd, sf)$ ) ratios with  $R^2(dd, ds)$  have been held fixed according to [5]; so they are in good agreement with our values. Even if ratios of configuration interaction integrals are let free (column [e] of table 1) values obtained for these parameters are not significantly different.

### 3.4 Interpretation of the experiment energy levels—predictions

Results, obtained with parameter values of Table 1, are presented in Table 4: experimental energy values, eigenvalues, difference between experimental and eigenvalues, calculated Lande  $g$  factor, experimental Lande  $g$  factor (all experimental values are from [4]). Then the dominant configuration (determined by summing over all basis states of each configuration), the experimental isotope shift [4], the total angular momentum  $J$  and the percentage composition of the level (3 largest eigenvector components) are given.

155 levels are represented with a standard average deviation of  $53 \text{ cm}^{-1}$ . But some imperfections in wave functions are visible for some levels through the isotope shift

and the Lande  $g$  factor. This is the case for  $\approx 12$  levels among 155. For some of these levels, when two close levels belong to different configurations, an inversion is observed in the assignment of these two levels. This can be seen especially for low  $J$  values, one example is given in Table 4 for the following levels with  $J = 2$ : 13149.733; 13951.627; 14191.0.50 and 15189.753 where two of them are inverted in assignment and for the two others, the dominant configuration is not compatible with the experimental isotopic shift. Our wave functions cannot be checked for all levels since few experimental data (Lande  $g$  factors, isotopic shifts) have been measured for levels  $> 19000 \text{ cm}^{-1}$ .

For levels lower than  $15000 \text{ cm}^{-1}$ , H. Crosswhite and H.M. Crosswhite [9] have shown that the contribution of the  $f^3d^3$  configuration to the eigenvectors for these low levels was less than 1%. Above  $15000 \text{ cm}^{-1}$ , this last configuration can perturb significantly the eigenvectors for some levels; especially, if this configuration, for which only one level has been observed ( $23084 \text{ cm}^{-1}$ ), starts at lower energy than Brewer's prediction ( $21000 \pm 4000 \text{ cm}^{-1}$ ) [10]. This has been already suggested by [5] and can be suspected from the number of extra levels which cannot be interpreted using Table 4 and the list given in [4]. Work is in progress on this subject.

## 4 Conclusion

The average deviation of  $53 \text{ cm}^{-1}$  for 155 experimental values demonstrates a good quality of the fs fit. All fs parameters are in good agreement with theoretical predictions and existing empirical values and are obtained with a good precision (< 10%).

Wave functions reproduce well the isotopic shift and the Lande  $g$  factor for most levels when they are available. The quality of the wave functions will be further tested by an extended analysis of the hyperfine constants for both configurations. A future work will try to take into account the next configuration  $f^3d^3$ . Some experimental work is in progress to identify some new levels belonging to this configuration.

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**Table 4.** Experimental energy values, eigenvalues, difference between experimental and eigenvalues, calculated Lande  $g$  factor, experimental Lande  $g$  factor [4]. Then the dominant configuration, the experimental isotope shift IS [4], the total angular momentum  $J$  and the percentage composition of the level (3 largest eigenvector components of the corresponding eigenvectors). Experimental energy values indicated with  $a^*$  are not taken into account for the fit. The notations are the following:  $5f36d7$  and  $5f36d2$  stand, respectively, for  $5f^3 6d7s^2$  and  $5f^3 6d^27s$  configurations; the state identification is given in 2 parts: the LS label for the  $f^3$  core (in parentheses) and the total LS.

Experimental level ( $\text{cm}^{-1}$ )	Calculated level ( $\text{cm}^{-1}$ )	$D$ (mK)	$g$ (cal.)	$g$ (exp.)	dominant configuration	IS (exp.) (mK)	$J =$	1 <sup>st</sup> component (%)		2 <sup>nd</sup> component (%)		3 <sup>rd</sup> component (%)	
								IS (exp.) (mK)	(%)	IS (exp.) (mK)	(%)	IS (exp.) (mK)	(%)
5988.061*	6236	0	5f36d7	28	.0	28.1	5f36d7 (4f) 3p	14.1	5f36d7 (2p) 3p	14.1	5f36d7 (4f) 5d		
13757	13757	0	5f36d7	.0	54.1	5f36d7 (4s) 5d	17.7	5f36d7 (4f) 3p	9.5	5f36d7 (2d) 1s			
15025.079	15036	-10.573	0	5f36d7	.0	48.8	5f36d7 (4f) 5d	15.3	5f36d7 (4s) 5d	12.4	5f36d7 (2p) 3p		
16568	16568	0	5f36d2	.0	57.4	5f36d2 (4i) 7f	14.3	5f36d2 (4f) 7f	6.5	5f36d2 (2h) 5d			
17949	17949	0	5f36d7	.0	47.8	5f36d7 (4g) 5d	6.1	5f36d7 (4f) 5d	5.4	5f36d7 (2f) 3p			
19160	19160	0	5f36d2	.0	34.5	5f36d2 (4s) 7f	20.5	5f36d2 (4f) 7f	8.0	5f36d2 (4i) 7f			
20240	20240	0	5f36d7	.0	0	5f36d2 (2p) 1s	25.3	5f36d7 (4d) 5d	22.1	5f36d7 (4f) 3p			
21595	21595	0	5f36d7	.0	22.5	5f36d7 (2d) 1s	21.5	5f36d7 (4d) 5d	17.6	5f36d7 (4f) 3p			
21831	21831	0	5f36d2	.0	28.9	5f36d2 (4f) 7f	17.8	5f36d2 (4s) 7f	11.2	5f36d2 (4f) 5d			
21989	21989	0	5f36d2	.0	8.8	5f36d2 (4g) 5d	10.2	5f36d2 (4f) 7f	9.9	5f36d2 (4i) 5d			
22624	22624	0	5f36d7	.0	26.2	5f36d7 (2d) 3p	31.5	5f36d7 (2d) 1s	13.8	5f36d7 (2p) 3p			
23904	23904	0	5f36d2	.0	16.2	5f36d2 (4g) 7f	10.7	5f36d7 (2d) 1s	8.3	5f36d2 (4f) 5d			
10113	-9.480	1.484	1.480	49	1.0	32.0	5f36d7 (4f) 5d	19.8	5f36d7 (4s) 5d	15.9	5f36d7 (2d) 3d		
12056	51.852	0.652	0.570	5f36d7	25	1.0	36.1	5f36d7 (4f) 5f	11.8	5f36d7 (4f) 3d	9.6	5f36d7 (2d) 3d	
13719.061	13651	67.709	1.996	1.830	5f36d7	1.0	59.3	5f36d7 (4f) 5p	9.1	5f36d7 (2d) 3s	8.7	5f36d7 (4f) 3p	
13826.895	13834	-6.970	0.879	5f36d7	1.0	26.6	5f36d7 (4s) 5d	19.0	5f36d7 (4f) 5f	10.0	5f36d7 (2p) 3d		
15045	15045	1.098	5f36d7	1.0	7.5	5f36d7 (4f) 3p	20.1	5f36d7 (4f) 5f	12.6	5f36d7 (2p) 3p			
15999.879*	16285	0.518	5f36d7	-493	1.0	38.0	5f36d7 (4g) 5f	15.6	5f36d7 (4g) 3d	8.1	5f36d2 (4i) 7f		
16304.815*	16506	0.920	5f36d2	1.0	25.3	5f36d2 (4i) 7f	9.7	5f36d7 (4g) 3d	6.9	5f36d2 (4f) 7f			
16304.825*	16684	-0.221	5f36d2	1.0	62.2	5f36d2 (4i) 7g	6.1	5f36d2 (2h) 5f	4.4	5f36d2 (4i) 5f			
17222.983*	17003	0.596	5f36d2	1.0	15.0	5f36d2 (4f) 7g	21.4	5f36d2 (4i) 7f	6.2	5f36d2 (4i) 7g			
17222.983*	17403	0.453	5f36d7	1.0	12.1	5f36d7 (4f) 3d	11.8	5f36d2 (4f) 7g	9.0	5f36d2 (4g) 5f			
18125.037	18162	-37.237	0.603	5f36d7	1.0	14.2	5f36d7 (4g) 3d	15.2	5f36d7 (4f) 3d	9.6	5f36d7 (4d) 5f		
18529	18529	1.014	5f36d7	1.0	29.3	5f36d7 (4s) 3d	18.9	5f36d7 (4f) 3p	8.8	5f36d7 (2p) 3d			
19063	19063	0.857	5f36d7	1.0	15.9	5f36d7 (4d) 5f	12.4	5f36d7 (4g) 5d	6.4	5f36d7 (4s) 5d			
19412	19412	0.981	5f36d2	1.0	25.5	5f36d2 (4s) 7f	14.1	5f36d2 (4f) 7g	13.7	5f36d2 (4f) 7f			
20070	20070	1.009	5f36d7	1.0	17.1	5f36d7 (4g) 5d	7.9	5f36d7 (4d) 5d	7.0	5f36d7 (2g) 3d			
20983	20983	1.588	5f36d2	1.0	12.2	5f36d2 (4f) 7d	6.9	5f36d7 (4d) 5d	5.3	5f36d2 (4f) 7d			
21059	21059	0.700	5f36d7	1.0	8.5	5f36d7 (2p) 3p	11.3	5f36d2 (4f) 7g	6.7	5f36d7 (4s) 5d			
21379	21379	0.763	5f36d7	1.0	13.7	5f36d7 (4d) 5d	13.1	5f36d2 (4f) 7g	6.9	5f36d7 (2p) 3p			
21489	21489	0.886	5f36d2	1.0	10.6	5f36d2 (4f) 7g	11.2	5f36d7 (4d) 5d	5.6	5f36d7 (4g) 5d			
21826	21826	1.066	5f36d2	1.0	3.2	5f36d2 (2d) 3d	12.4	5f36d2 (4f) 7g	10.3	5f36d2 (4f) 7d			
21923	21923	0.772	5f36d2	1.0	19.1	5f36d2 (4f) 7f	12.4	5f36d2 (4f) 7g	6.0	5f36d2 (4i) 5f			
22384	22384	0.981	5f36d7	1.0	15.0	5f36d7 (2d) 3p	20.8	5f36d7 (2p) 1p	10.5	5f36d7 (4f) 5d			
22508	22508	0.889	5f36d2	1.0	10.8	5f36d2 (4i) 5f	11.0	5f36d2 (4i) 5f	6.5	5f36d2 (4i) 3d			
22579	22579	0.923	5f36d2	1.0	8.2	5f36d2 (4f) 5d	12.6	5f36d2 (4s) 7f	12.4	5f36d2 (4f) 7f			

