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# High-Resolution Infrared Emission Spectrum of CaF

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The high-resolution infrared emission spectrum of calcium monofluoride has been observed with a Fourier transform spectrometer. A total of 790 rovibrational transitions, from the $v = 1 \rightarrow 0$ to $v = 8 \rightarrow 7$ bands have been assigned. This set of infrared data has been combined with existing microwave data to yield improved Dunham $Y_{ij}$ coefficients for the $X^2\Sigma^+$ electronic ground state of CaF. © 1995 Academic Press, Inc.

## INTRODUCTION

CaF has enjoyed a renewed interest in recent years primarily due to its potential astrochemical importance and in the study of Rydberg states. The existing work on CaF has almost exclusively been the study of optical transitions by various spectroscopic techniques. The rotational analysis of the $A^2\Pi$–$X^2\Sigma^+$ transition has been extensively studied using laser excitation (*1*), microwave–optical double resonance (*2*), and intermodulated fluorescence (*3*) spectroscopy. The analysis of nine bands of the $B^2\Sigma^+$–$X^2\Sigma^+$ transition by Dulick *et al.* (*4*), of the 0–0 band of the $C^2\Pi$–$X^2\Sigma^+$ system by Ernst *et al.* (*5*), and of both the $E^2\Sigma^+$–$A^2\Pi$ and $E'^2\Pi^+$–$A^2\Pi$ transitions by Bernath and Field (*6*) has also been carried out using similar methods. More recently the characterization of the $B'^2\Delta$ state was performed by Vergès *et al.* (*7*) using a Fourier transform spectrometer to detect krypton-ion laser-induced fluorescence. In addition, Childs *et al.* have measured an electric dipole moment of 3.07 D in the CaF $X^2\Sigma^+$ ($v = 0$) ground state (*8*), as well as the $v$ and $N$ dependence of the spin–rotation and hyperfine interactions (*9*, *10*).

With the recent confirmation of the detection of AlF toward the circumstellar envelope of the carbon star IRC + 10216 (*11*), Anderson *et al.* (*12*) recorded and analyzed the pure rotational spectrum of CaF in the four lowest vibrational levels of its ground state. Since calcium and aluminum have similar cosmic abundances, CaF may be detected in similar environments.

There has been extensive work on the Rydberg states of CaF by Field and coworkers (*13–16*). The large dipole moment of the $CaF^+$ ion-core causes extensive $l$-mixing of the Rydberg states, and CaF serves as a prototypical example of this type of Rydberg energy level pattern. In this paper, we present the first observation and analysis of the Fourier transform infrared emission spectrum of CaF.

## EXPERIMENTAL DETAILS

The high-resolution infrared emission spectrum of CaF was observed with a Bruker IFS 120 HR Fourier transform spectrometer. The gas-phase CaF was produced by heating $CaF_2$ powder to a temperature of 1600°C in a commercial CM Rapid Temp

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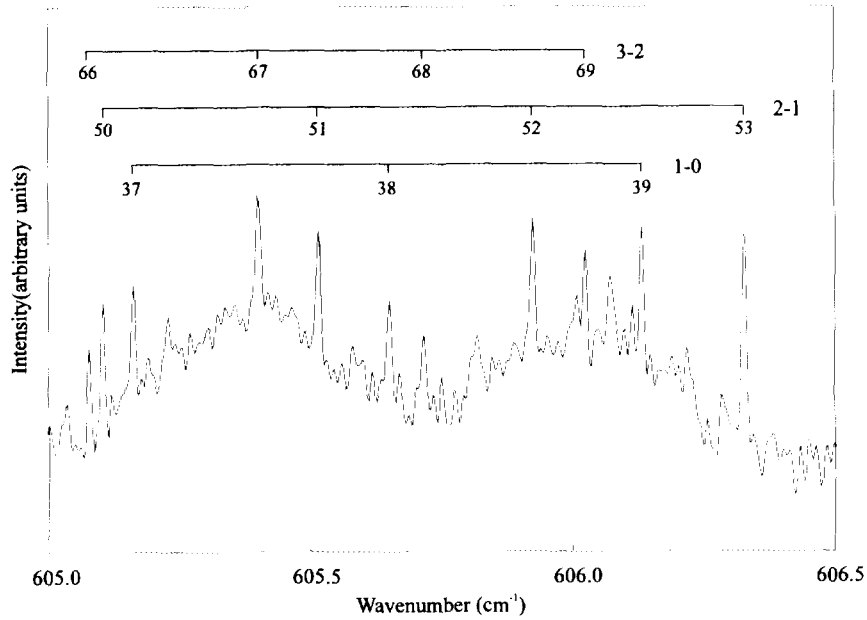


FIG. 1. A portion of the $R$ branch of the vibration–rotation spectrum of CaF. The 1–0, 2–1, and 3–2 bands are marked along with the $N''$ value.

Furnace. The cell design consisted of an alumina ($Al_2O_3$) tube 1.2 m in length protected inside by a carbon liner. The tube was centered in the furnace and slowly brought up to the operating temperature at a rate of 200°C/hr. Impurities were removed from the system by pumping on the cell up to a temperature of 1000°C. Argon buffer gas

TABLE I

Dunham Coefficients for the $X^2\Sigma^+$ Ground State of CaF

| Dunham Coefficient | Value ($cm^{-1}$) |
|---|---|
| $Y_{10}$ | 588.67608(29) |
| $Y_{20}$ | -2.91259(12) |
| $10^3 Y_{30}$ | 8.514(20) |
| $10^6 Y_{40}$ | -6.1(11) |
| $Y_{01}$ | 0.3437181(12) |
| $10^3 Y_{11}$ | -2.444671(93) |
| $10^6 Y_{21}$ | 4.917(20) |
| $10^8 Y_{31}$ | 2.77(12) |
| $10^7 Y_{02}$ | -4.6954(20) |
| $10^{10} Y_{12}$ | -1.29(11) |
| $10^{11} Y_{22}$ | 2.37(12) |

