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Fourier Transform Spectroscopy of the $A^2\Pi_i$–$X^2\Sigma^+$ System of CP

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The infrared emission spectrum of the $A^2\Pi_i$–$X^2\Sigma^+$ transition of CP has been observed using a high-resolution Fourier transform spectrometer in the 1.2- to 2.5-μm spectral region. This transition is analogous to the red system of CN and has not been directly observed prior to this study. Molecular constants were extracted from the line positions of the 1–0, 0–0, 0–1, 0–2, and 3–1 bands. © 1987 Academic Press, Inc.

INTRODUCTION

While CN is one of the most studied free radicals, relatively little is known about the isostructural radical CP. The existence of CP was first established spectroscopically by Herzberg (*1*) who observed the $B^2\Sigma^+$–$X^2\Sigma^+$ transition. Later, the rotational structure of the $B^2\Sigma^+$–$X^2\Sigma^+$ system of CP was analyzed by Bärwald *et al.* (*2*), who also provided estimates for the spectroscopic constants of the $A^2\Pi$ state from the $B^2\Sigma^+$–$A^2\Pi$ transition. The $B^2\Sigma^+$–$A^2\Pi$ transition has also been investigated by Chaudhry and Upadhya (*3*) and more recently by Tripathi *et al.* (*4*). There are a number of publications on the calculation of Franck–Condon factors, *r* centroids, and potential energy curves (*5–8*) of CP.

The bond dissociation energy (D_0^0 = 121 kcal/mol) was determined by Gingerich (*9*), Smoes *et al.* (*10*), and Kordis and Gingerich (*11*) by mass spectrometry. Kordis and Gingerich also detected the molecules C_2P, CP_2, and C_2P_2 and derived their atomization energies and standard heats of formation.

In the present study we report on the first observation of the infrared $A^2\Pi_i$–$X^2\Sigma^+$ electronic transition of CP, which is analogous to the red system of CN. The molecular constants obtained should be useful in the search for the CP free radical in stellar atmospheres and the interstellar medium.

EXPERIMENTAL DETAILS

The spectrum of CP was excited in an electrodeless quartz discharge tube with a 2450-MHz microwave oscillator. A mixture of 0.45 Torr of hydrogen and 0.04 Torr of white phosphorus vapor flowed through the cell.

The carbon atoms required for the production of CP came as an impurity in the discharge tube. The tube was coated with a carbon deposit from a previous experiment in which a mixture of methane, phosphorus vapor, and helium was discharged. This previous experiment was designed to produce CP, but the very strong emission from C_2 overwhelmed the $A^2\Pi$–$X^2\Sigma^+$ emission of CP. The best and clearest spectrum of CP was produced when only trace amounts of carbon were present. This observation

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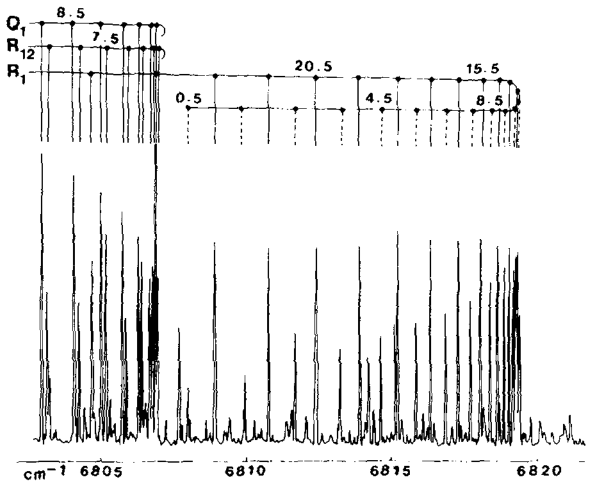

FIG. 1. Part of the rotational structure of the 0–0 band of the $A^2\Pi_{3/2}$–$X^2\Sigma^+$ transition near the $+B$ and $+3B$ bandheads.

agrees with the original work of Herzberg (*1*), who attributed the presence of carbon in his discharge to "tap grease and sealing wax."

The emission from the discharge was observed with the Fourier transform spectrometer associated with the National Solar Observatory[1] at Kitt Peak. Nine scans were coadded in 1 hr of integration. The unapodized resolution was set to 0.02 cm^{-1}. InSb detectors and a silicon filter restricted the spectrum to the 1800- to 8800-cm^{-1} region.

The molecules CO, PH, H_2, C_2, and P_2 were observed as well as emission from various atoms. The analysis of the vibration–rotation spectrum of PH is being published separately (*12*). The CO (*13*) and PH (*14*) lines were used to provide the absolute calibration of our spectra.

RESULTS AND DISCUSSION

The interferograms were transformed by standard methods to provide the spectrum. Some ringing was present, particularly near strong atomic lines, so the spectrum was slightly apodized. The final linewidth of the CP emission features was about 0.040 cm^{-1} (FWHM).

The line positions were extracted with the aid of a data reduction program called DECOMP developed at Kitt Peak. To find the peak positions, a Voigt lineshape function was fitted to the CP lines by a nonlinear least-squares procedure.

Five vibrational bands of the $A^2\Pi$–$X^2\Sigma^+$ transition were observed: 1–0, 0–0, 0–1, 0–2, and 3–1 (see Fig. 1). For the 3–1 band only the $^2\Pi_{3/2}$–$^2\Sigma^+$ subband was found because the Si filter prevented the observation of the corresponding $^2\Pi_{1/2}$–$^2\Sigma^+$ subband. The other bands either had poor Franck–Condon factors (e.g., 2–1) or were obscured by strong P_2 emission (e.g., 2–2).

[1] The National Solar Observatory is operated by the Association of Universities for Research in Astronomy, Inc., under contract with the National Science Foundation.

TABLE I

Observed Line Positions for the $A^2\Pi_i$–$X^2\Sigma^+$ Transition of CP (in cm^{-1})