Table 4. (continued)

Experimental level (cm <sup>-1</sup> )	Calculated level (cm <sup>-1</sup> )	D (mK)	<i>g</i> (cal.)	<i>g</i> (exp.)	dominant configuration	IS (exp.) (mK)	<i>J</i> =	1 <sup>st</sup> component (%)	2 <sup>nd</sup> component (%)	3 <sup>rd</sup> component (%)
23204	1.105	5f36d2	1.0	8.8	5f36d2 (4s) 5f	6.6	5f36d2 (4g) 7f	5.3	5f36d2 (4f) 7g	
23624	0.638	5f36d2	1.0	18.1	5f36d2 (4i) 5f	9.7	5f36d2 (4i) 5f	6.4	5f36d2 (4i) 5f	
23668	0.973	5f36d7	1.0	15.6	5f36d7 (2d) 3s	13.9	5f36d7 (2d) 3p	7.8	5f36d7 (2d) 3d	
23778	0.806	5f36d2	1.0	10.7	5f36d2 (4i) 5f	11.2	5f36d7 (2d) 3s	6.5	5f36d2 (4i) 5f	
7191.682	101.498	0.407	0.395	5f36d7	33	2.0	5f36d7 (4i) 5g	13.8	5f36d7 (2h) 3f	5.1
8856.992	8874	-17.594	0.612	0.640	5f36d7	34	2.0	42.2	5f36d7 (4f) 5g	16.4
10708.603	10732	-23.666	1.133	1.010	5f36d7	63	2.0	19.2	5f36d7 (4f) 5d	11.4
11973.586*	11875	0.848	0.915	5f36d7	72	2.0	15.6	5f36d7 (4g) 5g	16.1	5f36d7 (4f) 5g
13149.733*	13304	1.115	1.090	5f36d7	-493	2.0	5.2	5f36d7 (2p) 3p	13.0	5f36d7 (4g) 5g
13951.627*	13839	0.142	0.985	5f36d2	-69	2.0	58.1	5f36d2 (4i) 7h	10.4	5f36d2 (4i) 5g
14191.050*	14144	0.936	0.150	5f36d7	-550	2.0	45.8	5f36d7 (4g) 3f	10.7	5f36d7 (4s) 5d
15189.753	15156	33.438	1.190	1.270	5f36d7	-425	2.0	9.3	5f36d7 (4s) 3d	14.6
15347.918	15372	-24.482	1.402	5f36d7	2.0	24.0	5f36d7 (4f) 5p	15.9	5f36d7 (4f) 5d	12.5
15883.398*	15635	0.960	5f36d7	2.0	14.1	5f36d7 (2h) 3f	8.8	5f36d7 (4f) 3p	8.2	5f36d7 (2g) 1d
15883.398	15907	-23.174	0.721	5f36d7	2.0	11.5	5f36d7 (4f) 3f	13.5	5f36d7 (4g) 5g	8.3
16575.363	16466	109.491	0.911	5f36d2	2.0	15.9	5f36d2 (4i) 7f	16.6	5f36d2 (4i) 5p	9.3
16746.582	16700	46.357	0.890	5f36d2	2.0	14.2	5f36d2 (4i) 7h	21.3	5f36d2 (4i) 7f	9.4
16942.169	16934	8.272	1.033	5f36d7	2.0	14.7	5f36d7 (4s) 5d	7.5	5f36d7 (4f) 5g	6.0
17098.084	17104	-5.607	0.534	5f36d2	2.0	33.4	5f36d2 (4i) 7g	16.0	5f36d2 (4i) 7h	11.1
17268.440*	17696	1.127	5f36d2	2.0	1.6	5f36d2 (2d) 3d	17.7	5f36d7 (4g) 5f	11.6	5f36d2 (4f) 7g
17975	1.096	5f36d7	2.0	28.0	5f36d7 (4g) 5f	9.6	5f36d2 (4f) 7g	5.6	5f36d2 (4s) 7f	
18438.036	18490	-52.174	0.959	5f36d7	2.0	11.2	5f36d7 (2p) 3f	8.0	5f36d7 (4g) 5g	
19461.536	19467	-5.677	0.819	5f36d2	2.0	15.5	5f36d7 (4d) 5g	9.9	5f36d7 (2p) 3f	
19719.475	19683	36.338	0.923	5f36d7	2.0	14.8	5f36d2 (4f) 7g	11.0	5f36d2 (4i) 7h	
20098	0.464	5f36d2	2.0	18.6	5f36d7 (4d) 5f	7.6	5f36d7 (2d) 3f	5.3	5f36d2 (4s) 7f	
20367	1.089	5f36d7	2.0	29.7	5f36d2 (4f) 7h	14.6	5f36d2 (4i) 7h	8.0	5f36d7 (4g) 3d	
20453	1.243	5f36d2	2.0	4.2	5f36d7 (4f) 3p	10.7	5f36d7 (4g) 5d	6.4	5f36d2 (4f) 7g	
20661	1.002	5f36d2	2.0	6.9	5f36d2 (4f) 7p	6.5	5f36d7 (4d) 5f	5.2	5f36d2 (4i) 5g	
20866	1.017	5f36d7	2.0	14.3	5f36d2 (4i) 5g	8.9	5f36d2 (4f) 7p	5.0	5f36d2 (4i) 5g	
21243	1.040	5f36d7	2.0	15.1	5f36d2 (4i) 3f	7.5	5f36d2 (4i) 5g	7.4	5f36d2 (4i) 7g	
21367	1.105	5f36d7	2.0	9.5	5f36d7 (2d) 3f	6.7	5f36d7 (4s) 3d	6.1	5f36d7 (4d) 5d	
21578	0.847	5f36d7	2.0	8.3	5f36d7 (2g) 1d	7.7	5f36d7 (4g) 5d	6.6	5f36d7 (2g) 3f	
21799	1.071	5f36d7	2.0	13.1	5f36d2 (4i) 5g	6.7	5f36d2 (4i) 5f	5.8	5f36d7 (4g) 5d	
22022	1.241	5f36d2	2.0	9.8	5f36d7 (4f) 3d	5.9	5f36d7 (4d) 5d	5.0	5f36d2 (4i) 3p	
222161	1.105	5f36d2	2.0	4.8	5f36d7 (4g) 5d	11.8	5f36d2 (4f) 7f	6.6	5f36d2 (4f) 7g	
22425	1.045	5f36d7	2.0	1.8	5f36d2 (4f) 3f	6.4	5f36d2 (4f) 7d	4.2	5f36d7 (2d) 3p	
22515	0.923	5f36d2	2.0	11.8	5f36d7 (2d) 3p	10.5	5f36d2 (4f) 7g	7.9	5f36d7 (4d) 5g	
22572	1.355	5f36d2	2.0	2.4	5f36d2 (4g) 5g	7.8	5f36d2 (4i) 5f	4.8	5f36d2 (4i) 3f	
22931	1.125	5f36d2	2.0	20.7	5f36d2 (4f) 7g	7.4	5f36d2 (4f) 7p	6.8	5f36d2 (4s) 7p	
23044	0.898	5f36d7	2.0	4.9	5f36d2 (4s) 7f	6.1	5f36d2 (4f) 7f	6.0	5f36d2 (4i) 7f	
23126	1.009	5f36d2	2.0	5.1	5f36d7 (2p) 1d	12.6	5f36d7 (4d) 5g	10.5	5f36d7 (4d) 5f	
23255	0.789	5f36d2	2.0	0	5f36d2 (2f) 3d	8.6	5f36d7 (4f) 3f	5.9	5f36d7 (4d) 5d	
23411	0.824	5f36d2	2.0	19.2	5f36d2 (4g) 7h	8.2	5f36d2 (4f) 7f	6.4	5f36d2 (4s) 7f	
				6.8	5f36d2 (4i) 5g	5.7	5f36d2 (4i) 5g	5.5	5f36d2 (4i) 5f	

Table 4. (continued)