TABLE II

Observed Rovibrational Line Positions of the $X^2\Sigma^+$ State of CaF in $cm^{-1}$ [Observed-Calculated Values Are Shown in the Column Labeled $\Delta$ (in Units of $10^{-4}$ $cm^{-1}$)]

| 1 0 Band | | | | 2 1 Band | | | | 3 2 Band | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $N'$ | $N''$ | Observed | $\Delta$ | $N'$ | $N''$ | Observed | $\Delta$ | $N'$ | $N''$ | Observed | $\Delta$ |
| 67 | 68 | 525.7646 | -8 | 67 | 68 | 520.3938 | -13 | 57 | 58 | 524.6208 | -6 |
| 66 | 67 | 526.7509 | -2 | 65 | 66 | 522.3485 | -13 | 56 | 57 | 525.5521 | -12 |
| 65 | 66 | 527.7304 | -22 | 63 | 64 | 524.2887 | 7 | 55 | 56 | 526.4810 | -0 |
| 64 | 65 | 528.7105 | 5 | 62 | 63 | 525.2499 | -12 | 54 | 55 | 527.4041 | -4 |
| 63 | 64 | 529.6839 | 6 | 61 | 62 | 526.2097 | -1 | 53 | 54 | 528.3234 | -4 |
| 62 | 63 | 530.6538 | 13 | 60 | 61 | 527.1643 | -2 | 52 | 53 | 529.2398 | 10 |
| 61 | 62 | 531.6180 | 6 | 59 | 60 | 528.1149 | -1 | 51 | 52 | 530.1493 | -4 |
| 60 | 61 | 532.5798 | 16 | 58 | 59 | 529.0610 | -3 | 50 | 51 | 531.0557 | -5 |
| 59 | 60 | 533.5362 | 14 | 57 | 58 | 530.0035 | 1 | 49 | 50 | 531.9600 | 15 |
| 58 | 59 | 534.4843 | -30 | 56 | 57 | 530.9413 | -0 | 48 | 49 | 532.8551 | -15 |
| 57 | 58 | 535.4336 | -19 | 54 | 55 | 532.8039 | -6 | 46 | 47 | 534.6393 | -6 |
| 56 | 57 | 536.3776 | -19 | 52 | 53 | 534.6511 | 3 | 45 | 46 | 535.5265 | 14 |
| 55 | 56 | 537.3200 | 8 | 51 | 52 | 535.5688 | 12 | 43 | 44 | 537.2817 | -8 |
| 54 | 55 | 538.2546 | -2 | 50 | 51 | 536.4809 | 9 | 42 | 43 | 538.1559 | 12 |
| 52 | 53 | 540.1156 | 26 | 49 | 50 | 537.3876 | -6 | 41 | 42 | 539.0226 | -0 |
| 51 | 52 | 541.0361 | 4 | 48 | 49 | 538.2916 | -6 | 40 | 41 | 539.8844 | -18 |
| 50 | 51 | 541.9523 | -18 | 47 | 48 | 539.1909 | -9 | 39 | 40 | 540.7449 | -4 |
| 48 | 49 | 543.7787 | 6 | 46 | 47 | 540.0865 | -6 | 38 | 39 | 541.6017 | 16 |
| 47 | 48 | 544.6810 | -26 | 45 | 46 | 540.9806 | 25 | 37 | 38 | 542.4514 | 9 |
| 46 | 47 | 545.5818 | -29 | 44 | 45 | 541.8651 | 3 | 36 | 37 | 543.2964 | -1 |
| 45 | 46 | 546.4810 | -6 | 43 | 44 | 542.7467 | -4 | 35 | 36 | 544.1387 | 7 |
| 44 | 45 | 547.3747 | 7 | 42 | 43 | 543.6247 | -4 | 34 | 35 | 544.9746 | -6 |
| 43 | 44 | 548.2630 | 8 | 41 | 42 | 544.4984 | -3 | 33 | 34 | 545.8067 | -12 |
| 42 | 43 | 549.1449 | -9 | 40 | 41 | 545.3675 | -5 | 32 | 33 | 546.6365 | 3 |
| 41 | 42 | 550.0247 | -5 | 39 | 40 | 546.2323 | -4 | 31 | 32 | 547.4584 | -16 |
| 40 | 41 | 550.9005 | 4 | 38 | 39 | 547.0921 | -11 | 30 | 31 | 548.2807 | 13 |
| 39 | 40 | 551.7710 | 4 | 37 | 38 | 547.9486 | -6 | 29 | 30 | 549.0937 | -6 |
| 38 | 39 | 552.6380 | 12 | 36 | 37 | 548.8031 | 23 | 28 | 29 | 549.9037 | -10 |
| 37 | 38 | 553.4976 | -9 | 35 | 36 | 549.6477 | -3 | 27 | 28 | 550.7121 | 16 |
| 36 | 37 | 554.3560 | 3 | 34 | 35 | 550.4902 | -5 | 26 | 27 | 551.5117 | -1 |
| 35 | 36 | 555.2084 | -1 | 33 | 34 | 551.3294 | 4 | 25 | 26 | 552.3073 | -14 |
| 34 | 35 | 556.0572 | 4 | 32 | 33 | 552.1631 | 3 | 24 | 25 | 553.1009 | -2 |
| 33 | 34 | 556.9026 | 19 | 31 | 32 | 552.9911 | -11 | 23 | 24 | 553.8894 | 6 |
| 32 | 33 | 557.7398 | -2 | 30 | 31 | 553.8150 | -20 | 22 | 23 | 554.6724 | 4 |
| 30 | 31 | 559.4069 | 17 | 29 | 30 | 554.6349 | -24 | 21 | 22 | 555.4524 | 18 |
| 29 | 30 | 560.2305 | -5 | 28 | 29 | 555.4524 | -7 | 20 | 21 | 556.2247 | 0 |
| 28 | 29 | 561.0524 | 1 | 27 | 28 | 556.2659 | 14 | 19 | 20 | 556.9936 | -5 |
| 27 | 28 | 561.8699 | 9 | 26 | 27 | 557.0721 | 9 | 18 | 19 | 557.7587 | -3 |
| 26 | 27 | 562.6840 | 27 | 25 | 26 | 557.8728 | -6 | 17 | 18 | 558.5215 | 23 |
| 25 | 26 | 563.4890 | 2 | 24 | 25 | 558.6713 | 1 | 15 | 16 | 560.0265 | 7 |
| 24 | 25 | 564.2923 | 4 | 23 | 24 | 559.4645 | 2 | 14 | 15 | 560.7707 | -14 |
| 23 | 24 | 565.0905 | 1 | 22 | 23 | 560.2540 | 13 | 11 | 12 | 562.9818 | -14 |
| 22 | 23 | 565.8851 | 8 | 21 | 22 | 561.0371 | 4 | 9 | 10 | 564.4331 | -6 |
| 21 | 22 | 566.6717 | -18 | 20 | 21 | 561.8170 | 10 | 5 | 6 | 567.2779 | -2 |
| 19 | 20 | 568.2360 | -21 | 19 | 20 | 562.5896 | -11 | 5 | 4 | 574.7037 | -16 |
| 18 | 19 | 569.0129 | -5 | 18 | 19 | 563.3611 | 3 | 7 | 6 | 575.9949 | 23 |
| 17 | 18 | 569.7839 | -2 | 17 | 18 | 564.1259 | -4 | 8 | 7 | 576.6275 | -15 |
| 11 | 12 | 574.3110 | 11 | 16 | 17 | 564.8870 | -1 | 9 | 8 | 577.2577 | -27 |
| 9 | 10 | 575.7851 | 43 | 15 | 16 | 565.6445 | 12 | 10 | 9 | 577.8839 | -29 |
| 8 | 9 | 576.5105 | 15 | 13 | 14 | 567.1410 | -5 | 11 | 10 | 578.5058 | -26 |
| 7 | 8 | 577.2305 | -21 | 7 | 6 | 581.7221 | -14 | 12 | 11 | 579.1259 | 9 |
| 5 | 6 | 578.6629 | -23 | 11 | 10 | 584.2581 | 3 | 14 | 13 | 580.3445 | 14 |
| 4 | 5 | 579.3714 | -30 | 12 | 11 | 584.8796 | 6 | 16 | 15 | 581.5390 | -25 |