	$A^2\Pi_{1/2}$ - $X^2\Sigma^+$ 0-0					
	R_2	P_2	Q_2	R_{21}	P_{21}	Q_{21}
1.5	6964.5132(13)			6967.6323(19)		
2.5	-		6959.7234(53)	6969.4215(17)		
3.5	6964.7925(-37)	6953.3851(-35)	6958.3412(-17)	6971.0428(6)	6959.6493(-39)	
4.5	6964.6859(-19)	6950.4321(9)	6956.8016(8)	6972.4985(10)	6958.2584(-10)	
5.5	6964.4091(-34)	6947.3060(-11)	6955.0926(7)	6973.7862(5)	6956.6981(-10)	
6.5	6963.9707(6)	6944.0157(-7)	6953.2165(2)	6974.9058(-9)	6954.9704(-10)	6964.2924(5)
7.5	6963.3606(-1)	6940.5593(2)	6951.1741(3)	6975.8580(-24)	6953.0774(2)	6963.8310(0)
8.5	6962.5846(5)	6936.9355(3)	6948.9654(8)	6976.6482(13)	6951.0161(-1)	6963.2034(4)
9.5	6961.6420(15)	6933.1468(19)	-	6977.2686(27)	6948.7881(-4)	6962.4079(-1)
10.5	6960.5304(6)	6929.1886(6)	6944.0467(7)	6977.7222(46)	6946.3930(-10)	6961.4467(9)
11.5	6959.2528(9)	6925.0675(27)	6941.3363(-3)	6978.0020(2)	6943.8335(8)	6960.3170(5)
12.5	6957.8064(-3)	6920.7750(-1)	6938.4602(-2)	6978.1184(-2)	6941.1038(-10)	6959.0200(-1)
13.5	6956.1918(-26)	6916.3189(-1)	6935.4183(8)	6978.0667(-10)	6938.2114(13)	6957.5555(-9)
14.5	6954.4151(3)	6911.6963(-3)	6932.2085(6)	6977.8454(-38)	-	6955.9256(1)
15.5	6952.4676(-4)	6906.9081(1)	6928.8318(2)	6977.4629(-1)	6931.9200(-5)	6954.1278(4)
16.5	6950.3539(1)	6901.9537(7)	6925.2878(-8)	6976.9091(1)	6928.5238(-18)	6952.1620(0)
17.5	6948.0731(9)	6896.8316(-2)	6921.5797(8)	6976.1874(1)	6924.9638(-3)	6950.0295(3)
18.5	6945.6254(21)	6891.5447(3)	6917.7041(16)	6975.2976(0)	6921.2383(25)	6947.7294(2)
19.5	6943.0078(8)	6886.0911(2)	6913.6599(5)	6974.2399(-2)	6917.3408(-1)	6945.2627(10)
20.5	6940.2234(2)	6880.4722(10)	6909.4497(1)	6973.0136(-9)	6913.2793(1)	6942.6270(2)
21.5	6937.2723(3)	6874.6871(17)	6905.0737(6)	6971.6209(0)	6909.0509(0)	6939.8267(22)
22.5	6934.1524(-8)	6868.7344(9)	6900.5301(2)	6970.0596(5)	6904.6566(8)	6936.8532(-15)
23.5	6930.8641(-27)	6862.6170(14)	6895.8203(3)	6968.3285(-7)	6900.0921(-20)	6933.7172(-2)
24.5	6927.4132(2)	6856.3324(7)	6890.9444(9)	6966.4323(13)	6895.3650(-7)	6930.4120(-6)
25.5	6923.7921(7)	6849.8826(8)	6885.9007(5)	6964.3651(6)	6890.4701(-5)	6926.9406(5)
26.5	6920.0055(32)	6843.2667(8)	6880.6902(-1)	6962.1295(-2)	6885.4086(-2)	6923.2996(-4)
27.5	6916.0454(0)	6836.4841(0)	6875.3141(4)	6959.7234(-30)	6880.1801(-3)	6919.4919(-4)
28.5	6911.9200(-8)	6829.5368(4)	6869.7710(6)	6957.1551(5)	6874.7854(2)	6915.5187(18)
29.5	6907.6297(12)	6822.4239(11)	6864.0624(20)	6954.4151(9)	6869.2230(-4)	6911.3729(-9)
30.5	6903.1696(13)	6815.1435(2)	6858.1841(3)	6951.5053(1)	6863.4983(35)	6907.0629(0)
31.5	6898.5421(18)	6807.6966(-15)	6852.1417(13)	6948.4281(6)	6857.5990(-6)	6902.5842(0)
32.5	6893.7412(-33)	6800.0865(-5)	6845.9317(13)	6945.1843(32)	6851.5377(0)	6897.9388(11)
33.5	6888.7803(-4)	6792.3114(12)	6839.5541(5)	6941.7644(-14)	6845.3095(4)	6893.1223(-10)
34.5	6883.6502(11)	6784.3688(11)	6833.0109(7)	6938.1795(-21)	6838.9099(-40)	6888.1403(-7)
35.5	6878.3507(13)	6776.2632(38)	6826.3016(15)	6934.4245(-40)	6832.3507(-12)	6882.9911(4)
36.5	6872.8816(-1)	6767.9841(-14)	6819.4237(4)	6930.5106(42)	-	6877.6720(-5)
37.5	6867.2457(-3)	6759.5461(1)	6812.3789(-9)	6926.4157(6)	6818.7293(14)	6872.1862(-1)
38.5	6861.4406(-17)	6750.9389(-19)	6805.1639(-57)	6922.1536(-12)	6811.6678(20)	6866.5318(-3)
39.5	6855.4714(10)	6742.1670(-30)	6797.7942(15)	6917.7244(-8)	6804.4358(-13)	6860.7056(-42)
40.5	6849.3335(32)	6733.2367(30)	6790.2586(95)	6913.1276(12)		6854.7214(21)
41.5	6843.0240(19)	6724.1374(56)	-	6908.3588(6)		6848.5681(73)
42.5	6836.5473(16)	6714.8604(-41)	6774.6613(-7)	6903.4187(-20)		6842.2373(33)
43.5	6829.8994(-17)	6705.4332(15)	6766.6146(-37)	6898.3137(1)		6835.7393(2)
44.5	6823.0904(22)	6695.8356(21)	6758.4066(-14)	6893.0319(-52)		6829.0728(-31)
45.5	6816.1058(-12)	6686.0684(-14)	6750.0343(33)	6887.5956(46)		6822.2438(-7)

	$A^2\Pi_{3/2}$ - $X^2\Sigma^+$ 0-0					
	R_1	P_1	Q_1	R_{12}	P_{12}	Q_{12}
0.5	6807.9992(-29)					
1.5	6809.9297(-19)					6803.2579(32)
2.5	6911.6773(-41)					6802.0209(16)
3.5	6813.2511(-4)					6800.6024(-20)
4.5	6814.6419(0)			6806.7756(-10)		6799.0090(-11)
5.5	6815.8526(0)	6798.9103(22)	6806.6745(-1)	6806.4163(17)	6789.4716(16)	6797.2364(1)
6.5	6816.8833(-2)	6797.1154(-4)	6806.2932(-9)	6805.8731(1)	6786.1047(-5)	6795.2832(1)
7.5	6817.7343(-2)	6795.1433(-8)	6805.7335(-5)	6805.1542(22)	-	6793.1506(0)
8.5	6818.4052(-6)	6792.9929(-1)	6804.9934(-9)	6804.2522(9)	6778.8383(1)	6790.8388(0)
9.5	6818.8966(-6)	6790.6630(4)	6804.0750(-2)	6803.1721(9)	6774.9345(-17)	6788.3475(-2)
10.5	6819.2082(-6)	6788.1538(9)	6802.9763(-2)	6801.9125(10)	6770.8556(4)	6785.6772(-1)
11.5	6819.3417(12)	6785.4642(2)	6801.6981(-2)	6800.4735(11)	6766.5978(24)	6782.8271(-7)