Experimental level (cm <sup>-1</sup> )	Calculated level (cm <sup>-1</sup> )	D (mK)	g (cal.)	g (exp.)	dominant configuration	IS (exp.) (mK)	J =	1 <sup>st</sup> component (%)	2 <sup>nd</sup> component (%)	3 <sup>rd</sup> component (%)			
23648	0.942	5f36d2	2.0	4.7	5f36d2 (4i) 3f	5.9	5f36d2 (4g) 7h	4.0	5f36d7 (2g) 3d				
23708	1.222	5f36d2	2.0	11.1	5f36d2 (4f) 7f	8.0	5f36d2 (4g) 7h	6.8	5f36d2 (4f) 7d				
23831	0.690	5f36d2	2.0	23.3	5f36d2 (4i) 5g	7.7	5f36d2 (4i) 5g	4.3	5f36d2 (4i) 3f				
3868.486	-3.318	0.696	0.690	5f36d7	12	3.0	30.7	5f36d7 (4i) 5h	24.5	5f36d7 (4i) 3g	9.4		
7103.921	7071	33.366	0.781	0.775	5f36d7	24	3.0	3 0.8	5f36d7 (4i) 5g	26.9	5f36d7 (4i) 5h	11.5	
8878.547	8873	5.002	0.656	0.640	5f36d7	-19	3.0	39.8	5f36d7 (4i) 5h	14.5	5f36d7 (4i) 5g	13.7	
10540.266	10518	21.800	1.089	1.075	5f36d7	39	3.0	6.4	5f36d7 (4f) 3f	13.9	5f36d7 (4f) 7h	9.8	
10819.935*	11068	0.383	0.435	5f36d2	-494	3.0	47.1	5f36d2 (4i) 7i	10.7	5f36d2 (4f) 7i	10.3		
11788.926	11751	37.727	0.969	0.950	5f36d7	54	3.0	52.2	5f36d7 (4f) 5g	9.7	5f36d7 (2d) 3f	5.5	
11943.944	12003	-59.075	0.852	0.895	5f36d7	36	3.0	27.1	5f36d7 (4i) 3g	29.5	5f36d7 (4i) 5g	7.9	
13433.173	39.610	0.738	0.790	5f36d7	-59	3.0	29.3	5f36d7 (4g) 5h	7.2	5f36d2 (4i) 7i	5.6		
13936.705	13999	-62.661	1.046	5f36d7	64	3.0	6.8	5f36d7 (2g) 3d	12.1	5f36d7 (4f) 5f	8.2		
14281.945	14196	86.129	0.783	0.980	5f36d2	-213	3.0	35.0	5f36d2 (4i) 7h	7.4	5f36d2 (4i) 5g	7.0	
14576.689	14614	-36.998	0.528	0.528	5f36d2	53	3.0	37.6	5f36d2 (4i) 7i	12.3	5f36d2 (4f) 5h	5.4	
14774.231	14738	36.288	1.009	5f36d7	-46	3.0	7.7	5f36d7 (4f) 3d	9.7	5f36d7 (4f) 5p	7.1		
15169.850*	15011	1.003	5f36d7	-60	3.0	16.6	5f36d7 (4f) 5f	12.4	5f36d7 (4g) 5h	9.4	5f36d7 (4g) 3f	5p	
15560.498*	15247	0.908	5f36d2	-404	3.0	27.3	5f36d7 (4g) 5g	11.3	5f36d7 (2h) 3g	5.0	5f36d2 (4i) 7h		
15906.822	15849	57.737	1.224	5f36d7	3.0	20.8	5f36d7 (4f) 5d	8.3	5f36d7 (4g) 5g	8.3	5f36d7 (4s) 5d		
15986.814	16031	-44.288	1.216	5f36d7	3.0	21.7	5f36d7 (4s) 5d	6.7	5f36d7 (4f) 5d	6.5	5f36d7 (4f) 3d		
16530	1.263	5f36d2	3.0	15.3	5f36d2 (4i) 5f	14.2	5f36d2 (4i) 7f	9.8	5f36d7 (4s) 5d				
16983.306*	16864	1.048	5f36d2	-425	3.0	21.9	5f36d2 (4i) 7g	12.8	5f36d2 (4i) 5g	8.5	5f36d2 (4i) 5g		
17261.703	17298	-36.097	0.605	5f36d2	3.0	7.7	5f36d2 (4i) 5h	17.1	5f36d2 (4f) 7i	11.4	5f36d2 (4i) 7h		
17412	1.155	5f36d7	3.0	19.5	5f36d7 (4f) 5p	8.8	5f36d7 (4g) 5f	7.1	5f36d7 (4f) 3g				
17744	0.559	5f36d2	3.0	21.9	5f36d2 (4f) 7i	14.8	5f36d2 (4i) 7h	8.7	5f36d2 (4i) 7i				
18519.798*	18275	0.721	5f36d2	3.0	9.8	5f36d2 (4i) 5h	15.5	5f36d2 (4i) 7h	7.4	5f36d2 (4i) 7i			
18773.292	18700	73.285	0.933	5f36d7	3.0	5.9	5f36d7 (4d) 3g	11.9	5f36d7 (4f) 3g	7.2	5f36d7 (4g) 3g		
18947.691	19012	-63.983	1.060	5f36d7	3.0	9.5	5f36d7 (4f) 3g	10.5	5f36d7 (4f) 5d	9.4	5f36d7 (4f) 5f		
19246.546	19159	87.083	1.129	5f36d7	3.0	4.7	5f36d7 (2d) 3g	10.5	5f36d2 (4f) 7g	6.1	5f36d7 (4f) 5p		
19394.235*	19266	1.034	5f36d2	3.0	12.4	5f36d2 (4f) 7g	10.6	5f36d2 (4i) 5h	6.0	5f36d7 (4d) 5g			
19677.080*	19533	0.840	5f36d2	3.0	12.2	5f36d2 (4i) 5h	8.4	5f36d2 (4g) 7i	6.3	5f36d2 (4f) 7h			
19726	1.084	5f36d7	3.0	2.9	5f36d7 (4s) 3d	6.6	5f36d7 (4d) 5g	4.9	5f36d7 (4g) 5f				
19753	1.051	5f36d2	3.0	10.6	5f36d2 (4s) 7f	15.5	5f36d2 (4f) 7g	3.6	5f36d2 (4i) 5h				
20018	1.066	5f36d7	3.0	20.4	5f36d7 (4g) 5f	6.8	5f36d7 (4f) 3f	5.1	5f36d2 (4g) 7i				
20068	68.525	0.819	5f36d2	3.0	22.5	5f36d2 (4g) 7i	3.9	5f36d7 (4g) 5f	3.5	5f36d2 (4i) 7g			
20394	-48.602	1.081	0.980	5f36d7	-167	3.0	7.2	5f36d7 (2h) 3f	8.5	5f36d7 (4s) 3d	5.5	5f36d7 (4f) 3f	
20500	0.927	5f36d2	3.0	6.2	5f36d2 (4i) 5h	9.3	5f36d2 (4g) 7i	8.4	5f36d2 (4i) 7f				
20781.403	20726	54.933	0.910	5f36d2	3.0	17.9	5f36d2 (4f) 7h	4.5	5f36d7 (2d) 3f	4.5	5f36d2 (4i) 5h		
20345.095	20864	12.399	1.172	5f36d2	3.0	5.1	5f36d7 (4g) 3f	4.8	5f36d2 (4f) 7g	4.2	5f36d7 (4g) 5f		
21086	1.236	5f36d7	3.0	4.4	5f36d7 (4d) 5d	7.3	5f36d7 (4g) 5d	6.7	5f36d2 (4f) 7p				
21207	0.870	5f36d2	3.0	12.7	5f36d2 (4i) 5g	12.6	5f36d2 (4i) 3g	5.0	5f36d2 (4i) 5h				
21293	1.217	5f36d2	3.0	8.6	5f36d2 (4f) 7p	4.2	5f36d2 (4s) 7p	4.0	5f36d2 (4i) 7g				
21642	0.949	5f36d2	3.0	10.4	5f36d2 (4i) 7h	6.3	5f36d2 (4i) 5h	5.9	5f36d2 (4i) 5h				
21755	0.959	5f36d7	3.0	12.0	5f36d7 (2h) 3g	9.0	5f36d7 (4f) 3d	4.9	5f36d7 (2p) 1f				
21929	0.956	5f36d2	3.0	4.6	5f36d2 (4f) 5h	5.0	5f36d2 (4i) 7h	4.7	5f36d2 (4i) 5h				

Table 4. (continued)