TABLE II—*Continued*

| $N'$ | $N''$ | Observed | Δ | $N'$ | $N''$ | Observed | Δ | $N'$ | $N''$ | Observed | Δ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 5 | 586.8548 | -1 | 13 | 12 | 585.4946 | -6 | 17 | 16 | 582.1329 | -3 |
| 13 | 12 | 591.3029 | -24 | 14 | 13 | 586.1094 | 31 | 18 | 17 | 582.7201 | 3 |
| 16 | 15 | 593.1375 | -1 | 15 | 14 | 586.7148 | 22 | 20 | 19 | 583.8790 | 11 |
| 17 | 16 | 593.7408 | 26 | 16 | 15 | 587.3113 | -24 | 21 | 20 | 584.4499 | 5 |
| 18 | 17 | 594.3330 | -8 | 17 | 16 | 587.9104 | 5 | 22 | 21 | 585.0161 | 2 |
| 19 | 18 | 594.9259 | 15 | 18 | 17 | 588.5013 | 3 | 23 | 22 | 585.5780 | 8 |
| 20 | 19 | 595.5097 | -1 | 19 | 18 | 589.0861 | -9 | 24 | 23 | 586.1336 | 1 |
| 21 | 20 | 596.0912 | 10 | 20 | 19 | 589.6679 | -1 | 25 | 24 | 586.6872 | 25 |
| 22 | 21 | 596.6642 | -12 | 21 | 20 | 590.2443 | 3 | 26 | 25 | 587.2320 | 13 |
| 23 | 22 | 597.2350 | -5 | 22 | 21 | 590.8149 | 1 | 27 | 26 | 587.7707 | -9 |
| 24 | 23 | 597.7996 | -9 | 23 | 22 | 591.3821 | 16 | 28 | 27 | 588.3082 | 8 |
| 26 | 25 | 598.9147 | -4 | 24 | 23 | 591.9407 | -4 | 29 | 28 | 588.8393 | 12 |
| 27 | 26 | 599.4651 | 5 | 25 | 24 | 592.4969 | 3 | 30 | 29 | 589.3636 | 0 |
| 29 | 28 | 600.5491 | 8 | 26 | 25 | 593.0493 | 23 | 31 | 30 | 589.8852 | 13 |
| 30 | 29 | 601.0828 | 6 | 27 | 26 | 593.5918 | -4 | 32 | 31 | 590.3995 | 4 |
| 31 | 30 | 601.6091 | -19 | 28 | 27 | 594.1310 | -13 | 33 | 32 | 590.9089 | -1 |
| 32 | 31 | 602.1345 | -1 | 29 | 28 | 594.6669 | -3 | 34 | 33 | 591.4142 | 3 |
| 33 | 32 | 602.6517 | -12 | 30 | 29 | 595.1962 | -8 | 35 | 34 | 591.9138 | 4 |
| 34 | 33 | 603.1665 | 5 | 31 | 30 | 595.7210 | -5 | 36 | 35 | 592.4074 | -4 |
| 35 | 34 | 603.6740 | 1 | 32 | 31 | 596.2426 | 17 | 37 | 36 | 592.8969 | 0 |
| 36 | 35 | 604.1772 | 8 | 33 | 32 | 596.7541 | -10 | 38 | 37 | 593.3812 | 4 |
| 37 | 36 | 604.6743 | 5 | 34 | 33 | 597.2640 | 1 | 39 | 38 | 593.8597 | 4 |
| 38 | 37 | 605.1653 | -5 | 35 | 34 | 597.7669 | -7 | 40 | 39 | 594.3330 | 3 |
| 39 | 38 | 605.6527 | 1 | 36 | 35 | 598.2670 | 9 | 41 | 40 | 594.8023 | 15 |
| 40 | 39 | 606.1344 | 5 | 37 | 36 | 598.7597 | 4 | 42 | 41 | 595.2640 | 5 |
| 41 | 40 | 606.6100 | -0 | 38 | 37 | 599.2481 | 9 | 43 | 42 | 595.7210 | 1 |
| 42 | 41 | 607.0808 | 1 | 39 | 38 | 599.7296 | -3 | 44 | 43 | 596.1735 | 3 |
| 43 | 42 | 607.5474 | 13 | 40 | 39 | 600.2073 | 1 | 45 | 44 | 596.6191 | -9 |
| 44 | 43 | 608.0066 | 4 | 41 | 40 | 600.6801 | 8 | 46 | 45 | 597.0626 | 11 |
