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Low-Lying Electronic States of the ScF Molecule: Energies of the $a\ ^3\Delta$, $b\ ^3\Pi$, and $A\ ^1\Delta$ States

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Dispersed laser-induced fluorescence spectra of ScF have been recorded on a Fourier transform spectrometer. Most of the emission corresponds either to pure singlet or to pure triplet transitions, but excitation of perturbed levels of the $D\ ^1\Pi$ state results in fluorescence to both triplet and singlet states. The triplet states of ScF were thus located in energy with respect to the singlet ground state. Constants are reported for the observed low-lying singlet and triplet states: $A\ ^1\Delta$, $a\ ^3\Delta$, and $b\ ^3\Pi$. © 1993 Academic Press, Inc.

INTRODUCTION

The electronic structure and bonding in transition metal compounds have been extensively studied with a view to understanding the role of the *d* electrons. The ScF molecule provides a good starting point in such an investigation, because its electronic structure is relatively simple. Scandium is the first of the transition metal elements, with the fewest electrons, and (at least in the low-lying electronic states) only one *d* electron should be involved in the metal–ligand bond. As a result, scandium monofluoride has been extensively studied both experimentally and theoretically, and many of its low-lying electronic states are quite well characterized.

Absorption and emission spectroscopy of scandium monofluoride have allowed transitions involving low-lying singlet (*1–5*) and triplet states (*3, 6*) to be observed. McLeod and Weltner (*7*) used a matrix isolation experiment to show that the ground state of ScF was a $^1\Sigma^+$ state, but the energy gap between the ground state and the lowest triplet state remained an unknown quantity (*8, 9*). Ab initio calculations by Harrison in 1983 (*10*) gave a detailed picture of the electronic states of ScF up to the $Sc^+\ 3d^2$ dissociation limit, and in 1988 Langhoff *et al.* (*11*) published a theoretical study of ScF in which a more extensive atomic basis set was used to calculate electronic states of ScF up to 28 000 cm^{-1}. The permanent electric dipole moment of the ground state calculated in Ref. (*11*) is in full agreement with the value reported recently by Simard and co-workers (*12*), obtained from optical Stark splitting measurements.

By means of a laser-induced fluorescence experiment with a hot source, we were able to study rotationally simplified spectra without reducing the rotational or vibrational temperature of the molecules, thus obtaining data covering a wide range of rotational levels in various electronic states. By exciting perturbed upper state levels, which give transitions to singlet and triplet states simultaneously, we were also able to establish the energies of the low-lying triplet states with respect to the ground $X\ ^1\Sigma^+$ state.

EXPERIMENTAL DETAILS

ScF vapor was produced by placing a mixture of Sc and ScF_3 powder in the tantalum heater of a vacuum furnace, with argon as a buffer gas. This furnace has been described

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elsewhere (*13*). The operating pressure was typically 2–5 Torr, but in some cases it was increased to 30 Torr in order to enhance rotational relaxation. Heating the mixture to 1500–1800 K formed ScF vapor, which was excited by several fixed-frequency lines from an argon ion laser, and by the 568.2-nm line from a krypton ion laser. Both lasers were used in multimode operation. The Ar^+ laser was a Spectra Physics 2045, and allowed us to excite ScF with the 514.5-nm (3 W), 457.9-nm (1.9 W), 465.8-nm (0.5 W), and 454.5-nm (0.2 W) lines. The Kr^+ laser was a Coherent Innova 200-K3 model, which gave an output power of 1.3 W at 568.2 nm. Backward fluorescence from this source was collected with a pierced mirror to attenuate the laser line and focused into a fused silica optical fiber (core diameter, 1 mm). Care was taken to reduce the strong black body emission from the wall of the tantalum heater by placing a diaphragm in front of the optical fiber. The other end of the optical fiber was placed at the entrance aperture of a commercial Fourier transform spectrometer (Bomem DA3). Dispersed fluorescence spectra were recorded in the visible and near-infrared regions at a resolution varying from 0.04 to 0.10 cm^{-1} using either a Si detector or a photomultiplier tube. Recording times varied according to the intensity of the fluorescence signal, but were generally about 2 hr. The supply of scandium and scandium fluoride usually needed to be renewed after about 3 days of operation.