Experimental level (cm <sup>-1</sup> )	Calculated level (cm <sup>-1</sup> )	<i>D</i> (mK)	<i>g</i> (cal.)	<i>g</i> (exp.)	dominant configuration	IS (exp.) (mK)	<i>J</i> =	1 <sup>st</sup> component (%)	2 <sup>nd</sup> component (%)	3 <sup>rd</sup> component (%)				
21973	1.020	5f36d2	3.0	0.1	5f36d2 (2g) 1f	6.1	5f36d2 (4f) 7h	5.4	5f36d7 (2h) 3g					
22075	1.028	5f36d7	3.0	8.7	5f36d7 (4g) 5d	12.4	5f36d7 (4g) 5f	4.8	5f36d7 (2d) 3g					
22552	1.021	5f36d2	3.0	0	5f36d2 (2f) 1f	5.4	5f36d7 (4g) 3g	5.2	5f36d7 (2h) 1f					
22678.342*	1.053	0.830	5f36d2	-491	3.0	4.9	5f36d2 (4i) 3g	5.2	5f36d2 (4f) 7g					
22839	1.037	5f36d2	3.0	2.9	5f36d7 (2p) 3d	6.1	5f36d2 (4i) 5h	2.9	5f36d7 (2p) 1f					
22948	0.999	5f36d2	3.0	5.6	5f36d7 (2h) 1f	3.4	5f36d2 (4i) 5g	3.2	5f36d2 (4i) 3g					
23067	0.792	5f36d2	3.0	7.2	5f36d2 (4i) 5h	5.5	5f36d2 (2g) 5h	5.0	5f36d2 (4g) 5h					
13371.356	42.563	1.244	5f36d2	3.0	21.4	5f36d2 (4f) 7g	8.2	5f36d2 (4s) 7f	6.0	5f36d2 (4g) 7g				
23449.446	-25.659	1.136	1.210	5f36d2	3.0	3.5	5f36d7 (2d) 3f	6.1	5f36d2 (4f) 7f	5.3	5f36d2 (4i) 5h			
23567.566	67.568	1.016	5f36d2	3.0	6.0	5f36d7 (4d) 5f	7.1	5f36d2 (4f) 7g	6.7	5f36d7 (4g) 3g				
23663.641	-19.232	1.057	1.175	5f36d2	-500	3.0	8.7	5f36d2 (4f) 7f	4.0	5f36d2 (4f) 7s	3.8	5f36d7 (4g) 5d		
23753.142	-23.063	1.268	0.935	5f36d2	-555	3.0	8.6	5f36d2 (4f) 7d	8.2	5f36d2 (4f) 7g	5.9	5f36d2 (4f) 7s		
23908.874	-45.714	1.089	0.870	5f36d2	-588	3.0	4.3	5f36d2 (4f) 5h	5.8	5f36d2 (4f) 7d	4.5	5f36d7 (4d) 5f		
4453.419*	4335	0.671	0.680	5f36d7	6	4.0	67.5	5f36d7 (4i) 5i	14.5	5f36d7 (4i) 3h	6.5	5f36d7 (2h) 3h		
5991.314	-106.565	0.857	0.835	5f36d7	24	4.0	29.4	5f36d7 (4i) 5h	25.3	5f36d7 (4i) 3h	8.8	5f36d7 (4i) 5i		
8133.291	8236	-102.281	0.975	5f36d7	38	4.0	0	5f36d2 (2f) 1g	21.7	5f36d7 (4i) 5h	18.4	5f36d7 (4i) 3g		
10208.488	10236	-27.358	0.599	5f36d2	-373	4.0	40.3	5f36d2 (4i) 7k	16.3	5f36d7 (4g) 5i	7.1	5f36d2 (4i) 5h		
10557.037	10641	-84.068	0.838	5f36d7	-104	4.0	23.8	5f36d7 (4i) 5g	20.4	5f36d2 (4i) 7k	8.8	5f36d7 (4f) 5h		
11403.464	-44.646	0.774	0.805	5f36d7	-60	4.0	37.2	5f36d7 (4g) 5i	14.3	5f36d7 (4i) 5g	9.5	5f36d7 (4i) 5h		
11558.696*	11793	0.827	0.785	5f36d7	-256	4.0	22.7	5f36d7 (4f) 5h	17.9	5f36d2 (4i) 7i	8.9	5f36d7 (4g) 5i		
12362.448	-79.152	0.829	0.840	5f36d2	-215	4.0	28.5	5f36d2 (4i) 7i	20.7	5f36d7 (4f) 5h	8.6	5f36d7 (4i) 5h		
12627.560	12561	66.416	1.087	5f36d7	36	4.0	8.6	5f36d7 (4f) 3h	11.8	5f36d7 (4f) 5g	8.3	5f36d7 (4s) 5d		
12884.798	12921	-36.106	1.001	5f36d7	42	4.0	9.9	5f36d7 (2h) 3h	14.1	5f36d7 (4f) 5g	7.9	5f36d7 (2g) 3g		
13966	0.471	5f36d2	4.0	72.7	5f36d2 (4i) 7k	7.9	5f36d2 (2h) 5i	2.7	5f36d2 (4i) 7k					
14274.370	14349	-74.826	0.986	5f36d2	-520	4.0	16.3	5f36d2 (4i) 7h	10.5	5f36d2 (4f) 5h	4.7	5f36d7 (4g) 5h		
14411.306	14491	-79.620	1.235	0.545	5f36d7	-543	4.0	20.1	5f36d7 (4s) 5d	13.0	5f36d7 (4f) 5g	12.4	5f36d7 (4f) 5d	
15026.778	14961	65.995	0.939	1.010	5f36d7	4.0	17.8	5f36d7 (4f) 5g	15.7	5f36d7 (4g) 5h	12.6	5f36d2 (4i) 7i		
15778.044*	15231	0.861	0.861	5f36d2	4.0	28.2	5f36d2 (4i) 7i	12.3	5f36d7 (4f) 5g	7.8	5f36d2 (4f) 5d			
15778.044	15731	46.751	1.070	5f36d7	-296	4.0	25.3	5f36d7 (4i) 3g	10.4	5f36d7 (4i) 5g	9.3	5f36d7 (2h) 3g		
16047.611*	15922	1.050	0.960	5f36d7	-215	4.0	2.4	5f36d7 (2g) 3h	10.1	5f36d7 (4g) 5h	7.8	5f36d7 (4f) 5f		
16451.765	16420	31.377	0.926	5f36d2	-445	4.0	3.3	5f36d2 (4i) 3h	7.2	5f36d2 (4i) 7h	6.1	5f36d7 (4g) 5h		
16699.374	16708	-8.835	1.015	5f36d7	4.0	12.9	5f36d7 (4g) 5h	6.2	5f36d7 (4f) 3h	5.5	5f36d7 (4s) 5d			
17048.861	17067	-18.624	1.098	5f36d2	-331	4.0	5.6	5f36d2 (4i) 5g	10.0	5f36d2 (4i) 7g	9.3	5f36d2 (4i) 7h		
17217.089*	17412	0.997	5f36d7	4.0	0.7	5f36d2 (2d) 3h	6.8	5f36d7 (4i) 3g	6.2	5f36d7 (2h) 3h				
17533.315	17559	-25.21	1.223	5f36d7	-224	4.0	30.9	5f36d7 (4f) 5f	8.1	5f36d7 (4s) 5d	7.1	5f36d7 (4g) 3f		
17795.732*	17661	1.134	1.134	5f36d7	4.0	3.6	5f36d7 (2g) 1g	11.1	5f36d7 (4f) 5d	9.2	5f36d2 (4i) 7h			
17799.319	17875	-75.718	0.993	5f36d2	4.0	0	5f36d2 (2g) 1g	8.6	5f36d7 (4g) 5g	8.2	5f36d2 (4i) 5i			
18319.915	18350	-29.829	0.914	0.765	5f36d2	-571	4.0	7.3	5f36d2 (4i) 7h	14.2	5f36d2 (4i) 7g	8.1	5f36d2 (4i) 5h	
18412.703*	18622	1.014	1.014	5f36d7	-224	4.0	17.5	5f36d7 (4g) 5g	6.0	5f36d2 (4i) 7h	5.6	5f36d2 (4f) 7i		
18567.377*	18678	0.765	1.015	5f36d2	4.0	15.7	5f36d2 (4f) 7i	12.6	5f36d2 (4g) 7k	9.4	5f36d2 (4i) 5i			
19007.529	18975	32.178	1.028	5f36d2	-571	4.0	16.7	5f36d2 (4i) 7g	9.5	5f36d2 (4i) 5i	8.1	5f36d2 (4i) 7h		
19210.402	19211	-0.127	0.506	0.780	5f36d2	-538	4.0	64.7	5f36d2 (4g) 7k	6.2	5f36d2 (4f) 7i	5.2	5f36d2 (4i) 5i	
19555.755*	19321	1.121	1.055	5f36d7	4.0	14.0	5f36d7 (4f) 5d	8.7	5f36d7 (4f) 3h	5.7	5f36d7 (4f) 3g			
19664.647	19666	-1.619	1.055	5f36d2	4.0	10.9	5f36d2 (4i) 7f	11.3	5f36d2 (4i) 7f	5.1	5f36d2 (4i) 7h			

Table 4. (continued)