| 45 | 44 | 608.4599 | -10 | 42 | 41 | 601.1464 | 3 | 47 | 46 | 597.4976 | 0 |
| 46 | 45 | 608.9104 | 2 | 43 | 42 | 601.6091 | 16 | 48 | 47 | 597.9289 | 5 |
| 47 | 46 | 609.3522 | -20 | 44 | 43 | 602.0624 | -11 | 49 | 48 | 598.3559 | 21 |
| 48 | 47 | 609.7927 | 0 | 45 | 44 | 602.5144 | 1 | 50 | 49 | 598.7746 | 7 |
| 49 | 48 | 610.2263 | 6 | 46 | 45 | 602.9605 | 8 | 51 | 50 | 599.1886 | 0 |
| 50 | 49 | 610.6537 | 3 | 47 | 46 | 603.3976 | -21 | 52 | 51 | 599.5981 | 3 |
| 51 | 50 | 611.0754 | -3 | 48 | 47 | 603.8344 | 0 | 54 | 53 | 600.3979 | -21 |
| 52 | 51 | 611.4922 | -3 | 49 | 48 | 604.2642 | 6 | 55 | 54 | 600.7924 | -6 |
| 53 | 52 | 611.9035 | -4 | 50 | 49 | 604.6877 | 2 | 56 | 55 | 601.1800 | -6 |
| 54 | 53 | 612.3109 | 12 | 51 | 50 | 605.1068 | 9 | 57 | 56 | 601.5634 | 8 |
| 55 | 54 | 612.7105 | 4 | 52 | 51 | 605.5179 | -10 | 58 | 57 | 601.9390 | -1 |
| 56 | 55 | 613.1046 | -4 | 53 | 52 | 605.9270 | 5 | 59 | 58 | 602.3098 | -5 |
| 57 | 56 | 613.4937 | -7 | 54 | 53 | 606.3295 | 9 | 60 | 59 | 602.6759 | 1 |
| 58 | 57 | 613.8782 | -1 | 55 | 54 | 606.7261 | 9 | 61 | 60 | 603.0353 | -7 |
| 59 | 58 | 614.2576 | 9 | 56 | 55 | 607.1171 | 6 | 62 | 61 | 603.3882 | -24 |
| 60 | 59 | 614.6293 | -1 | 57 | 56 | 607.5012 | -10 | 63 | 62 | 603.7391 | -6 |
| 61 | 60 | 614.9971 | 3 | 58 | 57 | 607.8823 | -1 | 64 | 63 | 604.0830 | -2 |
| 62 | 61 | 615.3585 | 1 | 59 | 58 | 608.2571 | -0 | 65 | 64 | 604.4211 | -1 |
| 63 | 62 | 615.7142 | -4 | 60 | 59 | 608.6266 | 3 | 66 | 65 | 604.7521 | -16 |
| 64 | 63 | 616.0624 | -28 | 61 | 60 | 608.9903 | 3 | 67 | 66 | 605.0800 | -4 |
| 65 | 64 | 616.4104 | 4 | 62 | 61 | 609.3522 | 40 | 68 | 67 | 605.4035 | 18 |
| 66 | 65 | 616.7491 | -4 | 63 | 62 | 609.7002 | -5 | 69 | 68 | 605.7187 | 13 |
| 67 | 66 | 617.0816 | -16 | 64 | 63 | 610.0475 | -3 | 70 | 69 | 606.0269 | -5 |
| 68 | 67 | 617.4105 | -8 | 65 | 64 | 610.3894 | 2 | 71 | 70 | 606.3295 | -25 |
| 69 | 68 | 617.7327 | -11 | 66 | 65 | 610.7253 | 2 | 72 | 71 | 606.6309 | 2 |
| 70 | 69 | 618.0509 | 3 | 67 | 66 | 611.0552 | -1 | 73 | 72 | 606.9231 | -8 |
| 71 | 70 | 618.3627 | 10 | 68 | 67 | 611.3805 | 5 | 74 | 73 | 607.2124 | 9 |
| 72 | 71 | 618.6664 | -8 | 69 | 68 | 611.6988 | -2 | 76 | 75 | 607.7689 | -6 |
| 73 | 72 | 618.9674 | 4 | 70 | 69 | 612.0113 | -12 | 77 | 76 | 608.0395 | -5 |
| 74 | 73 | 619.2590 | -21 | 71 | 70 | 612.3210 | 7 | 78 | 77 | 608.3041 | -7 |
| 75 | 74 | 619.5485 | -9 | 72 | 71 | 612.6242 | 18 | 79 | 78 | 608.5639 | -0 |