RESULTS

We recorded laser-induced fluorescence transitions between a number of singlet and triplet states of ScF. The transitions we have observed are indicated in Fig. 1, which summarizes the experimentally known states of ScF and compares experimental and calculated (*11*) term values. Details of the excitation and subsequent emission associated with the different laser lines used are given in Table I. For the sake of consistency, we have adopted the labeling of the excited electronic states proposed in Ref. (*11*). The wavenumbers of the main fluorescence lines are listed in Table II.

The strongest features of the fluorescence spectra were bands belonging to the $D\,{}^1\Pi - X\,{}^1\Sigma^+$ and $D\,{}^1\Pi - A\,{}^1\Delta$ systems. Rotational relaxation was observed in both the D-X and D-A fluorescence, but the information for all other systems was limited to direct emission from the rovibronic level populated by the resonant pump transition. The presence of more than one series of lines for most of the observed transitions made it possible to deduce effective spectroscopic constants for the lower electronic states involved in fluorescence from a least-squares fit, which assumed that the rovibrational levels of each state could be expressed by the simple case (a) formula: $T_{v,J} = \sum_{lm} Y_{lm} (v + \frac{1}{2})^l \cdot (J(J+1))^m$.

The spectroscopic constants derived from fitting rotational and vibrational energies of the lower states observed in fluorescence to such a formula are presented in Table III. They allow the observed levels of the lower singlet states with $v \leq 10$ to be recalculated to within 0.04 cm^{-1}, and those of lower triplet states to within 0.2 cm^{-1}. Several factors contribute to the difficulties encountered in determining constants for the triplet states. In general, little rotational information was available, and this led us to constrain B_0 for the $a\,{}^3\Delta_{1,2}$ substates to take the values given in Ref. (*8*). Further approximation in the rotational constants arises because Λ-doubling has been neglected in this work. For the ${}^3\Pi - {}^3\Pi$, ${}^3\Pi - {}^3\Delta$, or ${}^3\Delta - {}^3\Delta$ transitions, we cannot tell which Λ-doubling components are involved. In the $D\,{}^1\Pi - a\,{}^3\Delta$ transitions, we can of course identify the parity of the upper state level from the pump transition, and hence the lower state components, but from the few R-Q and Q-P combination differences we can measure in the $a\,{}^3\Delta_{1,2}$ substates, we find that the splitting is negligible anyway. It

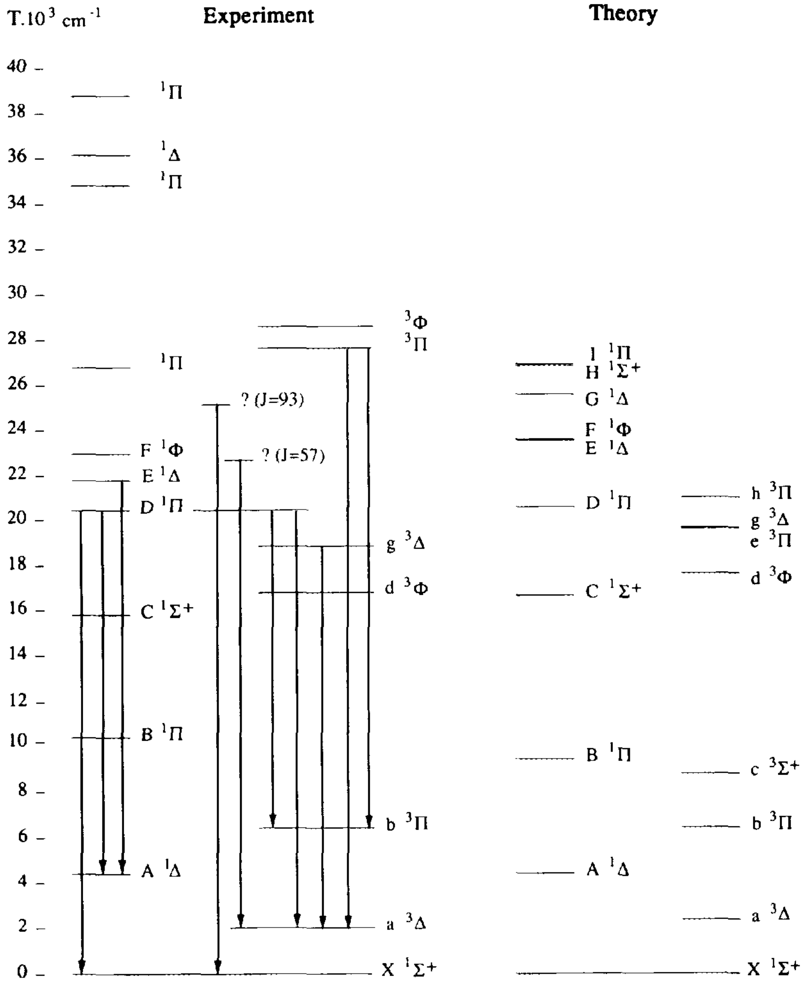

FIG. 1. Experimental and theoretical (*11*) term energies for the electronic states of ScF, indicating the transitions observed in fluorescence.