Experimental level (cm <sup>-1</sup> )	Calculated level (cm <sup>-1</sup> )	D (mK)	g (cal.)	g (exp.)	dominant configuration	IS (exp.) (mK)	J =	1 <sup>st</sup> component (%)	2 <sup>nd</sup> component (%)	3 <sup>rd</sup> component (%)			
19831.487	19880	-48.138	1.017	5f36d7	-517	4.0	21.7	5f36d7 (2h) 3f	7.1	5f36d7 (4i) 5i			
19907.079*	20028	1.077	1.040	5f36d7	-293	4.0	0	5f36d2 (2f) 1g	14.7	5f36d7 (2h) 3f			
20195.797	20155	40.446	0.977	0.985	5f36d2	-231	4.0	11.4	5f36d2 (4i) 5i	9.0	5f36d2 (4f) 7g		
20458.717	20468	-9.551	1.146	5f36d2	4.0	20.3	5f36d2 (4f) 7g	3.2	5f36d2 (4g) 7i	2.5	5f36d2 (4i) 7f		
20471.799	20516	-44.485	1.140	5f36d7	4.0	5.5	5f36d7 (2d) 1g	7.5	5f36d2 (4i) 7g	4.7	5f36d7 (4g) 5d		
20815.587*	20666	1.001	5f36d2	-519	4.0	18.0	5f36d2 (4f) 7h	7.4	5f36d2 (4i) 3h	7.1	5f36d2 (4i) 7g		
20945.871	20909	36.579	1.121	1.210	5f36d2	-474	4.0	15.8	5f36d2 (4s) 7f	9.3	5f36d2 (4g) 7i		
20967.290	20954	12.824	0.860	0.970	5f36d2	4.0	12.0	5f36d2 (4i) 7f	10.7	5f36d2 (4i) 5i	7.9	5f36d2 (4i) 5i	
21050.615	21097	-46.297	0.974	5f36d2	4.0	0	5f36d2 (2g) 1g	11.3	5f36d2 (4i) 7i	6.7	5f36d2 (4f) 7h		
21406.577	21422	-15.612	1.037	5f36d2	4.0	6.4	5f36d2 (4i) 5h	5.6	5f36d2 (4i) 5h	4.2	5f36d2 (4f) 7g		
21679.820	21728	-48.639	1.060	5f36d2	4.0	12.0	5f36d2 (4i) 7f	5.8	5f36d2 (4g) 7i	3.8	5f36d2 (4i) 5i		
21864	21864	1.169	5f36d2	4.0	3.8	5f36d7 (2h) 3g	5.9	5f36d7 (2d) 3g	5.0	5f36d7 (4d) 5f			
22149.776	22163	-13.357	0.824	0.995	5f36d2	4.0	17.5	5f36d2 (4i) 5i	7.0	5f36d2 (4i) 7i	6.6	5f36d2 (4i) 5h	
22293	22293	1.166	5f36d2	4.0	3.0	5f36d2 (4i) 3g	6.2	5f36d2 (4i) 7g	4.8	5f36d7 (4d) 5f			
22363.403	22355	8.372	0.995	5f36d2	4.0	8.1	5f36d7 (4g) 3h	8.7	5f36d2 (4f) 7h	4.5	5f36d7 (4d) 5g		
22492.342	22558	-65.806	1.088	0.920	5f36d2	-549	4.0	4.0	5f36d2 (4f) 7p	6.0	5f36d2 (4f) 7h		
22510.849	22596	-85.087	1.093	5f36d2	4.0	16.3	5f36d2 (4i) 7h	6.7	5f36d2 (4f) 7p	4.1	5f36d2 (4s) 7p		
22663	22663	1.032	5f36d2	4.0	6.6	5f36d7 (2d) 3f	5.9	5f36d2 (4i) 5i	5.6	5f36d7 (4g) 3h			
22842.594	22881	-38.746	1.000	5f36d2	4.0	2.9	5f36d2 (4i) 5i	3.9	5f36d2 (4i) 3h	3.6	5f36d2 (4i) 5g		
22964.313	22975	-10.991	0.958	5f36d2	4.0	6.9	5f36d2 (4i) 5h	3.9	5f36d2 (4f) 5i	3.1	5f36d2 (4i) 5i		
23040.775	23053	-11.957	1.035	5f36d2	4.0	0	5f36d2 (2f) 1g	5.9	5f36d2 (4i) 5h	4.6	5f36d2 (4i) 5j		
23129.137	23095	34.299	1.146	5f36d7	4.0	22.7	5f36d7 (4g) 5f	6.9	5f36d7 (2h) 3g	4.3	5f36d7 (4f) 3h		
23348	23367	1.028	5f36d2	4.0	12.8	5f36d2 (4i) 5h	4.6	5f36d2 (4f) 7h	4.4	5f36d2 (4i) 5h			
23622	23622	1.140	5f36d7	4.0	5.6	5f36d7 (4f) 3g	8.4	5f36d7 (4g) 5f	8.2	5f36d7 (4f) 5f			
23689	563	57.493	0.726	0.730	5f36d2	4.0	5.5	5f36d2 (4i) 3h	4.6	5f36d2 (4s) 7f	4.1	5f36d2 (4i) 5j	
5804	-42.486	0.893	0.885	5f36d7	0	5.0	5f36d2 (4f) 5i	3.9	5f36d2 (4i) 3h	3.4	5f36d2 (4i) 5j		
5762.079	7907	-43.061	0.932	0.940	5f36d7	25	5.0	62.2	5f36d7 (4i) 5i	14.9	5f36d7 (4i) 3h		
7864.204	31.451	0.541	0.535	5f36d2	-563	5.0	78.5	5f36d2 (4i) 7l	7.9	5f36d2 (2h) 5k	5.8	5f36d7 (2h) 3i	
10081.030	10342	-87.270	1.014	1.005	5f36d7	48	5.0	39.7	5f36d7 (4i) 5h	13.0	5f36d7 (4f) 5h	10.8	5f36d7 (4i) 3i
10254.999	13641	-9.376	0.985	1.005	5f36d7	49	5.0	6.6	5f36d7 (2h) 3i	12.0	5f36d7 (4i) 5i	11.4	5f36d7 (2g) 3i
11290.267*	11457	0.962	0.955	5f36d7	17	5.0	30.8	5f36d7 (4g) 5i	19.0	5f36d7 (4f) 5h	12.5	5f36d7 (4i) 5g	
11633.163	11691	-57.798	0.800	0.800	5f36d2	-550	5.0	58.7	5f36d2 (4i) 7k	6.3	5f36d2 (4i) 5i	6.3	5f36d2 (2h) 5i
11968.650*	12087	1.111	1.150	5f36d7	52	5.0	22.0	5f36d7 (4i) 5g	11.0	5f36d7 (4i) 5h	10.1	5f36d7 (4f) 5h	
13632.065	13641	-9.376	0.985	1.005	5f36d2	-452	5.0	39.9	5f36d2 (4i) 7i	7.0	5f36d7 (4g) 5i	6.3	5f36d2 (4f) 5h
13876.403	13873	3.701	1.043	1.060	5f36d7	-313	5.0	2.5	5f36d2 (4i) 1h	8.3	5f36d2 (4i) 7i	6.6	5f36d2 (4i) 7k
14344.522*	14245	1.042	1.010	5f36d7	-47	5.0	17.9	5f36d7 (4f) 5h	14.0	5f36d7 (4g) 5i	7.0	5f36d7 (4f) 5g	
14562.354	14543	19.421	0.786	1.060	5f36d2	29	5.0	46.4	5f36d2 (4i) 7k	9.2	5f36d2 (4i) 5k	8.0	5f36d2 (4i) 5k
14970.521*	14730	1.071	1.135	5f36d7	-552	5.0	12.4	5f36d7 (4f) 3h	20.5	5f36d7 (4i) 5g	10.5	5f36d7 (4g) 5i	
15542.022	15585	-42.915	1.013	1.005	5f36d2	-313	5.0	2.5	5f36d2 (4i) 1h	8.3	5f36d2 (4i) 7i	6.6	5f36d2 (4i) 7k
15799.241*	15957	1.047	1.020	5f36d7	-25	5.0	26.5	5f36d7 (4f) 5g	10.5	5f36d7 (2h) 3i	9.0	5f36d2 (4i) 7i	
16154.523*	16059	1.070	5f36d7	5.0	11.7	5f36d7 (4i) 3h	8.2	5f36d7 (4f) 5h	7.4	5f36d7 (2g) 3g	7.4	5f36d7 (2g) 3g	
16154.523	16183	-28.485	0.951	0.985	5f36d2	-462	5.0	2.2	5f36d2 (2h) 5h	11.2	5f36d2 (4i) 7i	9.3	5f36d7 (4f) 5g
16602.345	16688	-85.902	1.054	5f36d2	-514	5.0	27.1	5f36d2 (4i) 7h	8.3	5f36d2 (4i) 5h	6.9	5f36d2 (4i) 7h	

Table 4. (continued)