TABLE I—*Continued*

	$A^2\Pi_{3/2}$ - $X^2\Sigma^+$ 0-0					
	R_1	P_1	Q_1	R_{12}	P_{12}	Q_{12}
12.5	6819.2921(-2)	6782.5960(1)	6800.2405(-1)	6798.8533(-5)	6762.1576(8)	6779.7990(-1)
13.5	6819.0642(-1)	6779.5487(0)	6798.6031(-4)	6797.0550(-8)	6757.5394(-2)	6776.5912(-1)
14.5	6818.6554(-9)	6776.3219(-5)	6796.7870(1)	6795.0780(-4)	6752.7443(6)	6773.2047(2)
15.5	6818.0678(-6)	6772.9169(-2)	6794.7907(-3)	6792.9209(-8)	6747.7696(2)	6769.6380(-7)
16.5	6817.3005(-2)	6769.3330(3)	6792.6164(7)	6790.5850(-6)	6742.6163(-3)	6765.8941(1)
17.5	6816.3534(4)	6765.5695(0)	6790.2586(-25)	6788.0696(-6)	6737.2854(-2)	6761.9708(3)
18.5	6815.2269(14)	6761.6274(-1)	6787.7269(-3)	6785.3751(-5)	6731.7768(5)	6757.8681(-1)
19.5	6813.9178(-3)	6757.5074(8)	6785.0136(-4)	6782.5030(12)	6726.0893(4)	6753.5875(3)
20.5	6812.4307(-2)	6753.2065(-6)	6782.1213(-4)	6779.4487(-2)	6720.2235(0)	6749.1280(4)
21.5	6810.7634(-4)	6748.7287(-2)	6779.0502(0)	6776.2189(20)	6714.1784(-19)	6744.4895(0)
22.5	6808.9177(8)	6744.0721(-1)	6775.7993(-3)	6772.8063(5)	6707.9586(-6)	6739.6783(55)
23.5	6806.8873(-29)	6739.2366(-4)	6772.3700(0)	6769.2159(2)	6701.5606(1)	6734.6776(-2)
24.5	6804.6841(4)	6734.2237(2)	6768.7611(-3)	6765.4467(-1)	6694.9839(-4)	6729.5044(-1)
25.5	6802.2973(-2)	6729.0309(-7)	6764.9738(-1)	6761.5010(21)	6688.2253(-53)	6724.1488(-41)
26.5	6799.7301(-14)	6723.6616(1)	6761.0073(-2)	6757.3712(-10)	6681.3001(4)	6718.6195(-38)
27.5	6796.9853(-6)	6718.1129(-4)	6756.8621(-2)	6753.0664(-5)	6674.1937(22)	6712.9162(6)
28.5	6794.0589(-17)	6712.3864(-7)	6752.5383(0)	6748.5825(-3)	6666.9064(1)	6707.0299(0)
29.5	6790.9552(-5)	6706.4834(5)	6748.0361(4)	6743.9196(-5)	6659.4436(-6)	6700.9658(-7)
30.5	6787.6701(-11)	6700.4004(-5)	6743.3545(0)	6739.0800(11)	6651.8060(7)	6694.7253(1)
31.5	6784.2066(-6)	6694.1410(-1)	6738.4946(-2)	6734.0581(-12)	6643.9910(13)	6688.3064(0)
32.5	6780.5639(3)	6687.7046(9)	6733.4564(-2)	6728.8616(3)	-	6681.7075(-25)
33.5	6776.7400(-7)	6681.0887(-1)	6728.2397(-4)	6723.4846(-4)	6627.8316(24)	6674.9360(-2)
34.5	6772.7381(-2)	6674.2984(20)	6722.8476(24)	6717.9287(-18)	6619.4829(-16)	6667.9862(11)
35.5	6768.5559(-7)	6667.3278(10)	6717.2716(-6)	6712.1990(12)	6610.9643(6)	6660.8563(-5)
36.5	6764.1947(-8)	6660.1792(-7)	6711.5206(-4)	6706.2876(5)	6602.2654(-16)	6653.5518(5)
37.5	6759.6547(-6)	6652.8552(-8)	6705.5907(-10)	6700.1977(-8)	6593.3908(-36)	6646.0686(-4)
38.5	6754.9352(-6)	6645.3570(20)	6699.4847(2)	6693.9287(-33)	6584.3471(9)	-
39.5	6750.0343(-29)	6637.6764(-8)	6693.1974(-21)	6687.4852(-25)	6575.1224(-1)	6630.5741(4)
40.5	6744.9609(14)	6629.8231(4)	6686.7346(-20)	6680.8614(-43)	6565.7213(-21)	6622.5622(11)
41.5	6739.7057(29)	-	6680.0966(5)	6674.0674(13)	6556.1490(-2)	6614.3745(25)
42.5	6734.2711(39)	6613.5794(-45)	6673.2780(0)	6667.0869(-22)	6546.4012(13)	6606.0104(38)
43.5	6728.6521(-6)	6605.1998(-1)	6666.2807(-17)	6659.9371(25)	6536.4790(33)	6597.4647(-2)
44.5	6722.8476(-117)	6596.6423(27)	6659.1098(4)	6652.6016(-13)	6526.3766(-2)	6588.7483(13)
45.5	6716.8880(8)	6587.9015(-18)	6651.7571(-20)	6645.0932(-7)		6579.8539(7)
46.5	6710.7372(7)					

	$A^2\Pi_{1/2}$ - $X^2\Sigma^+$ 1-0					
	R_2	P_2	Q_2	R_{21}	P_{21}	Q_{21}
0.5				8015.9935(-26)		
1.5			8011.2476(-11)	8017.9213(-29)		8014.4189(52)
2.5	8014.9984(67)	8006.4976(-39)	8010.0070(-49)	8019.6746(7)	8011.2006(-17)	8014.7646(52)
3.5	8014.9984(-9)	8003.6781(-44)	8008.6024(55)	8021.2461(9)	8009.9483(13)	8014.9290(22)
4.5	8014.8251(-35)	8000.6850(-4)	8007.0017(-21)	8022.6388(7)	8008.5131(-4)	8014.9133(-25)
5.5	8014.4782(-13)	7997.5095(-8)	8005.2332(7)	8023.8559(34)	8006.9037(19)	8014.7294(28)
6.5	8013.9517(-4)	7994.1561(-11)	8003.2851(20)	8024.8898(14)	8005.1124(4)	8014.3601(11)
7.5	8013.2449(-13)	7990.6314(53)	8001.1566(10)	8025.7460(3)	8003.1450(10)	8013.8154(24)
8.5	8012.3638(19)	7986.9165(-7)	7998.8552(53)	8026.4240(-3)	8001.0014(35)	8013.0881(-5)
9.5	8011.2943(-49)	7983.0245(-59)	7996.3680(18)	8026.9217(-26)	7998.6740(2)	8012.1855(-3)
10.5	8010.0584(4)	7978.9677(19)	7993.7029(-15)	8027.2461(6)	7996.1716(1)	8011.1038(-7)
11.5	8008.6425(42)	7974.7246(12)	7990.8601(-43)	8027.3939(60)	7993.4915(4)	8009.8450(3)
12.5	8007.0383(-17)	7970.3035(2)	7987.8432(-32)	8027.3551(37)	7990.6314(-12)	8008.4071(6)
13.5	8005.2576(-56)	7965.7063(9)	7984.6500(-4)	8027.1363(3)	7987.5952(-9)	8006.7887(-10)
14.5	8003.3025(-53)	7960.9327(28)	7981.2764(2)	8026.7413(-3)	7984.3810(-5)	8004.9924(-19)
15.5	8001.1651(-86)	7955.9736(-32)	7977.7248(8)	8026.1696(14)	7980.9893(5)	8003.0203(-1)
16.5	7998.8552(-58)	7950.8455(-5)	7973.9947(9)	8025.4152(-5)	7977.4183(2)	8000.8677(-1)
17.5	7996.3680(-16)	7945.5380(4)	7970.0877(22)	8024.4825(-15)	7973.6668(-25)	7998.5361(-4)
18.5	7993.7029(34)	7940.0531(14)	7965.9947(-45)	8023.3734(3)	7969.7440(15)	7996.0289(24)
19.5	7990.8601(95)	7934.3883(0)	7961.7356(8)	8022.0825(-4)	7965.6356(-20)	7993.3374(-5)
20.5	7987.8254(25)	7928.5500(26)	7957.2931(7)	8020.6140(7)	7961.3550(3)	7990.4705(1)
21.5	7984.6193(29)	7922.5284(-6)	7952.6671(-48)	8018.9632(-12)	7956.8945(8)	7987.4245(3)
22.5	7981.2296(-14)	7916.3319(-13)	7947.8736(2)	8017.1359(-1)	7952.2540(-7)	7984.1996(5)
23.5	7977.6665(-2)	7909.9601(1)	7942.8973(4)	8015.1272(-8)	7947.4383(7)	7980.7950(-2)
24.5	7973.9236(1)	7903.4101(6)	7937.7401(-22)	8012.9397(-8)	7942.4434(8)	7977.2144(20)
25.5	7970.0013(0)	7896.6777(-39)	7932.4046(-51)	8010.5739(6)	7937.2740(46)	7973.4509(3)