is also possible that the simple case (a) expression is not particularly well suited to multiplet states for which $A\Lambda/B \sim 150$. The errors contained in this simplified treatment are carried over into the calculation of the molecular constants for the triplet states given in Table III. The simple expression for the energy levels is not appropriate for the excited states, which are poorly represented and often perturbed, and have not been considered in this work. We have therefore reproduced the measured wavenumbers in Table II.

Much of the laser-induced fluorescence we recorded was either purely singlet or purely triplet emission. However, the 454.5- and 465.8-nm lines from the Ar$^+$ laser excited perturbed levels of the $D\,{}^1\Pi$ state ($v' = 4$ and $v' = 2$, respectively), which resulted in fluorescence to both singlet and triplet states. Part of the spectrum excited by 454.5 nm, illustrating fluorescence to both $X\,{}^1\Sigma^+$ and $a\,{}^3\Delta_{1,2}$ states, is shown in Fig. 2. The energies of the triplet states observed through forbidden transitions with $\Delta S \neq 0$, (namely $b\,{}^3\Pi_1$ and $a\,{}^3\Delta_{1,2}$) could thus be established with respect to the

TABLE I

Laser Induced Fluorescence Transitions in ScF

Excitation				v" observed in fluorescence in low-lying state					
Laser (nm)	Line	(v'-v")	system	X $^1\Sigma$	A$^1\Delta$	a $^3\Delta_1$	a $^3\Delta_2$	b $^3\Pi_0$	b $^3\Pi_1$
457.9	R (44)	(5-2)	D $^1\Pi$ - X $^1\Sigma^+$	0-3, 5-10	4-7				
	Q (34)	(5-2)	D $^1\Pi$ - X $^1\Sigma^+$	0-3, 5-10	4-7				
514.5	R (59)	(1-2)	D $^1\Pi$ - X $^1\Sigma^+$	0-5	0-2				
	P (64)	(0-1)	D $^1\Pi$ - X $^1\Sigma^+$	0-5	0				
	R (53)	(0-1)	(?) E $^1\Delta$ - a $^3\Delta_3$		0				
	P (94)	(?-3)	? - X $^1\Sigma^+$	2-7, 9-13, 15					
454.5	R (32)	(4-1)	D $^1\Pi$ - X $^1\Sigma^+$	0-2, 4, 6-8	3-5	3, 4, 7, 10	3-5, 7-11		
	R (33)	(0-0)	$^3\Pi_0$ - b $^3\Pi_0$			0		0	
	R (36)	(0-0)	$^3\Pi_1$ - b $^3\Pi_1$				0		0
465.8	P (39)	(2-0)	D $^1\Pi$ - X $^1\Sigma^+$	0-6	1-3		0-2		0
	Q (57)	(?-0)	? - X $^1\Sigma^+$			2-5, 7-9			
568.0	R (52)	(1-0)	g $^3\Delta_1$ - a $^3\Delta_1$			0-5	1		
	R (47)	(1-0)	g $^3\Delta_1$ - a $^3\Delta_1$			0-4			

singlet states directly, and from triplet–triplet transitions involving these states (either observed here or previously reported (*8, 9*)), the energies of the known triplet states of ScF could be determined.