Experimental level ( $\text{cm}^{-1}$ )	Calculated level ( $\text{cm}^{-1}$ )	$D$ (mK)	$g$ (cal.)	$g$ (exp.)	dominant configuration	IS (exp.) (mK)	$J =$	1 <sup>st</sup> component (%)		2 <sup>nd</sup> component (%)		3 <sup>rd</sup> component (%)		
								IS (exp.) (%)	IS (exp.) (%)	IS (exp.) (%)	IS (exp.) (%)	IS (exp.) (%)	IS (exp.) (%)	
17461.027	17431	30.489	0.984	5f36d2	5.0	8.0	5f36d2 (4i) 5k	9.2	5f36d2 (4i) 7i	9.1	5f36d2 (4i) 5k	9.1		
17589.426	17605	-15.355	0.804	5f36d2	-530	5.0	18.5	5f36d2 (4i) 5k	19.1	5f36d2 (4i) 5k	9.6	5f36d2 (4i) 5k	9.6	
17882.529	17901	-18.777	0.988	5f36d7	-31	5.0	11.1	5f36d7 (2g) 3i	8.1	5f36d7 (2h) 3h	7.1	5f36d7 (2g) 3i	7.1	
18065.155*	18227	1.060	0.815	5f36d7	5.0	41.7	5f36d7 (4g) 5h	5.5	5f36d7 (2h) 3h	4.4	5f36d7 (2h) 3g	4.4		
18214.588*	18479	1.064		5f36d7	5.0	10.1	5f36d7 (4g) 5g	8.1	5f36d7 (4g) 5h	7.0	5f36d7 (2h) 3g	7.0		
18518.682	18498	20.89	0.889	5f36d2	5.0	16.2	5f36d2 (4i) 5k	6.5	5f36d2 (4i) 5k	5.3	5f36d2 (4i) 5k	5.3		
18964.117	18977	-12.411	1.010	5f36d2	5.0	10.4	5f36d7 (4g) 3i	8.3	5f36d2 (4i) 5k	4.9	5f36d7 (2k) 3i	4.9		
19068.395	19009	59.001	1.047	5f36d2	5.0	1.2	5f36d2 (2h) 3g	7.5	5f36d7 (4g) 3i	6.0	5f36d7 (4f) 5g	6.0		
19148.706	19207	-58.636	1.042	1.020	5f36d2	-275	5.0	7.4	5f36d2 (4i) 5i	10.3	5f36d7 (4i) 5h	4.8		
19403.921*	19447	1.110		5f36d7	5.0	28.3	5f36d7 (4i) 3g	4.9	5f36d7 (2k) 1h	4.0	5f36d2 (4f) 7i	4.0		
19670.851	19728	-57.264	1.092	1.125	5f36d2	5.0	1.4	5f36d2 (4i) 5f	8.0	5f36d2 (4i) 7i	7.6	5f36d2 (4i) 7i	7.6	
19959.940	19931	28.616	1.003	1.100	5f36d2	-323	5.0	8.5	5f36d7 (2h) 1h	14.2	5f36d7 (4i) 5f	4.5	5f36d7 (4f) 3g	4.5
20139.067	20042	97.431	1.024	5f36d2	5.0	15.4	5f36d7 (4f) 5f	5.6	5f36d7 (2h) 1h	4.1	5f36d2 (4g) 7i	4.1		
20331.345	20430	-98.243	0.825	1.030	5f36d2	-481	5.0	47.5	5f36d2 (4g) 7k	6.8	5f36d2 (4i) 5k	2.3	5f36d2 (4i) 5k	2.3
20525.894	20522	3.934	1.052	5f36d2	5.0	4.9	5f36d2 (4i) 3i	10.6	5f36d2 (4i) 7h	5.9	5f36d2 (4i) 5k	5.9		
20777.053	20710	66.765	0.855	5f36d2	5.0	22.2	5f36d2 (4i) 5k	15.4	5f36d2 (4g) 7k	3.4	5f36d2 (4f) 7i	3.4		
20916.213	20914	2.232	1.057	0.985	5f36d7	5.0	0	5f36d2 (2f) 1h	7.1	5f36d2 (4g) 7k	6.5	5f36d7 (4g) 5g	6.5	
21116.726	21083	33.485	0.980	5f36d2	5.0	13.5	5f36d2 (4i) 7i	6.2	5f36d2 (4f) 7i	3.9	5f36d2 (2h) 5k	3.9		
21196.797	21215	-18.747	1.111	1.000	5f36d7	5.0	7.9	5f36d7 (2h) 3g	5.5	5f36d7 (2h) 3h	5.2	5f36d7 (4f) 3g	5.2	
21455.604	21422	33.115	1.100	5f36d2	5.0	12.1	5f36d2 (4i) 5i	8.4	5f36d2 (4s) 7f	6.1	5f36d2 (4i) 7f	6.1		
21562.672	21509	53.432	1.107	5f36d2	5.0	17.9	5f36d2 (4f) 7g	9.5	5f36d2 (4i) 5k	5.1	5f36d7 (4g) 5g	5.1		
21608.903	21632	-23.111	1.032	5f36d2	5.0	8.1	5f36d2 (4f) 7i	7.4	5f36d2 (4f) 7g	4.8	5f36d2 (4i) 5k	4.8		
21620.822*	21741	1.047		5f36d2	5.0	6.7	5f36d7 (2h) 3h	6.0	5f36d7 (4g) 5f	4.8	5f36d7 (4g) 5g	4.8		
21861		1.105		5f36d2	5.0	19.2	5f36d2 (4i) 7g	3.8	5f36d2 (4i) 5i	3.7	5f36d2 (4i) 5i	3.7		
22047		1.073		5f36d2	5.0	7.9	5f36d2 (4i) 3i	13.1	5f36d2 (4i) 7g	4.0	5f36d2 (4i) 5i	4.0		
22154		1.050		5f36d7	5.0	5.5	5f36d7 (2k) 3h	6.1	5f36d7 (4g) 3i	5.7	5f36d7 (4g) 5h	5.7		
22229		1.116		5f36d2	5.0	11.0	5f36d2 (4f) 7h	5.6	5f36d2 (4s) 7f	2.4	5f36d7 (2d) 3g	2.4		
22390		1.146		5f36d7	5.0	4.4	5f36d7 (4g) 3g	5.3	5f36d7 (2d) 3g	4.7	5f36d2 (4f) 7g	4.7		
22559		1.116		5f36d2	5.0	9.2	5f36d2 (4s) 7f	6.3	5f36d2 (4i) 5i	3.9	5f36d2 (4f) 7f	3.9		
22908		0.964		5f36d2	5.0	0.1	5f36d2 (2g) 1h	10.8	5f36d7 (2k) 3i	9.2	5f36d2 (4g) 7i	9.2		
22975		1.001		5f36d2	5.0	13.6	5f36d7 (2k) 3i	4.5	5f36d7 (4g) 3i	3.7	5f36d7 (4g) 3h	3.7		
23051		1.015		5f36d2	5.0	29.1	5f36d2 (4g) 7i	5.7	5f36d7 (2k) 3i	4.3	5f36d2 (4i) 7i	4.3		
23367		1.056		5f36d2	5.0	10.1	5f36d2 (4i) 5i	7.8	5f36d2 (4f) 7h	7.3	5f36d2 (4i) 5i	7.3		
23437		1.076		5f36d7	5.0	7.6	5f36d7 (2h) 3g	8.5	5f36d7 (2g) 1h	7.5	5f36d7 (4f) 3g	7.5		
23625		1.191		5f36d2	5.0	13.0	5f36d2 (4i) 7f	6.3	5f36d2 (4s) 7f	4.4	5f36d2 (4i) 5h	4.4		
23859		1.072		5f36d2	5.0	9.2	5f36d2 (4i) 7h	4.5	5f36d2 (4f) 7g	3.7	5f36d2 (4f) 7f	3.7		
23948		1.035		5f36d2	5.0	4.0	5f36d2 (4i) 3i	4.9	5f36d2 (4i) 5i	3.0	5f36d2 (4i) 3i	3.0		
0	-22	21.846	0.754	0.750	5f36d7	0	6.0	72.9	5f36d7 (4i) 5l	13.5	5f36d7 (2h) 3k	5.4		
4225.707	4222	53.786	0.920	5f36d7	25	6.0	81.8	5f36d7 (4i) 5k	7.1	5f36d7 (2h) 3i	3.5	5f36d7 (4i) 3i	3.5	
6249.029	6219	30.182	0.612	0.625	5f36d2	-545	6.0	77.4	5f36d2 (4i) 7m	9.0	5f36d2 (2h) 5l	4.2	5f36d2 (4i) 5l	4.2
7005.532	7013	-7.885	0.954	0.950	5f36d7	5	6.0	15.3	5f36d7 (4i) 3i	17.8	5f36d7 (2h) 3k	14.1	5f36d7 (4i) 5l	14.1
10288.617	10263	26.088	1.036	1.035	5f36d7	37	6.0	62.8	5f36d7 (4i) 5i	7.0	5f36d7 (2h) 3k	5.4	5f36d7 (4i) 3i	5.4
10987.587*	11119	1.025	1.035	5f36d7	28	6.0	3.0	5f36d7 (2h) 3i	15.7	5f36d7 (4i) 3k	13.9	5f36d7 (4i) 5h	13.9	
11457.312	11475	-17.739	0.814	0.810	5f36d2	-550	6.0	63.4	5f36d2 (4i) 7l	6.8	5f36d2 (2h) 5k	4.8	5f36d2 (4i) 5l	4.8

Table 4. (continued)