TABLE I—*Continued*

$A^2\Pi_{1/2} - X^2\Sigma^+$ 1-0

	R_2	P_2	Q_2	R_{21}	P_{21}	Q_{21}
26.5	7965.9005(3)	7889.7763(-1)	7926.8979(-12)	8008.0281(18)	7931.9165(-18)	7969.5082(-17)
27.5	7961.6207(8)	7882.6951(11)	7921.2123(20)	8005.2991(-5)	7926.3869(-22)	7965.3886(-16)
28.5	7957.1601(-5)	7875.4338(-4)	7915.3434(-2)	8002.3936(6)	7920.6814(-5)	7961.0969(55)
29.5	7952.5200(-22)	7867.9970(-3)	7909.3012(24)	7999.3010(-55)	7914.7981(15)	7956.6137(1)
30.5	7947.7061(15)	7860.3780(-51)	7903.0768(8)	7996.0289(-111)	7908.7304(-29)	7951.9563(-3)
31.5	7942.7085(6)	7852.5915(-3)	7896.6777(26)	7992.5944(10)	7902.4919(0)	7947.1202(-3)
32.5	7937.5326(7)	7844.6248(14)	7890.0965(3)	7988.9655(-12)	7896.0715(-10)	7942.1090(38)
33.5	7932.1755(-12)	7836.4795(17)	7883.3418(25)	7985.1631(33)	7889.4738(-12)	7936.9098(-9)
34.5	7926.6404(-18)	7828.1556(5)	7876.4044(1)	7981.1738(11)	7882.9651(-44)	7931.5373(4)
35.5	7920.9322(39)	7819.6562(8)	7869.2893(-19)	7977.0046(-7)	7875.7409(-51)	7925.9827(-11)
36.5	7915.0364(13)	7810.9838(52)	7861.9996(-5)	7972.6555(-20)	7868.6154(11)	7920.2525(11)
37.5	7908.9582(-43)	7802.1204(-45)	7854.5315(6)	7968.1326(34)	7861.3078(31)	7914.3403(6)
38.5	7902.7111(7)	7793.0940(-1)	7846.8827(-10)	7963.4187(-18)	7853.8182(12)	7908.2471(-14)
39.5	7896.2772(-17)	7783.8873(9)	7839.0596(12)	7958.5315(4)	7846.1534(22)	7901.9772(-7)
40.5	7889.6669(-9)	7774.4984(-35)	7831.0547(-4)	7953.4603(-8)	7838.3130(56)	7895.5284(6)
41.5	7882.8810(37)	7764.9377(-27)	7822.8738(2)	7948.2111(6)	7830.2802(-53)	7888.8998(15)
42.5	7875.9068(-3)	7755.2014(-6)	7814.5165(23)	7942.7810(20)	7822.0813(-42)	7882.0919(28)
43.5	7868.7598(24)	7745.2829(-39)	7805.9691(-76)	7937.1691(24)	7813.7038(-37)	7875.1050(45)
44.5	7861.4269(-11)	7735.1946(-2)	7797.2636(25)	7931.3741(5)		7867.9350(28)
45.5	7853.9209(19)	7724.9246(-15)	7788.3664(-11)	7925.3998(3)		7860.5818(-25)