DISCUSSION

At this point, we were able to compare theoretical and experimental term energies for the known electronic states of ScF (see Fig. 1 and Table IV). The theoretical values are the (MRCI + Q + rel) values given in Table IX of Ref. (*11*), for which quadruple excitation terms and a relativistic correction are taken into account after the multireference configuration interaction calculation. Experimental values for the electronic states which were not observed in this work are from Refs. (*4–6, 8*). There is a good match between theoretical constants and the experimentally determined parameters of both multiplicities, particularly for the low-lying states. The molecular constants quoted in Table III confirm earlier experimental results (values available from Refs. (*4, 8*) are given in faint type in Table III), which concerned only the lowest vibrational levels of the $X\ ^1\Sigma^+$, $A\ ^1\Delta$, and $a\ ^3\Delta$ electronic states. Our measurements, which are from Fourier transform records rather than from spectra taken on photographic plates, should be more reliable than the older data in terms of wavenumber calibration, but more importantly, our extension of the observed vibrational levels in the $X\ ^1\Sigma^+$, $A\ ^1\Delta$, and $a\ ^3\Delta$ states ought to make this set of parameters useful for future work.

A few comments arise from the spectra themselves. Although the $D\ ^1\Pi$ state of ScF is well known (it has been referred to in the past (*3, 8, 9*) as $E\ ^1\Pi$), and the low-lying $A\ ^1\Delta$ state has also been studied (*4*), the D-A transition had not been identified before. The strong D-A and D-X fluorescence progressions observed here have extended the range of known vibrational levels to $v = 7$ in $A\ ^1\Delta$, and up to $v = 15$ in the X state. The upper states involved in laser-induced fluorescence experiments are frequently poorly represented because of the selectivity of the technique, and although we observed

TABLE II

Measured Wavenumbers of Main Fluorescence Lines in ScF (cm^{-1})

Fluorescence excited by 454.5 nm

D $^1\Pi$ - A $^1\Delta$

v"	R (32)	Q (33)	P (34)
5	15088.057	15064.946	15041.145
4	15700.501	15677.234	15653.263
3	16318.935	16295.500	16271.362

D $^1\Pi$ - a $^3\Delta_2$

v"	R (32)	P (34)
11	14072.571	14027.455
10	14653.022	14607.577
9	15239.214	15193.445
7	16429.035	16382.606
5	17642.432	17595.352
4	18258.126	18210.697
3	18879.857	18832.094
2	19507.702	-

$^3\Pi_0$ - a$^3\Delta_1$

v"	R (33)	Q (34)	P (35)
0	26309.345	26284.878	26259.706

$^3\Pi_1$ - a$^3\Delta_2$

v"	R (36)	Q (37)	P (38)
0	26295.732	26268.814	26241.17

D $^1\Pi$ -X $^1\Sigma^+$

v"	R (32)	P (34)
8	17118.788	17068.984
7	17794.515	17744.356
6	18477.170	18426.659
4	19863.417	19812.201
2	21277.868	21225.942
1	21995.769	21943.493
0	22720.850	22668.216

D $^1\Pi$ - a $^3\Delta_1$

v"	R (32)	P (34)
10	14715.515	14670.578
7	16491.417	16445.518
4	18320.394	18273.500
3	18942.082	18894.880

$^3\Pi_0$ - b$^3\Pi_0$

v"	R (33)	P (35)
0	21995.78	21948.01

$^3\Pi_1$ - b$^3\Pi_1$

v"	R (36)	P (38)
0	21995.78	21943.08

Fluorescence excited by 457.9 nm

D $^1\Pi$ - A $^1\Delta$

v"	R (44)	Q (45)	P (46)
7	14473.224	14442.233	14410.559
6	15071.595	15040.386	15008.492
5	15675.832	15644.401	15612.280
4	16285.998	16254.346	16221.997

D $^1\Pi$ - A $^1\Delta$

v"	R (33)	Q (34)	P (35)
7	14463.066	14439.620	14415.446
6	15063.561	15039.925	15015.598
5	15669.899	15646.097	15621.598
4	16282.191	16258.215	16233.544

D $^1\Pi$ -X $^1\Sigma^+$

v"	R (44)	P (46)
10	16360.616	16294.086
9	17020.214	16953.181
8	17686.572	17619.114
7	18359.905	18291.940
6	19040.133	18971.689
5	19727.314	19658.391
3	21122.735	21052.850
2	21831.043	21760.693
1	22546.511	22475.663
0	23269.135	23197.806

D $^1\Pi$ - X $^1\Sigma^+$

v"	Q (34)
10	16343.808
9	17005.448
8	17673.936
7	18349.310
6	19031.618
5	19720.881
3	21120.487
2	21831.043
1	22548.451
0	23273.176

Fluorescence excited by 465.8 nm

D $^1\Pi$ - A $^1\Delta$

v"	R (37)	Q (38)	P (39)
3	15134.716	15107.755	15080.093
2	15758.305	15731.156	15703.299
1	16387.975	16360.631	16332.581