Experimental level (cm <sup>-1</sup> )	Calculated level (cm <sup>-1</sup> )	<i>D</i> (mK)	<i>g</i> (cal.)	<i>g</i> (exp.)	dominant configuration	IS (exp.) (mK)	<i>J</i> =	1 <sup>st</sup> component (%)	2 <sup>nd</sup> component (%)	3 <sup>rd</sup> component (%)
12910.507	12930	-19.356	1.031	1.015	5f36d7	0	6.0	18.9	5f36d7 (4i) 3i	8.6
13361.397	13361	0.799	1.030	1.015	5f36d7	-200	6.0	1.8	5f36d7 (2k) 1i	10.1
13402.537	13459	-56.956	0.997	0.995	5f36d2	-285	6.0	40.2	5f36d2 (4i) 5k	4.4
14174.348	14217	-42.951	1.139	1.145	5f36d7	56	6.0	28.4	5f36d7 (4i) 5h	16.7
14543.776	14550	-6.583	0.847	0.810	5f36d2	-503	6.0	9.8	5f36d2 (4i) 5l	10.4
15435.243	15481	-45.782	0.980	1.050	5f36d2	-94	6.0	5.6	5f36d2 (4i) 3k	8.0
15804.313*	15633		1.084	1.100	5f36d2	-404	6.0	0	5f36d2 (2i) 1i	10.5
15906.340*	15717		1.049		5f36d2		6.0	27.4	5f36d2 (4i) 7i	7.2
16376.313	16312	63.976	1.143		5f36d7	-20	6.0	15.8	5f36d7 (4i) 5h	11.1
16847.021	16813	33.798	1.105		5f36d7		6.0	40.8	5f36d7 (4f) 5i	5.2
17102.856*	17363		0.827		5f36d2	-555	6.0	28.9	5f36d2 (4i) 5l	9.9
17572.941	17588	-15.032	1.090		5f36d7	35	6.0	13.6	5f36d7 (2k) 3k	9.6
17572.941*	17863	1.025			5f36d2		6.0	17.1	5f36d2 (4i) 7i	7.1
18005.947	17948	57.488	1.051		5f36d2	-535	6.0	4.2	5f36d2 (4i) 3i	12.9
18111.753	18064	47.807	0.987	0.990	5f36d7		6.0	23.8	5f36d7 (2k) 3k	11.8
18359.990*	18659		1.024		5f36d2	-353	6.0	4.7	5f36d2 (4i) 5k	10.2
18591.225*	18748		0.867		5f36d2	-580	6.0	16.0	5f36d2 (4i) 5l	13.0
19016.882	18942	74.643	1.167		5f36d7		6.0	22.4	5f36d7 (4f) 5g	17.1
19685.138*	19499		0.996		5f36d2	-506	6.0	13.5	5f36d2 (4i) 7k	14.4
19914.311	19880	34.647	1.084		5f36d2		6.0	0.3	5f36d2 (4g) 5h	4.6
20353.022*	19993	1.094			5f36d7		6.0	14.0	5f36d2 (4i) 3h	9.9
20353.022	20305	47.587	0.956		5f36d2		6.0	12.6	5f36d2 (4i) 5l	7.9
20697.644	20713	-15.058	1.174		5f36d7		6.0	19.8	5f36d7 (4g) 5g	12.5
20731.172	20740	-8.951	1.066		5f36d7		6.0	14.3	5f36d7 (2g) 3i	11.8
10922.725*	21052	1.024			5f36d2		6.0	10.9	5f36d2 (4i) 7h	9.7
21170.637*	21321		1.032		5f36d7		6.0	7.9	5f36d7 (4f) 3h	10.9
21354.123	21356	-1.832	1.069		5f36d2		6.0	9.1	5f36d2 (4i) 5k	4.2
21488.644	21475	13.900	1.065		5f36d2		6.0	18.8	5f36d2 (4f) 7i	4.6
21576.700*	21727	1.040			5f36d2		6.0	3.3	5f36d2 (4i) 5g	13.9
21706.851*	21840		1.071		5f36d2		6.0	8.6	5f36d7 (2k) 3i	10.6
21973.746	21970	3.543	1.092		5f36d2		6.0	8.6	5f36d7 (4g) 5h	6.5
22171.940	22126	47.206	1.074		5f36d2		6.0	4.5	5f36d2 (4i) 5j	16.7
22276.7	22230	1.096			5f36d2		6.0	30.7	5f36d2 (4g) 7k	5.5
22336	22349	-35.091	1.023		5f36d7		6.0	14.3	5f36d2 (4i) 5k	6.4
22454.331	22249		1.051		5f36d2		6.0	20.8	5f36d7 (2i) 3k	5.3
23049	23267	1.085			5f36d2		6.0	9.5	5f36d2 (4i) 3k	7.7
23381	23381	1.112			5f36d2		6.0	10.3	5f36d7 (4g) 3i	10.0
23642	23642	1.124			5f36d2		6.0	2.4	5f36d2 (4i) 5k	6.5
23712	23712	1.091			5f36d2		6.0	19.1	5f36d2 (4g) 7i	5.6
23913	3831	-30.627	0.926	0.925	5f36d7	13	7.0	81.7	5f36d2 (4f) 7g	6.9
3800.829	7326.118	7272	54.217	1.016	5f36d7	-17	7.0	65.3	5f36d7 (4i) 3l	3.9

Table 4. (continued)

Experimental level (cm <sup>-1</sup> )	Calculated level (cm <sup>-1</sup> )	<i>D</i> (mK)	<i>g</i> (cal.)	<i>g</i> (exp.)	dominant configuration	IS (exp.) (mK)	<i>J</i> =	1 <sup>st</sup> component (%)		2 <sup>nd</sup> component (%)		3 <sup>rd</sup> component (%)	
								IS (exp.) (%)	1 <sup>st</sup> component (%)	2 <sup>nd</sup> component (%)	3 <sup>rd</sup> component (%)		
8118.632	8098	20.108	0.834	0.845	5f36d2	-511	7.0	68.6	5f36d2 (4i) 7m	7.2	5f36d2 (2h) 5l	6.2	5f36d2 (4i) 5m
10069.177*	9946	0.942	0.930	5f36d7	-44	7.0	40.3	5f36d7 (4i) 3l	18.7	5f36d7 (4i) 5k	5.7	5f36d7 (2k) 3l	
11677.036	11648	29.274	1.093	1.095	5f36d7	32	7.0	29.5	5f36d7 (4i) 5i	25.3	5f36d7 (4i) 3k	14.4	5f36d7 (4i) 7m
12826.316	12825	1.321	0.888	0.890	5f36d2	-530	7.0	25.1	5f36d2 (4i) 5m	13.0	5f36d2 (4i) 7l	12.7	5f36d2 (4i) 7m
13346.912	13302	44.887	1.082	0.985	5f36d7	-342	7.0	7.8	5f36d7 (2h) 3k	25.7	5f36d7 (4i) 5l	8.9	5f36d2 (4i) 7l
13567.946	13524	44.229	0.926	1.010	5f36d2	-218	7.0	36.6	5f36d2 (4i) 7l	22.4	5f36d2 (4i) 5m	3.4	5f36d2 (4i) 5l
14790.989	14713	78.029	1.106	1.110	5f36d7	52	7.0	24.3	5f36d7 (4i) 3k	17.3	5f36d7 (4i) 5h	9.1	5f36d7 (2h) 3k
15353.798	15373	-19.594	1.092	1.065	5f36d2	-537	7.0	46.1	5f36d2 (4i) 7k	11.3	5f36d2 (4i) 5k	6.7	5f36d2 (4i) 7l
15712.861	15696	16.912	0.996	1.030	5f36d2	-436	7.0	2.7	5f36d2 (2h) 3k	16.2	5f36d2 (4i) 7l	16.0	5f36d2 (4i) 5m
16766.128*	16626	1.077	5f36d7	-431	7.0	9.9	5f36d7 (4i) 3i	11.6	5f36d7 (4i) 5j	9.9	5f36d7 (4i) 3k		
16980.556*	16872	1.167	5f36d7	7.0	26.5	5f36d7 (4i) 5h	21.9	5f36d7 (4i) 3i	9.6	5f36d7 (2h) 3i			
17669	17669	1.125	5f36d2	7.0	26.9	5f36d2 (4i) 7i	8.5	5f36d2 (4i) 7k	6.5	5f36d2 (4i) 7k			
17928.965*	17801	1.076	1.150	5f36d7	-448	7.0	4.1	5f36d7 (2g) 3i	14.5	5f36d7 (2k) 3k	10.2	5f36d7 (4i) 5h	
18068.167	18130	-61.518	0.994	5f36d2	-330	7.0	13.0	5f36d2 (4i) 5l	12.3	5f36d2 (4i) 7k	10.9	5f36d2 (4i) 5l	
18898	18898	1.085	5f36d7	7.0	21.7	5f36d7 (4g) 5i	12.9	5f36d7 (4f) 5h	6.0	5f36d7 (2i) 3k			
19043	19043	0.975	5f36d2	7.0	21.1	5f36d2 (4i) 5m	10.8	5f36d2 (4i) 7k	6.2	5f36d7 (4f) 5h			
19181.6690	19178	2.950	0.853	5f36d2	7.0	38.1	5f36d2 (4i) 5m	10.2	5f36d2 (4i) 5m	5.6	5f36d2 (2h) 3l		
19758.723*	19621	1.013	5f36d2	-446	7.0	8.9	5f36d2 (4i) 3l	11.3	5f36d2 (4i) 3l	7.8	5f36d2 (4i) 7l		
19998.952*	19714	1.035	5f36d7	7.0	7.6	5f36d7 (2h) 1k	8.3	5f36d2 (4i) 5l	6.7	5f36d7 (4f) 5h			
19998.952	20008	-9.481	1.048	5f36d2	7.0	10.7	5f36d2 (4i) 5l	8.8	5f36d2 (4i) 7i	5.7	5f36d2 (4f) 7i		
20180.590*	20454	1.099	5f36d2	7.0	21.2	5f36d2 (4i) 7k	15.3	5f36d2 (4i) 7i	8.4	5f36d2 (4f) 7i			
20680.816*	20828	1.120	5f36d2	-570	7.0	14.4	5f36d7 (2h) 3i	11.9	5f36d7 (4g) 5h	7.9	5f36d2 (4i) 7h		
20932	20932	0.993	5f36d2	7.0	13.2	5f36d2 (4i) 3l	9.9	5f36d2 (4i) 5m	7.4	5f36d7 (4g) 5i			
21228.034*	21089	1.131	5f36d2	-532	7.0	9.5	5f36d7 (4g) 5h	12.6	5f36d7 (4g) 5i	11.5	5f36d7 (2h) 3i		
21329.057	21307	21.680	1.071	5f36d7	7.0	8.6	5f36d7 (2k) 3i	13.7	5f36d7 (4g) 5i	11.6	5f36d7 (2h) 3k		
21630.980	21678	-46.721	1.032	5f36d2	7.0	24.0	5f36d2 (4i) 5l	4.0	5f36d2 (4i) 7h	3.0	5f36d2 (4i) 7i		
21777.731	21806	-28.675	1.058	5f36d7	7.0	19.2	5f36d7 (2k) 3k	7.0	5f36d7 (2k) 3l	5.4	5f36d2 (4i) 7i		
22135.838	22087	48.439	0.993	5f36d2	7.0	7.3	5f36d2 (4i) 5l	9.0	5f36d2 (4i) 5l	7.0	5f36d2 (4i) 5l		
22268.937	22344	-75.386	1.029	5f36d2	7.0	10.7	5f36d2 (4i) 5k	9.3	5f36d2 (4i) 5l	7.4	5f36d2 (4i) 5l		
22440.595*	22611	1.067	5f36d2	7.0	0.3	5f36d2 (2g) 3i	7.7	5f36d2 (4i) 3l	5.9	5f36d2 (4i) 5l			
22885.513	22839	46.723	1.075	5f36d2	7.0	9.0	5f36d2 (4i) 5k	10.9	5f36d2 (4i) 7h	7.0	5f36d2 (4i) 3l		
22991.838*	23340	1.078	5f36d7	7.0	9.8	5f36d7 (2i) 3l	8.0	5f36d7 (2h) 3i	7.6	5f36d7 (2i) 3l			
23570.963*	23409	1.108	5f36d2	7.0	11.3	5f36d2 (4i) 7h	5.8	5f36d2 (4i) 3l	4.6	5f36d7 (2i) 3l			
23690	23761	1.101	5f36d2	7.0	18.6	5f36d2 (4f) 7i	12.5	5f36d2 (4g) 7k	4.3	5f36d2 (4i) 5l			
23927	23927	1.035	5f36d2	7.0	6.6	5f36d2 (4i) 3l	7.6	5f36d2 (4i) 5l	6.3	5f36d2 (4f) 7i			
23982	23982	1.100	5f36d2	7.0	8.9	5f36d2 (4i) 3l	7.3	5f36d2 (4g) 7k	6.4	5f36d2 (4i) 5k			
7645.645	7689	-43.293	1.043	1.040	5f36d7	30	8.0	88.9	5f36d7 (4i) 5l	3.3	5f36d2 (4i) 5l	2.5	5f36d7 (2h) 3k
10347.345	10327	20.757	1.074	1.030	5f36d7	-299	8.0	49.0	5f36d7 (4i) 5k	19.0	5f36d2 (4i) 7m	8.3	5f36d7 (4i) 3l
10685.887	10596	90.183	1.007	1.065	5f36d2	-186	8.0	57.4	5f36d2 (4i) 7m	20.7	5f36d7 (4i) 5k	4.6	5f36d2 (4i) 5m
14501.807*	14272	1.030	1.035	5f36d7	-23	8.0	35.5	5f36d7 (4i) 3l	20.5	5f36d7 (4i) 5k	16.1	5f36d7 (2k) 3m	
14841.798*	14622	1.154	1.160	5f36d7	51	8.0	43.1	5f36d7 (4i) 5i	21.3	5f36d7 (4i) 3k	13.1	5f36d7 (2k) 3k	
15458.492	15438	20.352	1.080	5f36d2	-508	8.0	47.9	5f36d2 (4i) 7l	11.9	5f36d2 (4i) 5l	7.7	5f36d2 (4i) 7k	
16244.486	16269	-24.861	0.953	0.960	5f36d2	-580	8.0	43.3	5f36d2 (4i) 5m	14.4	5f36d2 (4i) 7m	9.4	5f36d2 (4i) 5m