TABLE II—*Continued*

| $N'$ | $N''$ | Observed | Δ | $N'$ | $N''$ | Observed | Δ | $N'$ | $N''$ | Observed | Δ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 76 | 75 | 619.8316 | -5 | 73 | 72 | 612.9190 | 1 | 80 | 79 | 608.8163 | -10 |
| 77 | 76 | 620.1090 | -0 | 74 | 73 | 613.2099 | 2 | 81 | 80 | 609.0631 | -19 |
| 78 | 77 | 620.3800 | -2 | 75 | 74 | 613.4937 | -11 | 82 | 81 | 609.3060 | -9 |
| 79 | 78 | 620.6457 | 0 | 76 | 75 | 613.7740 | -2 | 86 | 85 | 610.2164 | -4 |
| 80 | 79 | 620.9052 | -1 | 77 | 76 | 614.0484 | 6 | 88 | 87 | 610.6378 | 7 |
| 81 | 80 | 621.1580 | -12 | 78 | 77 | 614.3162 | 3 | 89 | 88 | 610.8402 | 17 |
| 82 | 81 | 621.4089 | 16 | 79 | 78 | 614.5782 | 1 | 90 | 89 | 611.0349 | 9 |
| 83 | 82 | 621.6494 | -2 | 80 | 79 | 614.8335 | -11 | 91 | 90 | 611.2221 | -17 |
| 84 | 83 | 621.8865 | 4 | 81 | 80 | 615.0843 | -11 | 92 | 91 | 611.4073 | -4 |
| 85 | 84 | 622.1179 | 11 | 82 | 81 | 615.3328 | 24 | 93 | 92 | 611.5842 | -15 |
| 86 | 85 | 622.3420 | 5 | 83 | 82 | 615.5698 | 3 | 94 | 93 | 611.7555 | -23 |
| 87 | 86 | 622.5630 | 25 | 84 | 83 | 615.8016 | -14 | 95 | 94 | 611.9226 | -14 |
| 88 | 87 | 622.7741 | 4 | 85 | 84 | 616.0295 | -11 | 96 | 95 | 612.0848 | 3 |
| 90 | 89 | 623.1820 | -3 | 86 | 85 | 616.2529 | 5 | 97 | 96 | 612.2379 | -9 |
| 91 | 90 | 623.3766 | -12 | 87 | 86 | 616.4675 | -9 | 99 | 98 | 612.5286 | -13 |
| 92 | 91 | 623.5662 | -12 | 88 | 87 | 616.6752 | -34 | 101 | 100 | 612.7941 | -32 |
| 93 | 92 | 623.7478 | -31 | 89 | 88 | 616.8828 | -1 | 106 | 105 | 613.3631 | 22 |
| 94 | 93 | 623.9278 | -9 | 90 | 89 | 617.0816 | 2 | 111 | 110 | 613.7740 | 0 |
| 97 | 96 | 624.4269 | 7 | 91 | 90 | 617.2725 | -14 | 116 | 115 | 614.0356 | 6 |
| 98 | 97 | 624.5810 | 9 | 92 | 91 | 617.4589 | -18 | 121 | 120 | 614.1448 | 21 |
| 99 | 98 | 624.7254 | -27 | 93 | 92 | 617.6437 | 22 | | | | |
| 101 | 100 | 625.0064 | 5 | 94 | 93 | 617.8182 | 18 | | | | |
| | | | | 95 | 94 | 617.9868 | 14 | | | | |
| | | | | 96 | 95 | 618.1493 | 9 | | | | |
| | | | | 97 | 96 | 618.3054 | -2 | | | | |
| | | | | 98 | 97 | 618.4566 | -1 | | | | |
| | | | | 99 | 98 | 618.6030 | 10 | | | | |
| | | | | 101 | 100 | 618.8730 | -15 | | | | |
| | | | | 102 | 101 | 619.0006 | -13 | | | | |
| | | | | 104 | 103 | 619.2370 | -14 | | | | |
| | | | | 107 | 106 | 619.5485 | 6 | | | | |
| | | | | 109 | 108 | 619.7249 | 8 | | | | |
| | | | | 113 | 112 | 620.0043 | 12 | | | | |
| | | | | 114 | 113 | 620.0575 | -2 | | | | |
| | | | | 115 | 114 | 620.1090 | 30 | | | | |
| | 4 3 Band | | | | 5 4 Band | | | | 6 5 Band | | |
| 56 | 57 | 520.2155 | 3 | 50 | 51 | 520.3546 | -37 | 44 | 45 | 520.3268 | -16 |
| 50 | 51 | 525.6825 | 2 | 48 | 49 | 522.1330 | -21 | 39 | 40 | 524.5811 | -11 |
| 49 | 50 | 526.5799 | 11 | 42 | 43 | 527.3655 | 17 | 38 | 39 | 525.4193 | -7 |
| 48 | 49 | 527.4710 | 1 | 41 | 42 | 528.2179 | -23 | 36 | 37 | 527.0805 | -22 |
| 47 | 48 | 528.3598 | 10 | 40 | 41 | 529.0726 | 2 | 31 | 32 | 531.1615 | -18 |
| 46 | 47 | 529.2398 | -27 | 39 | 40 | 529.9206 | 4 | 28 | 29 | 533.5601 | 13 |
| 45 | 46 | 530.1222 | 3 | 38 | 39 | 530.7644 | 8 | 26 | 27 | 535.1358 | 21 |
| 41 | 42 | 533.5986 | 21 | 37 | 38 | 531.6026 | -2 | 24 | 25 | 536.6902 | -5 |
| 40 | 41 | 534.4544 | 1 | 35 | 36 | 533.2673 | -7 | 22 | 23 | 538.2280 | -19 |
| 39 | 40 | 535.3094 | 16 | 34 | 35 | 534.0927 | -13 | 21 | 22 | 538.9932 | 5 |
| 38 | 39 | 536.1562 | -7 | 33 | 34 | 534.9153 | -4 | 18 | 19 | 541.2531 | -8 |
| 37 | 38 | 537.0015 | -2 | 30 | 31 | 537.3547 | 5 | 17 | 18 | 541.9963 | -23 |
| 36 | 37 | 537.8420 | -1 | 29 | 30 | 538.1559 | -22 | 12 | 13 | 545.6570 | 37 |
| 35 | 36 | 538.6768 | -12 | 28 | 29 | 538.9532 | -45 | 4 | 3 | 557.2067 | -6 |
| 33 | 34 | 540.3357 | -11 | 24 | 25 | 542.1124 | 13 | 6 | 5 | 558.4756 | -7 |
| 31 | 32 | 541.9773 | -6 | 23 | 24 | 542.8882 | 1 | 7 | 6 | 559.1066 | 31 |
| 30 | 31 | 542.7912 | -6 | 22 | 23 | 543.6632 | 25 | 8 | 7 | 559.7234 | -25 |
| 27 | 28 | 545.2041 | -25 | 18 | 19 | 546.7014 | -43 | 9 | 8 | 560.3470 | 36 |
| 26 | 27 | 546.0036 | 10 | 16 | 17 | 548.1975 | -34 | 10 | 9 | 560.9607 | 46 |
| 25 | 26 | 546.7942 | 1 | 12 | 13 | 551.1344 | -15 | 11 | 10 | 561.5682 | 43 |
| 24 | 25 | 547.5803 | -7 | 11 | 12 | 551.8590 | 10 | 14 | 13 | 563.3611 | 31 |
| 23 | 24 | 548.3618 | -17 | 8 | 9 | 553.9965 | -2 | 15 | 14 | 563.9467 | 5 |