D$^1\Pi$ - a$^3\Delta_2$

v"	R (37)	Q (38)	P (39)
3	-	17668.080	-
2	18322.099	18294.838	-
1	18955.222	18927.770	18899.603
0	19594.534	19566.895	19538.535

? - a$^3\Delta_1$

v"	R (56)	P (58)
9	14205.352	-
8	14792.146	14714.247
7	15384.777	15306.328
5	16587.771	16508.202
4	17198.164	17118.071
3	17814.640	17733.936
2	18437.190	18355.909

D $^1\Pi$ -X $^1\Sigma^+$

v"	R(37)	P(39)
6	17285.275	17227.278
5	17973.975	17915.573
4	18669.686	18610.876
3	19372.435	19313.220
2	20082.271	20022.650
1	20799.247	20739.213
0	21523.389	21462.832

D $^1\Pi$ - b$^3\Pi_1$

v"	R (37)	P (39)
0	15293.455	15239.242

Fluorescence excited by 514.5 nm

D $^1\Pi$ - A $^1\Delta$

v"	R (59)	Q (60)	P (61)
2	15169.689	15127.063	15083.742
1	15794.015	15751.090	15707.464
0	16424.451	16381.223	16337.285

D $^1\Pi$ - A $^1\Delta$

v"	R (62)	Q (63)	P (64)
0	15821.922	15776.579	15730.530

? - X $^1\Sigma^+$

v"	R (92)	P (94)
15	11819.581	11690.183
13	13044.026	12912.593
12	13666.101	13533.684
11	14294.896	14161.496
10	14930.431	14796.050
9	15572.737	15437.378
7	16877.829	16740.492
6	17540.690	17402.361
5	18210.508	18071.190
4	18887.271	18746.965
3	19571.076	19429.770
2	20261.939	20119.654

D $^1\Pi$ -X $^1\Sigma^+$

v"	R (59)	P (61)
5	17338.280	17246.990
4	18028.342	17936.414
3	18725.442	18632.878
2	19429.770	19336.413
1	20140.922	20047.073
0	20859.397	20764.900

D $^1\Pi$ -X $^1\Sigma^+$

v"	R (62)	P (64)
5	16729.443	-
4	17418.614	17322.211
3	18114.749	18017.678
2	18817.961	18720.217
1	19528.299	19429.770
0	20245.817	20146.719

E $^1\Delta$ - A $^1\Delta$

v"	R(53)	P(55)
0	17567.212	17488.555

Fluorescence excited by 568.0 nm

g $^3\Delta_1$ - a $^3\Delta_2$

v"	R (52)	Q (53)	P (54)
1	16890.063	16851.912	16813.061

g $^3\Delta_1$ - a $^3\Delta_1$

v"	R(47)	P(49)
8	12671.553	-
5	14470.154	-
4	15082.276	15014.578
3	15701.254	15633.068
2	16326.320	16257.654
1	16957.538	16888.378
0	17594.890	17525.301

g $^3\Delta_1$ - a $^3\Delta_1$

v"	R (52)	P (54)
8	12677.360	-
5	14476.509	14402.409
4	15088.008	15013.379
3	15705.542	15630.387
2	16329.156	16253.477
1	16958.920	16882.710
0	17594.890	17518.134

TABLE III

Constants (cm^{-1}) for some Low-Lying States of ScF

	$X\,^1\Sigma^+$	$A\,^1\Delta$	$a\,^3\Delta_1$	$a\,^3\Delta_2$	$b\,^3\Pi_0$	$b\,^3\Pi_1$
T_e	0.0	4586.0(3)	1953.8(8)	2011.7(4)	6240(2)$^{(b)}$	6287(1)$^{(b)}$
ω_e	735.00 735.6	645.54(3)	649.3(2) 648.9	649.3(3) 648.9		
$\omega_e x_e$	3.604(3) 3.8	3.101(9)	3.17(6)	3.17(6) 3.03		
10^3 $\omega_e y_e$	6.2(2)	7.2(7)	9(3)	9.4(3)		
B_e	0.39514(2) 0.3950	0.36486(2) 0.3651	0.36234$^{(a)}$ 0.3623	0.3665$^{(a)}$ 0.3665	0.346$^{(c)}$	0.352$^{(c)}$
10^3 α_e	2.638(5) 2.66	2.53(7) 2.9	2.58(4) 2.5	2.57(1) 2.54		
10^6 γ_e		6.0(9)	11(4)	7(1)		
10^7 D_e	4.618(20)	4.68(3)	4.0(1)	5.0(1)		
10^{10} β_e	4(3)					