$A^2\Pi_{3/2} - X^2\Sigma^+$ 1-0

	R_1	P_1	Q_1	R_{12}	P_{12}	Q_{12}
1.5				7857.2052(-25)		7853.7020(-32)
2.5	7862.0632(-16)	7853.6581(-7)	7857.1573(-41)	7857.3469(15)		7852.4379(-39)
3.5	7863.5853(6)	7852.3791(22)	7857.2873(68)	7857.2873(-50)		7850.9906(27)
4.5	7864.9145(8)	7850.9031(-13)	7857.2052(-36)	7857.0479(-5)		7849.3442(9)
5.5	7866.0533(15)	7849.2382(-31)	7856.9473(9)	7856.6135(-4)		7847.5085(4)
6.5	7866.9988(-2)	7847.3893(17)	7856.4931(-2)	7855.9888(2)	7836.3741(-29)	7845.4831(7)
7.5	7867.7553(1)	7845.3456(23)	7855.8504(9)	7855.1727(1)	7832.7600(-5)	7843.2662(0)
8.5	7868.3265(61)	7843.1095(10)	7855.0154(4)	7854.1681(22)	7828.9530(-7)	7840.8590(-4)
9.5	7868.6930(-16)	7840.6814(-18)	7853.9887(-10)	7852.9676(-9)	7824.9563(-5)	7838.2637(15)
10.5	7868.8737(-40)	7838.0696(21)	7852.7735(-3)	7851.5809(5)	7820.7718(20)	7835.4752(6)
11.5	7868.8727(29)	7835.2582(-32)	7851.3725(53)	7850.0024(7)	7816.3787(-140)	7832.4969(3)
12.5	7868.6690(-19)	7832.2668(19)	7849.7698(-1)	7848.2323(-1)	7811.8266(9)	7829.3284(0)
13.5	7868.2850(41)	7829.0776(-4)	7847.9820(0)	7846.2703(-22)	7807.0686(-3)	7825.9695(-4)
14.5	7867.7008(10)	7825.7008(-2)	7846.0034(-2)	7844.1246(27)	7802.1204(-19)	7822.4211(0)
15.5	7866.9282(5)	7822.1295(-42)	7843.8345(0)	7841.7815(6)	7796.9817(-43)	7818.6824(2)
16.5	7865.9644(-1)	7818.3762(-1)	7841.4750(1)	7839.2493(-1)	7791.6632(31)	7814.7504(-30)
17.5	7864.8100(-2)	7814.4309(21)	7838.9249(1)	7836.5281(7)	7786.1467(19)	7810.6345(2)
18.5	7863.4659(11)	7810.2855(-58)	7836.1840(-3)	7833.6155(6)	7780.4383(-18)	7806.3253(-1)
19.5	7861.9277(-7)	7805.9691(53)	7833.2527(-6)	7830.5135(14)	7774.5398(-62)	7801.8268(2)
20.5	7860.2003(-7)	7801.4459(-5)	7830.1308(-12)	7827.2192(2)	7768.4635(7)	7797.1379(0)
21.5	7858.2829(4)	7796.7385(-7)	7826.8206(3)	7823.7352(-4)	7762.1902(-4)	7792.2602(6)
22.5	7856.1728(-2)	7791.8403(-20)	-	7820.0619(-1)	7755.7299(6)	7787.1919(4)
23.5	7853.8730(4)	7786.7558(0)	7819.6292(30)	7816.2023(42)	7749.0804(11)	7781.9325(-15)
24.5	7851.3725(-86)	7781.4793(-3)	7815.7436(-2)	7812.1442(0)	7742.2409(5)	7776.4874(5)
25.5	7848.6980(-7)	7776.0120(-20)	7811.6753(40)	7807.9013(12)	7735.2094(-36)	7770.8523(20)
26.5	7845.8250(-4)	7770.3591(2)	7807.4086(-1)	7803.4659(-2)	7727.9955(-16)	7765.0291(46)
27.5	7842.7599(-13)	7764.5139(-7)	7802.9555(-7)	7798.8424(2)	7720.5944(16)	7759.0098(3)
28.5	7839.5057(-5)	7758.4807(-3)	7798.3146(9)	7794.0283(0)	7712.9990(-12)	7752.8078(25)
29.5	7836.0621(18)	7752.2575(-7)	7793.4800(-13)	7789.0243(-4)	7705.2173(-22)	7746.4129(9)
30.5	7832.4246(10)	7745.8460(-4)	7788.4588(-3)	7783.8382(69)	7697.2517(9)	7739.8302(4)
31.5	7828.5961(0)	7739.2483(26)	7783.2469(-3)	7778.4474(-9)	7689.0952(9)	7733.0595(7)
32.5	7824.5823(43)	7732.4586(25)	7777.8457(1)	7772.8741(-15)	7680.7526(26)	7726.0995(5)
33.5	7820.3686(-6)	7725.4792(14)	7772.2547(3)	7767.1147(12)	7672.2192(11)	7718.9506(1)
34.5	7815.9678(-19)	7718.3087(-21)	7766.4753(16)	7761.1652(33)	7663.5011(23)	7711.6138(2)
35.5	7811.3790(-7)	7710.9507(-46)	7760.5039(3)	7755.0155(-54)	7654.5893(-29)	7704.0866(-16)
36.5	7806.5974(-17)	7703.4118(5)	7754.3445(4)	7748.6908(1)		7696-3747(2)
37.5	7801.6282(1)	7695.6786(-5)	7747.9963(10)	7742.1702(-11)		7688.4700(-26)
38.5	7796.4655(-11)	7687.7578(-8)	7741.4559(-15)	7735.4617(-11)		7680.3839(14)
39.5	7791.1143(-5)	7679.6492(-9)	7734.7292(-11)	7728.5648(-5)		7672.1053(7)
40.5	7785.5753(27)	7671.3545(10)	7727.8141(-2)	7721.4767(-21)		7663.6351(-36)

TABLE I—*Continued*

$A^2\Pi_{1/2} - X^2\Sigma^+$ 0-1

	R_2	P_2	Q_2	R_{21}	P_{21}	Q_{21}
1.5	5738.4184(-21)		5734.8325(-26)	5741.5127(-24)		
2.5	5738.6833(14)	5730.1220(-17)	5733.6596(-30)	5743.3286(1)		5738.3699(-43)
3.5	5738.7906(21)	5727.3771(-38)	5732.3353(1)	5744.9862(-6)	5733.6011(33)	5738.6198(26)
4.5	5738.7357(-43)	5724.4857(24)	5730.8529(-1)	5746.4908(8)	5732.2499(-20)	5738.7092(40)
5.5	5738.5362(-2)	5721.4214(-97)	5729.2167(8)	5747.8377(-4)	5730.7503(-9)	5738.6298(-84)
6.5	5738.1786(7)	5718.2269(27)	5727.4223(-17)	5749.0311(2)	5729.0946(-11)	5738.4121(-41)
7.5	5737.6654(12)	5714.8640(14)	5725.4714(-60)	5750.0688(3)	5727.2848(-5)	5738.0428(37)
8.5	5736.9944(-10)	5711.3378(-87)	5723.3762(3)	5750.9515(8)	5725.3195(-6)	5737.5021(-48)
9.5	5736.1672(-43)	5707.6758(-1)	5721.1205(8)	5751.6774(-2)	5723.1996(-6)	5736.8194(-3)
10.5	5735.1899(-26)	5703.8508(1)	5718.7093(6)	5752.2490(-1)	5720.9254(0)	5735.9811(39)
11.5	5734.0583(1)	5699.8718(7)	5716.1433(4)	5752.6657(7)	5718.4963(4)	5734.9801(4)
12.5	5732.7683(-4)	5695.7374(3)	5713.4228(4)	5752.9253(-1)	5715.9110(-7)	5733.8279(10)
13.5	5731.3243(3)	5691.4482(-4)	5710.5477(6)	5753.0309(6)	5713.1729(3)	5732.5192(2)
14.5	5729.7260(20)	5687.0051(-8)	5707.5174(3)	5752.9791(-3)	5710.2792(3)	5731.0542(-16)
15.5	5727.9693(5)	5682.4034(-54)	5704.3327(3)	5752.7726(-3)	5707.2316(12)	5729.4374(1)
16.5	5726.0581(-1)	5677.6580(6)	5700.9977(47)	5752.4106(0)	5704.0278(6)	5727.6638(3)
17.5	5723.9918(-4)	5672.7517(-1)	5697.4991(3)	5751.8923(-1)	-	5725.7347(3)
18.5	5721.7715(7)	5667.6921(2)	5693.8502(2)	5751.2187(3)	-	5723.6491(-8)
19.5	5719.3944(4)	5662.4780(1)	5690.0433(-31)	5750.3877(-7)	5693.4897(5)	5721.4129(29)
20.5	5716.8617(-1)	5657.1103(5)	5686.0891(10)	5749.4029(5)	5689.6603(-68)	-
21.5	5714.1745(5)	5651.5869(-6)	5681.9754(3)	5748.2582(-22)	5785.6918(14)	5716.4660(20)
22.5	5711.3357(49)	5645.9107(-4)	5677.7079(4)	5746.9624(2)	5681.5582(-7)	5713.7572(-6)
23.5	5708.3319(-1)	5640.0813(6)	5673.2852(1)	-	5677.2733(6)	5710.8954(-6)
24.5	5705.1774(-2)	5634.0927(-36)	5668.7083(2)	5743.8969(-3)	5672.8323(4)	5707.8778(-9)
25.5	5701.8717(42)	5627.9565(-14)	5663.9748(-15)	5742.1294(-8)	5668.2335(-3)	5704.7055(-3)
26.5	5698.4011(-8)	5621.6669(14)	5659.0881(-18)	5740.2071(2)	5663.4863(2)	5701.3809(36)
27.5	5694.7801(-4)	5615.2184(-8)	5654.0485(-3)	5738.1278(6)	5658.5812(0)	5697.8929(-2)
28.5	5691.0027(-7)	5608.6180(-10)	5648.8533(3)	5735.8812(-97)	5653.5204(-12)	5694.2512(-21)
29.5	5687.0716(10)	5601.8628(-21)	5643.5028(2)	5733.4976(-5)	5648.3047(-26)	5690.4571(-6)
30.5	5682.9773(-47)	5594.9568(-2)	5637.9975(1)	5730.9552(65)	5642.9392(9)	-
31.5	5678.7387(11)	-	5632.3397(21)	5728.2413(-13)	5637.4145(-2)	5682.4034(42)
32.5	5674.3374(1)	5580.6815(17)	5626.5214(-18)	5725.3816(19)	5631.7360(-4)	5678.1381(18)
33.5	5669.7823(12)	5573.3108(2)	5620.5547(7)	5722.3612(12)	5625.9037(3)	5673.7176(1)
34.5	5665.0681(-9)	5565.7860(-17)	5614.4300(-2)	5719.1827(-8)	5619.9155(-2)	5669.1441(13)
35.5	5660.2007(-3)	5558.1103(-8)	5608.1515(-2)	5715.8510(10)	5613.7725(-9)	5664.4114(-9)
36.5	5655.1756(-14)	5550.2816(8)	5601.7197(12)	5712.3588(-7)	5607.4752(-12)	5659.5256(-1)
37.5	5649.9968(-2)	5542.2968(-1)	5595.1318(11)	5708.7114(-6)	5601.0270(22)	5654.4889(57)
38.5	5644.6603(-6)	5534.1543(-52)	5588.3880(-3)	5704.9071(-3)	5594.4163(-22)	5649.2845(-2)
39.5	5639.1708(20)	5525.8660(-25)	5581.4906(-5)	5700.9411(-45)	5587.6594(21)	5643.9293(-8)
40.5	5633.5189(-17)	5517.4264(25)	5574.4392(-2)	5696.8258(-8)	5580.7302(-117)	5638.4199(4)
41.5	5627.7145(-17)	5508.8282(23)		5692.5510(8)	5573.6664(-52)	
42.5	5621.7541(-16)	5500.0739(-6)		5688.1171(5)	5566.4445(-22)	
43.5	5615.6381(-9)	5491.1728(32)		5683.5253(-2)	5559.0669(-2)	
44.5	5609.3658(-3)	5482.1059(-55)			5551.5421(92)	
45.5	5602.9331(-39)	5472.9024(26)			5543.8470(29)	