TABLE II—*Continued*

| $N'$ | $N''$ | Observed | Δ | $N'$ | $N''$ | Observed | Δ | $N'$ | $N''$ | Observed | Δ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 21 | 22 | 549.9129 | -18 | 3 | 4 | 557.4708 | 37 | 16 | 15 | 564.5263 | -31 |
| 20 | 21 | 550.6845 | 11 | 1 | 0 | 560.8229 | 39 | 17 | 16 | 565.1062 | -16 |
| 19 | 20 | 551.4468 | -9 | 5 | 4 | 563.4128 | -15 | 18 | 17 | 565.6766 | -45 |
| 18 | 19 | 552.2048 | -25 | 7 | 6 | 564.6887 | 58 | 21 | 20 | 567.3681 | -32 |
| 16 | 17 | 553.7123 | -4 | 8 | 7 | 565.3131 | 32 | 22 | 21 | 567.9249 | 2 |
| 15 | 16 | 554.4596 | 11 | 11 | 10 | 567.1584 | -33 | 23 | 22 | 568.4702 | -29 |
| 14 | 15 | 555.1998 | 1 | 14 | 13 | 568.9665 | -27 | 24 | 23 | 569.0129 | -36 |
| 13 | 14 | 555.9362 | -1 | 15 | 14 | 569.5570 | -49 | 25 | 24 | 569.5570 | 21 |
| 12 | 13 | 556.6689 | 7 | 24 | 23 | 574.6717 | 4 | 35 | 34 | 574.6589 | -1 |
| 11 | 12 | 557.3942 | -13 | 25 | 24 | 575.2146 | 7 | 36 | 35 | 575.1409 | -3 |
| 10 | 11 | 558.1205 | 25 | 26 | 25 | 575.7526 | 11 | 37 | 36 | 575.6184 | 1 |
| 6 | 7 | 560.9607 | -7 | 27 | 26 | 576.2871 | 32 | 38 | 37 | 576.0899 | -3 |
| 15 | 14 | 575.2296 | 17 | 28 | 27 | 576.8110 | -2 | 39 | 38 | 576.5574 | 5 |
| 16 | 15 | 575.8209 | 8 | 29 | 28 | 577.3324 | -11 | 40 | 39 | 577.0195 | 11 |
| 17 | 16 | 576.4076 | 4 | 30 | 29 | 577.8498 | -8 | 41 | 40 | 577.4753 | 6 |
| 18 | 17 | 576.9897 | 3 | 31 | 30 | 578.3661 | 34 | 42 | 41 | 577.9267 | 9 |
| 19 | 18 | 577.5654 | -12 | 32 | 31 | 578.8693 | -2 | 43 | 42 | 578.3751 | 36 |
| 20 | 19 | 578.1388 | 1 | 33 | 32 | 579.3714 | 1 | 44 | 43 | 578.8121 | -1 |
| 21 | 20 | 578.7062 | 4 | 34 | 33 | 579.8684 | 5 | 45 | 44 | 579.2479 | 4 |
| 22 | 21 | 579.2693 | 14 | 35 | 34 | 580.3608 | 16 | 46 | 45 | 579.6771 | -4 |
| 23 | 22 | 579.8273 | 24 | 36 | 35 | 580.8444 | -11 | 47 | 46 | 580.1011 | -12 |
| 24 | 23 | 580.3762 | -6 | 37 | 36 | 581.3270 | 4 | 48 | 47 | 580.5229 | 10 |
| 25 | 24 | 580.9235 | -2 | 38 | 37 | 581.8021 | -3 | 49 | 48 | 580.9409 | 49 |
| 26 | 25 | 581.4665 | 10 | 39 | 38 | 582.2734 | 4 | 50 | 49 | 581.3452 | 3 |
| 27 | 26 | 582.0013 | -9 | 40 | 39 | 582.7388 | 4 | 51 | 50 | 581.7493 | 8 |
| 28 | 27 | 582.5360 | 23 | 41 | 40 | 583.1966 | -20 | 52 | 51 | 582.1472 | 5 |
| 29 | 28 | 583.0592 | -9 | 42 | 41 | 583.6540 | 5 | 54 | 53 | 582.9285 | 14 |
| 30 | 29 | 583.5813 | -1 | 43 | 42 | 584.1003 | -29 | 55 | 54 | 583.3050 | -42 |
| 31 | 30 | 584.1003 | 27 | 44 | 43 | 584.5449 | -27 | 56 | 55 | 583.6865 | 6 |
| 32 | 31 | 584.6091 | 5 | 45 | 44 | 584.9852 | -15 | 57 | 56 | 584.0578 | 5 |
| 33 | 32 | 585.1164 | 19 | 46 | 45 | 585.4207 | 2 | 58 | 57 | 584.4230 | -3 |
| 34 | 33 | 585.6147 | -5 | 47 | 46 | 585.8493 | 2 | 59 | 58 | 584.7861 | 22 |
| 35 | 34 | 586.1094 | -12 | 48 | 47 | 586.2736 | 13 | 60 | 59 | 585.1400 | 10 |
| 36 | 35 | 586.6012 | 3 | 49 | 48 | 586.6877 | -25 | 61 | 60 | 585.4946 | 59 |
| 37 | 36 | 587.0854 | -6 | 50 | 49 | 587.1023 | -4 | 62 | 61 | 585.8330 | 1 |
| 38 | 37 | 587.5654 | -4 | 51 | 50 | 587.5097 | -3 | 63 | 62 | 586.1716 | -1 |
| 39 | 38 | 588.0413 | 10 | 52 | 51 | 587.9104 | -14 | 64 | 63 | 586.5045 | -6 |
| 40 | 39 | 588.5099 | 1 | 53 | 52 | 588.3082 | -1 | 65 | 64 | 586.8334 | 4 |
| 41 | 40 | 588.9723 | -15 | 54 | 53 | 588.7000 | 6 | 66 | 65 | 587.1552 | -1 |
| 42 | 41 | 589.4320 | -6 | 55 | 54 | 589.0861 | 11 | 67 | 66 | 587.4722 | 0 |
| 43 | 42 | 589.8852 | -10 | 56 | 55 | 589.4652 | -2 | 68 | 67 | 587.7849 | 13 |
| 44 | 43 | 590.3352 | 7 | 57 | 56 | 589.8401 | -2 | 69 | 68 | 588.0892 | -2 |
| 45 | 44 | 590.7776 | 2 | 58 | 57 | 590.2083 | -14 | 70 | 69 | 588.3879 | -18 |
| 46 | 45 | 591.2144 | -7 | 59 | 58 | 590.5739 | 2 | 72 | 71 | 588.9723 | -13 |
| 47 | 46 | 591.6479 | 5 | 60 | 59 | 590.9320 | -4 | 74 | 73 | 589.5331 | -23 |
| 48 | 47 | 592.0754 | 10 | 61 | 60 | 591.2862 | 7 | 75 | 74 | 589.8094 | 16 |
| 49 | 48 | 592.4969 | 9 | 62 | 61 | 591.6335 | 4 | 77 | 76 | 590.3352 | -7 |
| 50 | 49 | 592.9125 | 2 | 63 | 62 | 591.9742 | -12 | 78 | 77 | 590.5894 | -21 |
| 51 | 50 | 593.3220 | -12 | 64 | 63 | 592.3121 | 1 | 81 | 80 | 591.3231 | -14 |
| 52 | 51 | 593.7292 | 5 | 65 | 64 | 592.6426 | -6 | 82 | 81 | 591.5573 | -3 |
| 53 | 52 | 594.1310 | 22 | 66 | 65 | 592.9668 | -20 | 89 | 88 | 593.0298 | 5 |
| 54 | 53 | 594.5246 | 10 | 67 | 66 | 593.2888 | -3 | 91 | 90 | 593.3981 | 0 |
| 55 | 54 | 594.9139 | 10 | 68 | 67 | 593.6035 | -1 | 92 | 91 | 593.5744 | 6 |
| 56 | 55 | 595.2947 | -22 | 69 | 68 | 593.9109 | -19 | 93 | 92 | 593.7408 | -31 |
| 57 | 56 | 595.6738 | -14 | 70 | 69 | 594.2166 | 4 | 94 | 93 | 593.9109 | 28 |
| 58 | 57 | 596.0467 | -16 | 73 | 72 | 595.0943 | 10 | 96 | 95 | 594.2166 | -23 |
| 59 | 58 | 596.4172 | 13 | 74 | 73 | 595.3759 | 15 | 100 | 99 | 594.7721 | 14 |
| 61 | 60 | 597.1336 | -9 | 75 | 74 | 595.6507 | 7 | 102 | 101 | 595.0093 | -21 |
| 62 | 61 | 597.4862 | 6 | 76 | 75 | 595.9183 | -16 | 107 | 106 | 595.5097 | -1 |
| 63 | 62 | 597.8304 | -9 | 77 | 76 | 596.1849 | 7 | | | | |