[a] Deduced from B_0 given in Ref. (*8*).
[b] T_0.
[c] B_0 estimated from $\Delta_2 F$.

some rotational relaxation in $D\,^1\Pi$, these lines showed that levels with $v' \geqslant 2$ are strongly perturbed. It is hoped that future experiments will furnish enough data to make it possible to deperturb these levels, giving information about the perturbing triplet state at the same time.

These perturbations explain the appearance of transitions with $\Delta S \neq 0$, which were

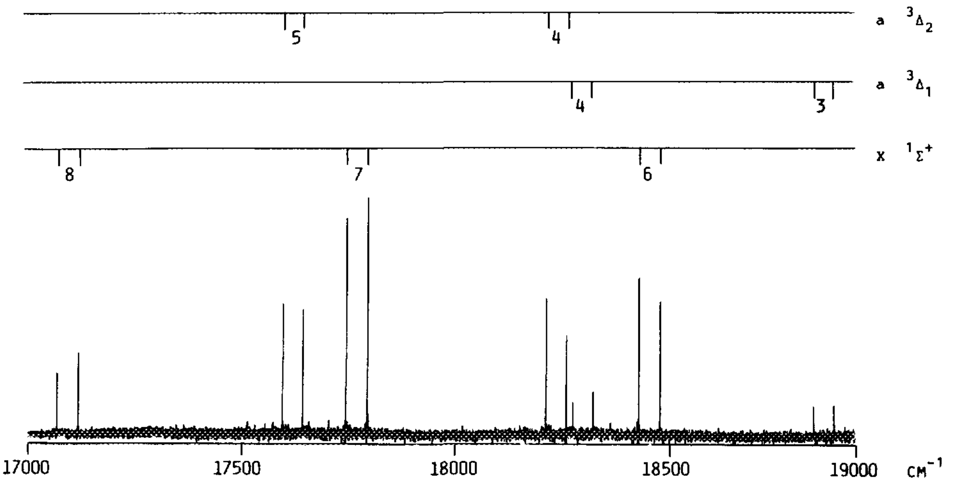

FIG. 2. Part of the fluorescence spectrum of ScF excited by 454.5 nm, showing transitions to both singlet and triplet states. The laser pumps $J' = 33$, $v' = 4$ in $D^1\Pi$. Vibrational numbering is given for the $X\,^1\Sigma^+$, $a^3\Delta_1$, and $a^3\Delta_2$ states.

TABLE IV

Comparison of Experimental and Ab Initio (Ref 11) T_e and R_e Values

State	T_e (cm^{-1})		R_e (Å)	
	Expt	Calc	Expt	Calc
$^1\Pi$	38806.1 [1,2]	-	1.854_3 [1,2]	-
$^1\Pi$	35009 [1]	-	1.82_7 [1,2]	-
$^1\Delta$	31549.25 [2,4]	-	1.8125 [2,4]	-
$^3\Phi_3$	29139.8 [1,2]	-	1.915_3 [1,2]	-
$^3\Phi_2$	29049.2 [1,2]	-	1.923_1 [1,2]	-
$^3\Pi_1$	28252.5 [2]	-	-	-
$^3\Pi_0$	28208.5 [2]	-	-	-
$^1\Pi$	26891.5 [1]	27755	1.909_8 [1]	1.924
F $^1\Phi$	22903.6 [2,3]	24026	1.8674 [2,3]	1.875
E $^1\Delta$	22105.0 [2,3]	23791	1.8937 [2,3]	1.899
D $^1\Pi$	20383.5 [1]	21150	1.864_8 [1]	1.873
g $^3\Delta_2$	19139 [3]	20449	-	-
g $^3\Delta_1$	19067 [3]	-	-	-
d $^3\Phi_3$	17328.5 [1]	18364	1.896_1 [1,2]	1.894
d $^3\Phi_2$	17227.4 [1]	-	1.901_8 [1,2]	-
C $^1\Sigma^+$	16164.7 [1]	16769	1.906_5 [1]	1.928
B $^1\Pi$	$\leq$ 10735.5 [1]	9578	1.9181 [1]	1.928
b $^3\Pi_1$	6287 [2]	6434	$<$ 1.894 [2]	1.902
b $^3\Pi_0$	6240 [2]	-	$<$ 1.909 [2]	-
A $^1\Delta$	4586.6	4482	1.8600	1.884
a $^3\Delta_2$	2011.7	2362	1.855_9 [1]	1.876
a $^3\Delta_1$	1953.8	-	1.866_6 [1]	-
X $^1\Sigma^+$	0.0	0.0	1.7873	1.796

[1] Value taken from Ref. (*8*).