$A^2\Pi_{3/2} - X^2\Sigma^+$ 0-1

	R_1	P_1	Q_1	R_{12}	P_{12}	Q_{12}
0.5	5581.8785(37)					
1.5	5583.8127(-36)		5580.2913(55)			5577.1687(55)
2.5	5585.5924(24)		5580.6414(-61)	5580.9035(-28)		5575.9604(-33)
3.5	5587.1933(-28)	5575.8997(7)	5580.8344(-72)	5580.9505(-8)	5569.6560(18)	5574.5969(2)
4.5	5588.6354(10)	5574.5082(-53)	5580.8640(-41)	5580.8313(26)	5566.7069(-8)	5573.0637(15)
5.5	5589.9056(6)	-	5580.7300(30)	5580.5385(-1)	5563.5937(-3)	5571.3603(0)
6.5	5591.0077(0)	5571.2377(-23)	5580.4190(7)	5580.0740(-68)	-	5569.4962(53)
7.5	5591.9471(45)	-	5579.9418(-3)	5579.4560(5)	5556.8671(23)	5567.4559(18)
8.5	5592.7093(-4)	5567.3023(54)	5579.2985(3)	5578.6631(5)	5553.2511(16)	5565.2499(-1)
9.5	5593.3087(-2)	5565.0785(42)	5578.4870(2)	5577.6998(-24)	5549.4666(-6)	5562.8786(0)
10.5	5593.7354(-48)	5562.6842(-2)	-	5576.5683(-59)	5545.5049(-130)	5560.3379(-21)
11.5	5594.0110(73)	5560.1264(-8)	5576.3620(6)	5575.2852(65)	5541.3783(-235)	5557.6340(-1)
12.5	5594.0996(4)	5557.4035(7)	5575.0474(-1)	5573.8174(16)	5537.1217(29)	5554.7620(10)
13.5	5594.0211(-57)	5554.5114(1)	5573.5657(-4)	5572.1852(-2)	5532.6688(-4)	5551.7205(-4)
14.5	5593.7870(5)	5551.4517(-10)	5571.9177(5)	5570.3890(14)	5528.0534(5)	5548.5136(-1)