TABLE II—*Continued*

| $N'$ | $N''$ | Observed | Δ | $N'$ | $N''$ | Observed | Δ | $N'$ | $N''$ | Observed | Δ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 64 | 63 | 598.1703 | -10 | 78 | 77 | 596.4432 | 4 | | | | |
| 65 | 64 | 598.5084 | 25 | 79 | 78 | 596.6960 | 2 | | | | |
| 66 | 65 | 598.8356 | 6 | 80 | 79 | 596.9407 | -25 | | | | |
| 67 | 66 | 599.1566 | -17 | 81 | 80 | 597.1859 | 11 | | | | |
| 68 | 67 | 599.4770 | 7 | 82 | 81 | 597.4168 | -40 | | | | |
| 69 | 68 | 599.7879 | -7 | 83 | 82 | 597.6493 | -17 | | | | |
| 70 | 69 | 600.0926 | -29 | 84 | 83 | 597.8770 | 14 | | | | |
| 71 | 70 | 600.3979 | 13 | 86 | 85 | 598.3094 | 20 | | | | |
| 72 | 71 | 600.6928 | 6 | 89 | 88 | 598.9147 | 26 | | | | |
| 73 | 72 | 600.9805 | -16 | 92 | 91 | 599.4651 | 4 | | | | |
| 75 | 74 | 601.5456 | 5 | 94 | 93 | 599.8042 | 0 | | | | |
| 76 | 75 | 601.8187 | 5 | 99 | 98 | 600.5491 | -13 | | | | |
| 78 | 77 | 602.3477 | 5 | 100 | 99 | 600.6801 | -19 | | | | |
| 80 | 79 | 602.8550 | 14 | 101 | 100 | 600.8087 | 10 | | | | |
| 81 | 80 | 603.0981 | -1 | 104 | 103 | 601.1464 | -30 | | | | |
| 82 | 81 | 603.3328 | -43 | 112 | 111 | 601.8004 | 25 | | | | |
| 85 | 84 | 604.0186 | -8 | | | | | | | | |
| 90 | 89 | 605.0387 | -25 | | | | | | | | |
| 94 | 93 | 605.7530 | -10 | | | | | | | | |
| 96 | 95 | 606.0756 | 4 | | | | | | | | |
| 100 | 99 | 606.6460 | -12 | | | | | | | | |
| 103 | 102 | 607.0142 | 4 | | | | | | | | |
| 116 | 115 | 607.9793 | 5 | | | | | | | | |
| 118 | 117 | 608.0395 | 32 | | | | | | | | |
| | 7 6 Band | | | | 8 7 Band | | | | | | |
| 18 | 19 | 535.8498 | -29 | 16 | 17 | 531.9600 | -46 | | | | |
| 15 | 16 | 538.0617 | 40 | 13 | 14 | 534.1317 | 48 | | | | |
| 14 | 15 | 538.7899 | 64 | 9 | 10 | 536.9443 | -18 | | | | |
| 10 | 11 | 541.6454 | 42 | 7 | 8 | 538.3268 | -13 | | | | |
| 7 | 8 | 543.7294 | -65 | 3 | 4 | 541.0361 | -3 | | | | |
| 3 | 2 | 551.0509 | -52 | 2 | 3 | 541.7102 | 84 | | | | |
| 8 | 7 | 554.1877 | -55 | 4 | 3 | 546.2323 | 44 | | | | |
| 9 | 8 | 554.8083 | 21 | 9 | 8 | 549.3116 | -66 | | | | |
| 13 | 12 | 557.2067 | -28 | 12 | 11 | 551.1111 | -34 | | | | |
| 15 | 14 | 558.3828 | 9 | 16 | 15 | 553.4411 | -6 | | | | |
| 16 | 15 | 558.9603 | -4 | 24 | 23 | 557.8630 | 30 | | | | |
| 17 | 16 | 559.5356 | 10 | 27 | 26 | 559.4362 | 13 | | | | |
| 20 | 19 | 561.2244 | -23 | 29 | 28 | 560.4609 | 13 | | | | |
| 24 | 23 | 563.4128 | -3 | 30 | 29 | 560.9607 | -38 | | | | |
| 25 | 24 | 563.9467 | -5 | 33 | 32 | 562.4489 | 2 | | | | |
| 26 | 25 | 564.4775 | 12 | 35 | 34 | 563.4128 | 1 | | | | |
| 31 | 30 | 567.0448 | -13 | 36 | 35 | 563.8939 | 68 | | | | |
| 33 | 32 | 568.0429 | 45 | 37 | 36 | 564.3583 | 19 | | | | |
| 34 | 33 | 568.5302 | 33 | 38 | 37 | 564.8213 | 9 | | | | |
| 35 | 34 | 569.0129 | 26 | 39 | 38 | 565.2807 | 14 | | | | |
| 37 | 36 | 569.9572 | -45 | 40 | 39 | 565.7276 | -56 | | | | |
| 47 | 46 | 574.4079 | 6 | 41 | 40 | 566.1817 | -1 | | | | |
| 48 | 47 | 574.8211 | -20 | 46 | 45 | 568.3498 | 28 | | | | |
| 50 | 49 | 575.6416 | 28 | 47 | 46 | 568.7653 | 9 | | | | |
| 52 | 51 | 576.4328 | -5 | 48 | 47 | 569.1729 | -37 | | | | |
| 53 | 52 | 576.8214 | -12 | 50 | 49 | 569.9814 | -36 | | | | |
| 55 | 54 | 577.5853 | 1 | 64 | 63 | 575.0491 | 5 | | | | |
| 56 | 55 | 577.9573 | -11 | 65 | 64 | 575.3664 | -35 | | | | |
| 57 | 56 | 578.3247 | -15 | 66 | 65 | 575.6828 | -29 | | | | |
| 58 | 57 | 578.6934 | 46 | 67 | 66 | 575.9949 | -12 | | | | |
| 59 | 58 | 579.0475 | 16 | 70 | 69 | 576.8930 | -15 | | | | |
| 60 | 59 | 579.3982 | 6 | 72 | 71 | 577.4632 | -27 | | | | |
| 61 | 60 | 579.7411 | -29 | 73 | 72 | 577.7416 | -17 | | | | |