[2] Constant for $v = 0$.

[3] Value taken from Ref. (*6*).

[4] Value taken from Ref. (*5*).

the focus of this study. In studying the forbidden bands, we found that different fluorescence patterns were seen following excitation to different levels of $D\ ^1\Pi$. From $v' = 2$ in $D\ ^1\Pi$ we observed a *P*, *R* doublet in fluorescence to $b\ ^3\Pi_1$ and a *P*, *Q*, *R* triplet in fluorescence to $a\ ^3\Delta_2$, whereas Fig. 2 illustrates that from the more strongly perturbed $v' = 4$ level of $D\ ^1\Pi$, *P*, *R* doublets were seen in fluorescence both to $a\ ^3\Delta_1$ and to $a\ ^3\Delta_2$. A transition with $\Delta S \neq 0$ is also the most likely explanation for the series of fluorescence lines with $J' = 93$ excited by 514.5 nm and for the fluorescence with $J' = 57$ excited by 465.8 nm (see Tables I and II). The upper levels do not correspond to a known singlet state and probably belong to either the $e\ ^3\Pi$ or the $h\ ^3\Pi$ state calculated in Ref. (*11*). Another instance of singlet–triplet excitation seems to occur in the pump transition $R(53)$ (0–1) $E\ ^1\Delta \leftarrow a\ ^3\Delta_3$, which is resonant with the 514.5-nm line of the argon laser and gives rise to the $E\ ^1\Delta$–$A\ ^1\Delta$ fluorescence series in Table II. The $E\ ^1\Delta$ state is already known (*4*), and the only likely lower state for this excitation is the $a\ ^3\Delta_3$ state.

The 454.5-nm line of the argon ion laser coincides with transitions involving two components in the (0–0) band of the strong violet degraded triplet system which has been discussed before (*3, 6, 9–11*). Fluorescence close to the laser line consists of P, R doublets (see Table II), corresponding to a transition with $\Delta\Lambda = 0$. At shorter wavelengths, a second system is observed in fluorescence, which shows R, Q, and P lines. The combination differences between these lines, which are observed around 26 300 cm^{-1}, agree with calculated combination differences for the $a\ ^3\Delta_{1,2}$ substates, and the P, Q, R triplet is characteristic of a transition with $\Delta\Lambda = -1$. We therefore assign the upper state for both these transitions as $^3\Pi$, and from the newly established energy of $a\ ^3\Delta$, we find that the upper $^3\Pi$ state lies at about 28 000 cm^{-1}, and is above the range of states calculated in Ref. (*11*). We have not given this state a label for this reason, but it is very likely that the upper state is the fourth $^3\Pi$ state calculated by Harrison (*10*) to have $T_e = 32\ 000\ \text{cm}^{-1}$ and $R_e = 1.932$ Å. Although the term energy calculated in Ref. (*10*) is higher than observed, the prediction for its internuclear distance matches rather well. The violet system is thus reassigned as $^3\Pi \rightarrow b\ ^3\Pi$, confirming suggestions made both by Harrison and by Langhoff and coauthors (*11*), that this system does not involve the $a\ ^3\Delta$ state.

CONCLUSION

Laser-induced fluorescence spectra have allowed us to measure the energy gap between the lowest singlet and the lowest triplet states in ScF, and have extended the range of observed vibrational levels in the low-lying electronic states. The $D\ ^1\Pi - A\ ^1\Delta$ and $^3\Pi - b\ ^3\Pi$ transitions have been identified, and a new triplet transition, $^3\Pi_{0,1} \rightarrow a\ ^3\Delta_{1,2}$, has been recorded. Preliminary spectroscopic constants are reported for a number of low-lying states, which confirm the quality of existing ab initio calculations for a number of electronic states in scandium monofluoride.

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