Table 4. (continued)

Experimental level ( $\text{cm}^{-1}$ )	Calculated level ( $\text{cm}^{-1}$ )	$D$ (mK)	$g$ (cal.)	$g$ (exp.)	dominant configuration	IS (exp.) (mK)	$J =$	1 <sup>st</sup> component (%)	2 <sup>nd</sup> component (%)	3 <sup>rd</sup> component (%)
17428.301*	17183	46.931	1.093	1.120	5f36d7	-460	8.0	21.3	5f36d7 (4i) 3k	22.2
17540.417	17493	1.127	5f36d2	-183	8.0	10.6	5f36d2 (4i) 5k	26.0	5f36d2 (4i) 7k	19.3
18200	18200	0.986	5f36d7	8.0	26.0	5f36d7 (2k) 3m	18.4	5f36d7 (4i) 3l	12.0	5f36d7 (4i) 5i
18621.395	18659	-28.644	0.898	5f36d2	-189	8.0	33.7	5f36d2 (4i) 5n	7.2	5f36d2 (2k) 3m
18938.085	18855	83.441	1.083	5f36d2	-330	8.0	5.4	5f36d2 (4i) 5l	12.1	5f36d2 (4i) 7l
19142.951*	19515	1.070	5f36d7	-474	8.0	0	5f36d2 (2f) 3k	12.2	5f36d7 (2k) 3m	
19761.706	19828	-66.187	1.128	5f36d2	-409	8.0	25.0	5f36d2 (4i) 7k	10.4	5f36d2 (4i) 7l
20178.161*	20303	1.097	5f36d2	8.0	17.6	5f36d2 (4i) 7l	9.7	5f36d2 (4i) 7k	8.5	5f36d2 (4i) 3m
20738.236	20782	-44.031	1.082	5f36d7	8.0	18.6	5f36d7 (4g) 5i	13.1	5f36d7 (2k) 3l	6.9
21174.671	21171	3.480	0.985	5f36d2	8.0	0	5f36d2 (2i) 1l	13.0	5f36d2 (4i) 5m	11.8
21584	21655	1.070	5f36d2	8.0	6.3	5f36d2 (4i) 5m	11.9	5f36d2 (4i) 7k	8.7	5f36d2 (4i) 5n
22200.841	22162	38.398	1.033	5f36d2	8.0	22.4	5f36d7 (2k) 3l	14.7	5f36d7 (2k) 1l	7.3
22447.933*	22652	1.057	5f36d2	8.0	17.1	5f36d2 (4i) 5m	12.9	5f36d2 (4i) 7k	8.5	5f36d2 (4i) 5m
23001	23128	1.091	5f36d2	8.0	13.0	5f36d2 (4i) 7k	16.7	5f36d2 (4i) 5m	8.1	5f36d2 (4i) 5l
23234	23583	1.053	5f36d7	8.0	14.2	5f36d2 (4i) 3m	10.0	5f36d2 (4i) 7h	6.9	5f36d2 (4f) 7l
23909	28.870	1.124	1.120	5f36d7	9.0	21.3	5f36d7 (2l) 3m	13.7	5f36d7 (2l) 1l	7.9
11308.153	11279	-2.763	1.116	1.090	5f36d2	-451	9.0	18.4	5f36d2 (4i) 5l	7.0
13127.925	13131	1.129	1.175	5f36d7	12	9.0	15.1	5f36d2 (4i) 3m	8.5	5f36d2 (4i) 5l
13535.186*	13313	1.111	1.140	5f36d2	-538	9.0	19.5	5f36d2 (4i) 7h	7.9	5f36d2 (4i) 5k
17882.936*	17696	1.089	1.100	5f36d7	13	9.0	22.8	5f36d7 (4i) 3l	6.0	5f36d7 (2k) 3m
18511.121*	18049	1.091	1.085	5f36d2	-512	9.0	43.4	5f36d2 (4i) 7m	27.1	5f36d7 (4i) 5k
19297.381*	19093	-28.648	1.104	1.135	5f36d2	-547	9.0	8.5	5f36d7 (2k) 3l	37.0
19509.520	19538	-28.648	1.094	1.094	5f36d2	-817	9.0	25.6	5f36d2 (4i) 5m	28.8
20677.968*	20467	1.037	5f36d7	9.0	40.2	5f36d2 (4i) 7l	9.0	5f36d2 (4i) 7k	14.6	5f36d2 (4i) 5n
21136	21614	16.486	1.196	5f36d2	9.0	23.6	5f36d7 (2l) 3n	24.3	5f36d7 (4i) 5l	16.7
22358	79.812	1.163	5f36d2	9.0	41.1	5f36d7 (2k) 3m	14.3	5f36d7 (4i) 3l	8.6	5f36d7 (2k) 3m
22923	1.018	5f36d7	9.0	14.3	5f36d2 (4i) 7l	12.6	5f36d2 (4f) 7i	12.2	5f36d2 (4i) 7k	
23390	1.066	5f36d2	9.0	0.2	5f36d2 (2k) 3l	14.3	5f36d7 (2k) 3l	13.3	5f36d7 (2l) 3m	
23524	1.089	5f36d2	9.0	17.0	5f36d7 (2l) 3m	12.8	5f36d7 (2k) 3l	9.8	5f36d2 (4i) 7k	
23752	1.088	5f36d7	63	10.0	82.3	5f36d7 (4i) 5l	11.3	5f36d7 (2k) 3m	3.5	5f36d2 (4i) 5l
14845.326*	14693	1.186	1.200	5f36d2	-499	10.0	86.3	5f36d2 (4i) 5m	3.9	5f36d2 (4i) 5m
16040.500	16102	-61.397	1.142	1.160	5f36d2	-519	10.0	64.5	5f36d2 (4i) 5m	2.0
20945.148	20927	17.919	1.197	1.210	5f36d2	-511	10.0	44.6	5f36d2 (4i) 5l	5.3
22641.083	36.216	1.230	5f36d2	1.146	5f36d2	10.0	38.2	5f36d2 (4i) 5m	17.3	5f36d2 (4i) 5m
23303.476*	23182	1.089	5f36d7	10.0	43.9	5f36d7 (2k) 3m	18.6	5f36d7 (2l) 3n	9.5	5f36d2 (4i) 5l
23600	18992	-58.459	1.197	1.225	5f36d2	-502	11.0	88.8	5f36d2 (4i) 5n	1.9
23673.434	23698	-24.160	1.243	1.239	5f36d2	-501	11.0	69.9	5f36d2 (4i) 5m	9.3
21835	1.239	5f36d2	12.0	86.6	5f36d2 (4i) 7m	9.5	5f36d2 (2k) 5n	3.0	5f36d2 (4i) 5m	

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