TABLE I—*Continued*

$A^2\Pi_{3/2} - X^2\Sigma^+$ 0-1

	R_1	P_1	Q_1	R_{12}	P_{12}	Q_{12}
15.5	5593.3781(-2)	5548.2289(20)	5570.1008(-1)	5568.4230(5)	5523.2704(2)	5545.1394(-1)
16.5	5592.8012(-10)	5544.8381(38)	5568.1170(-2)	5566.2904(4)	5518.3137(-73)	5541.5981(-3)
17.5	5592.0573(-9)	5541.2747(0)	5565.9660(-2)	5563.9912(10)	5513.2055(0)	5537.8903(-2)
18.5	5591.1474(11)	5537.5482(0)	5563.6462(-17)	5561.5237(6)	5507.9237(-1)	5534.0153(-4)
19.5	5590.0662(-3)	5533.6553(3)	5561.1625(1)	5558.8906(17)	5502.4763(4)	5529.9759(16)
20.5	5588.8182(-6)	5529.5947(-3)	5558.5092(-4)	5556.0875(0)	5496.8668(47)	5525.7656(-6)
21.5	5587.4026(-7)	5525.3688(3)	5555.6889(-8)	5553.1230(41)	5491.0819(-5)	5521.3911(-4)
22.5	5585.8186(-13)	5520.9750(-3)	5552.7032(5)	-	5485.1319(-49)	5516.8499(-5)
23.5	5584.0669(-19)	5516.4151(-5)	5549.5483(-3)	5546.6804(-4)	5479.0255(-1)	5512.1425(-4)
24.5	5582.1489(-10)	5511.6891(-5)	5546.2271(-5)	5543.2104(-10)	5472.7497(8)	5507.2680(-11)
25.5	5580.0634(2)	5506.7977(4)	5542.7391(-5)	5539.5739(-11)	5466.3051(-16)	5502.2305(15)
26.5	5577.8084(-4)	5501.7397(9)	5539.0830(-17)	5535.7712(-6)	-	5497.0224(-5)
27.5	5575.3842(-25)	5496.5142(1)	5535.2632(1)	5531.8004(-16)	5452.9279(13)	5491.6513(6)
28.5	5572.7967(-2)	5491.1262(28)	5531.2749(2)	5527.6641(-13)	5445.9847(-42)	5486.1115(-11)
29.5	5570.0394(-2)	5485.5665(-3)	5527.1192(-4)	5523.3617(-6)	5438.8850(-14)	5480.4094(8)
30.5	5567.1147(1)	5479.8430(-13)	5522.7976(-4)	5518.8926(0)	5431.6214(24)	5474.5382(-7)
31.5	5564.0239(17)	5473.9496(-66)	5518.3137(39)	5514.2558(-7)	5424.1867(-3)	5468.5026(-10)
32.5	5560.7620(-3)	5467.9158(135)	5513.6547(-6)	5509.4528(-13)	5416.5907(3)	5462.3033(5)
33.5	5557.3322(-27)	5461.6887(57)	5508.8326(-17)	5504.4869(16)	5408.8300(5)	5455.9369(3)
34.5	5553.7410(9)	5455.2933(-50)	5503.8472(1)	5499.3514(10)	5400.9072(27)	5449.4050(-1)
35.5	-	5448.7485(2)	5498.6927(-10)	5494.0626(132)	5392.8146(-7)	5442.7064(-20)
36.5	5546.0475(-12)	5442.0362(31)	5493.3728(-13)	5488.5857(33)	-	5435.8460(-6)
37.5	5541.9547(26)	5435.1510(-18)	5487.8889(3)	5482.9489(-5)	5376.1520(67)	5428.8196(-3)
38.5	5537.6882(-2)	5428.1114(38)	5482.2368(-4)	5477.1493(-13)	5367.5639(-10)	5421.6282(-2)
39.5	5533.2572(-4)	5420.8978(2)	5476.4166(-33)	5471.1858(-3)	5358.8226(17)	5414.2705(-17)
40.5	5528.6636(39)	5413.5231(2)	5470.4374(6)	5465.0543(-16)	5349.9171(35)	5406.7516(3)
41.5	-	5405.9826(-10)	5464.2883(2)	5458.7615(13)	5340.8446(14)	5399.0698(37)
42.5	5518.9633(2)	5398.2743(-55)	5457.9742(3)	5452.2987(-3)	-	5391.2181(16)
43.5	5513.8656(11)	5390.4127(10)	5451.4974(32)		5322.2161(25)	5383.1994(-34)
44.5	5508.5987(-4)	-	5444.8512(20)		5312.6510(-37)	5375.0263(14)
45.5	5503.1537(-134)	5374.1843(12)	5438.0376(-14)		5302.9361(28)	5366.6834(2)

$A^2\Pi_{1/2} - X^2\Sigma^+$ 0-2

	R_2	P_2	Q_2	R_{21}	P_{21}	Q_{21}
0.5				4527.1027(31)		
1.5				4529.0826(26)		
2.5		4517.7461(-25)		4530.9162(-13)		
3.5		4515.0547(9)	4520.0092(12)	4532.6093(-26)		
4.5	4526.4709(-19)	4512.2126(-36)	4518.5843(-15)	4534.1633(2)	4519.9217(-33)	
5.5	4526.3544(131)	4509.2346(-13)	4517.0177(-31)	4535.5696(-16)	4518.4854(11)	4526.3699(-14)
6.5	4526.0679(12)	4506.1136(6)	-	4536.8334(-27)	4516.9004(-4)	4526.2225(12)
7.5	4525.6494(4)	4502.8477(2)	4513.4609(-13)	4537.9572(-5)	4515.1739(-6)	4525.9327(44)
8.5	4525.0889(6)	4499.4381(-13)	4511.4717(29)	4538.9393(33)	4513.3061(7)	4525.4934(12)
9.5	4524.3826(-18)	4495.8885(-3)	4509.3320(-6)	4539.7691(-18)	4511.2940(5)	4524.9090(-40)
10.5	4523.5367(-7)	4492.1938(-18)	4507.0529(-7)	4540.4630(6)	4509.1389(1)	4524.1895(-11)
11.5	4522.5485(13)	4488.3588(-13)	4504.6315(-4)	4541.0110(5)	4506.8417(3)	4523.3267(16)
12.5	4521.4125(-12)	4484.3821(0)	4502.0668(-6)	4541.4158(8)	4504.3986(-26)	4522.3158(-7)
13.5	4520.1360(-11)	4480.2624(7)	4499.3596(-6)	4541.6756(-3)	4501.8200(17)	4521.1646(0)
14.5	4518.7172(0)	4476.0005(15)	4496.5102(-1)	4541.7889(-43)	4499.0929(3)	4519.8697(2)
15.5	4517.1544(4)	4471.5925(-15)	4493.5167(-10)	4541.7687(20)	4496.2260(17)	4518.4313(2)
16.5	4515.4459(-16)	4467.0468(0)	4490.3818(-6)	4541.5973(7)	4493.2155(23)	4516.8515(20)
17.5	4513.5980(3)	4462.3562(-11)	4487.1048(5)	4541.2820(-6)	4490.0611(17)	4515.1232(-14)
18.5	4511.6046(1)	4457.5262(6)	4483.6825(-12)	4540.8253(6)	4486.7637(8)	4513.2588(25)
19.5	4509.4690(11)	4452.5514(-4)	4480.1198(-5)	4540.2224(-6)	-	4511.2477(31)
20.5	4507.1896(17)	4447.4365(7)	4476.4140(-2)	4539.4815(43)	4479.7430(11)	4509.0941(45)
21.5	4504.7640(-4)	4442.1771(-7)	4472.5653(-2)	4538.5866(-8)	4476.0132(-42)	4506.7944(33)
22.5	4502.1973(-1)	4436.7796(19)	4468.5755(14)	4537.5550(15)	-	4504.3471(-20)
23.5	4499.4823(-46)	4431.2356(-1)	4464.4438(37)	4536.3748(-7)	4468.1411(7)	4501.7629(-8)
24.5	4496.6332(3)	4425.5504(-12)	4460.1667(33)	4535.0505(-27)	4463.9879(0)	4499.0358(10)
25.5	4493.6355(3)	4419.7262(6)	4455.7467(27)	4533.5869(2)	4459.6968(40)	4496.1623(0)
26.5	4490.4906(-34)	4413.7578(2)	4451.1812(-9)	4531.9763(5)	4455.2562(12)	4493.1460(-2)
27.5	4487.2109(17)	4407.6488(10)	-	4530.2166(-40)	4450.6742(-4)	4489.9849(-16)
28.5	4483.7801(-6)	4401.3956(-6)	4441.6274(-29)	4528.3208(-1)	4445.9551(36)	4486.6815(-17)
29.5	4480.2085(1)	-	4436.6409(5)	4526.2768(1)	4441.0908(50)	4483.2382(20)