TABLE II—*Continued*

| $N'$ | $N''$ | Observed | Δ | $N'$ | $N''$ | Observed | Δ | $N'$ | $N''$ | Observed | Δ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 62 | 61 | 580.0835 | -13 | 75 | 74 | 578.2780 | -36 | | | | |
| 63 | 62 | 580.4225 | 22 | 76 | 75 | 578.5441 | 17 | | | | |
| 64 | 63 | 580.7512 | 9 | 77 | 76 | 578.7990 | 14 | | | | |
| 65 | 64 | 581.0737 | -11 | 78 | 77 | 579.0475 | 2 | | | | |
| 66 | 65 | 581.3934 | -6 | 79 | 78 | 579.2902 | -11 | | | | |
| 67 | 66 | 581.7102 | 26 | 80 | 79 | 579.5373 | 74 | | | | |
| 68 | 67 | 582.0140 | -17 | 81 | 80 | 579.7639 | 12 | | | | |
| 71 | 70 | 582.9101 | 29 | | | | | | | | |
| 72 | 71 | 583.1966 | 34 | | | | | | | | |
| 75 | 74 | 584.0193 | 11 | | | | | | | | |
| 76 | 75 | 584.2843 | 23 | | | | | | | | |
| 77 | 76 | 584.5449 | 45 | | | | | | | | |
| 82 | 81 | 585.7463 | -13 | | | | | | | | |
| 84 | 83 | 586.1938 | 28 | | | | | | | | |
| 85 | 84 | 586.4028 | -14 | | | | | | | | |
| 88 | 87 | 587.0081 | -16 | | | | | | | | |
| 91 | 90 | 587.5654 | 15 | | | | | | | | |

(5 Torr) was then introduced to prevent any deposition of solid material onto the KRS-5 cell windows. The high-resolution spectrum was recorded at a resolution of 0.01 $cm^{-1}$ over the spectral range 350–750 $cm^{-1}$ with a liquid-helium-cooled Si:B detector and a KBr beamsplitter. The upper limit of 750 $cm^{-1}$ was set by a cold filter attached to the detector, while a combination of detector response and KBr beamsplitter transmission effectively set the lower limit to 350 $cm^{-1}$. The final spectrum consisted of 100 coadded scans. A portion of the spectrum showing part of the *R* branches of the first few bands can be seen in Fig. 1.

## RESULTS

Rotational lines were measured using PC-DECOMP, a spectral analysis program written by J. Brault, which fits the line profiles with Voigt lineshape functions. Assignment of the CaF bands was performed using an interactive color Loomis–Wood program. The overall spectrum of CaF was then calibrated with respect to pure rotational HF lines (*17*) which were present as an impurity. Although CaF has a $^2\Sigma^+$

TABLE III

Spectroscopic Constants for the $X^2\Sigma^+$ Ground State of CaF (in $cm^{-1}$)

| v | $T_v$ | $B_v$ | $10^7 D_v$ |
|---|---|---|---|
| 0 | 0 | 0.342488337(90) | 4.68963(90) |
| 1 | 582.847759(110) | 0.340053845(52) | 4.69073(85) |
| 2 | 1159.946892(192) | 0.337629480(50) | 4.69135(82) |
| 3 | 1731.34856(21) | 0.335215331(50) | 4.69150(79) |
| 4 | 2297.10325(27) | 0.332811563(112) | 4.69110(77) |
| 5 | 2857.26144(37) | 0.330418358(181) | 4.69019(77) |
| 6 | 3411.87316(45) | 0.32803600(23) | 4.68889(76) |
| 7 | 3960.98951(61) | 0.32566419(35) | 4.68674(84) |
| 8 | 4504.65944(73) | 0.32330425(51) | 4.68533(98) |

ground state, no spin–rotation splitting was observed; therefore, data reduction was performed by fitting the data to the conventional Dunham expression

$$E(v, N) = \sum_{ij} Y_{ij}\left(v + \frac{1}{2}\right)^i [N(N+1)]^j.$$

The microwave lines (*10*) were corrected for the effects of fine and hyperfine structure and were added to the fit. The Dunham coefficients obtained are shown in Table I. The equilibrium internuclear distance of 1.9516386(35) Å was calculated from the $Y_{01}$ Dunham coefficient and found to be in agreement with that reported by Dulick *et al.*, (*4*). The infrared rovibrational line positions are found in Table II, and spectroscopic constants for the $X^2\Sigma^+$ ground state of CaF are given in Table III.

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