TABLE I—*Continued*

	$A^2\Pi_{1/2}$ - $X^2\Sigma^+$ 0-2					
	R_2	P_2	Q_2	R_{21}	P_{21}	Q_{21}
30.5	4476.4934(9)	4388.4683(8)	4431.5088(9)	4524.0867(-12)	4436.0796(21)	4479.6446(-10)
31.5	4472.6300(-28)	4381.7892(-13)	4426.2334(5)	4521.7553(8)	4430.9278(12)	4475.9106(-6)
32.5	4468.6284(-9)	4374.9774(55)	4420.8158(6)	4519.2736(-28)	4425.6376(45)	4472.0343(13)
33.5	4464.4862(42)	4368.0136(21)	4415.2534(-15)	4516.6518(-18)	4420.1985(15)	4468.0098(-13)
34.5	-	4360.9101(6)	4409.5510(-11)	4513.8915(55)	4414.6194(12)	4463.8429(-24)
35.5	4455.7529(-30)	4353.6668(8)	4403.7045(-21)	4510.9710(-25)	4408.8981(12)	4459.5351(-7)
36.6	4451.1793(23)	4346.2800(-8)	4397.7182(-4)	4507.9145(-16)	4403.0294(-36)	4455.0845(22)
37.5	-	4338.7525(-17)	4391.5897(17)	4504.7116(-22)	4397.0277(12)	4450.4839(-11)
38.5	4441.5848(-27)	4331.0859(-1)	4385.3151(3)	4501.3667(3)	4390.8776(1)	4445.7444(7)
39.5	4436.5764(-4)	4323.2720(-44)	4378.8952(-39)	4497.8735(-5)	4384.5852(-7)	4440.8568(-17)
40.5	4431.4189(-32)	4315.3286(32)	4372.3409(0)	4494.2348(-16)	4378.1519(2)	4435.8316(23)

	$A^2\Pi_{3/2}$ - $X^2\Sigma^+$ 0-2					
	R_1	P_1	Q_1	R_{12}	P_{12}	Q_{12}
0.5	4369.4302(24)					
1.5	4371.3815(3)			4368.2859(33)		4364.7570(49)
2.5	4373.1787(-3)	4364.7070(10)	4368.2261(-104)	4368.5273(-39)		4363.5883(-3)
3.5	4374.8199(-12)	4363.5370(130)	4368.4653(-13)	4368.6251(9)		4362.2724(28)
4.5	4376.3058(-17)	4362.1949(84)	4368.5419(7)	4368.5569(-47)	4354.4362(-44)	4360.7996(45)
5.5	4377.6352(-29)	4360.6931(-5)	4368.4526(-75)	4368.3422(-12)	4351.4010(22)	4359.1667(16)
6.5	4378.8093(-36)	4359.0425(-27)	4368.2261(26)	4367.9654(-43)	4348.2017(-1)	4357.3779(-19)
7.5	4379.8315(-3)	4357.2390(-24)	4367.8294(-19)	4367.4369(-34)	4344.8468(-28)	4355.4390(0)
8.5	4380.6946(-4)	4355.2840(19)	4367.2825(-10)	4366.7576(21)	4341.3451(28)	4353.3417(-12)
9.5	4381.4017(-5)	4353.1665(-11)	4366.5792(-9)	4365.9158(8)	4337.6817(17)	4351.0949(34)
10.5	4381.9508(-28)	4350.8947(-31)	4365.7215(2)	4364.9251(60)	4333.8640(12)	4348.6852(3)
11.5	4382.3489(-2)	4348.4753(26)	4364.7070(1)	4363.7667(-10)	4329.8872(-35)	4346.1230(-1)
12.5	4382.5903(16)	4345.8905(-19)	4363.5370(0)	4362.4599(-9)	4325.7691(53)	4343.4051(-10)
13.5	4382.6721(-4)	4343.1569(0)	4362.2094(-23)	4361.0035(50)	4321.4804(-19)	4340.5335(-5)
14.5	4382.5986(-17)	4340.2671(7)	4360.7302(-7)	4359.3794(-14)	4317.0480(19)	4337.5106(37)
15.5	4382.3725(3)	4337.2187(-21)	4359.0934(-14)	4357.6086(9)	4312.4542(-12)	4334.3239(-9)
16.5	4381.9883(1)	4334.0192(-11)	4357.3041(9)	4355.6817(23)	4307.7160(56)	4330.9892(14)
17.5	4381.4496(13)	4330.6667(19)	4355.3561(-3)	4353.5956(-1)	4302.8116(6)	4327.4953(-7)
18.5	4380.7527(1)	4327.1512(-34)	4353.2541(-2)	4351.3584(16)	4297.7541(-34)	4323.8485(-9)
19.5	4379.9013(3)	4323.4896(1)	4350.9956(-13)	4348.9633(6)	4292.5488(-10)	4320.0482(1)
20.5	4378.8948(12)	4319.6670(-28)	4348.5836(-8)	4346.4124(-12)	4287.1890(8)	4316.0908(-15)
21.5	4377.7291(-13)	4315.6947(-8)	4346.0165(-3)	4343.7084(-9)	4281.6692(-35)	4311.9829(10)
22.5	4376.4089(-24)	4311.5639(-27)	4343.2944(4)	4340.8484(-16)	4275.9999(-35)	4307.7160(-10)
23.5	4374.9403(38)	4307.2839(6)	4340.4160(-3)	4337.8347(-11)	4270.1818(12)	4303.2975(-3)
24.5	4373.3046(-13)	4302.8461(4)	4337.3846(10)	4334.6661(-5)	4264.2033(-9)	4298.7237(-7)
25.5	4371.5229(33)	4298.2569(31)	4334.1957(-3)	4331.3479(52)	4258.0739(-5)	4293.9954(-13)
26.5	4369.5765(-12)	4293.5038(-39)	4330.8508(-28)	4327.8678(38)	4251.7898(-16)	4289.1130(-20)
27.5	4367.4816(15)	4288.6015(-60)	4327.3569(4)	4324.2338(32)	4245.3540(-13)	4284.0791(-2)
28.5	4365.2242(-27)	4283.5542(8)	4323.7089(43)	4320.4418(-8)	4238.7652(-10)	4278.8897(-1)
29.5	4362.8204(23)	4278.3471(18)	4319.8979(-3)	4316.4963(-37)	4232.0219(-23)	4273.5437(-27)
30.5	4360.2521(-18)	4272.9800(-35)	4315.9346(-26)	4312.3990(-41)	4225.1275(-20)	4268.0490(-4)
31.5	4357.5308(-33)	4267.4703(22)	4311.8227(9)	4308.1531(14)	4218.0841(19)	4262.3988(0)
32.5	4354.6601(11)	4261.7987(-4)	4307.5519(-1)	4303.7449(-12)	4210.8803(-22)	4256.5932(-16)
33.5	4351.6272(-13)	4255.9725(-41)	4303.1266(-13)	4299.1895(32)	4203.5319(14)	4250.6361(-14)
34.5	4348.4471(45)	4250.0064(56)	4298.5493(-3)	4294.4795(72)	4196.0288(25)	4244.5261(-8)
35.5	4345.0984(-32)	4243.8723(5)	4293.8173(1)	4289.6057(14)	4188.3694(-8)	4238.2625(-8)
36.5	4341.6014(-39)	4237.5895(-2)	4288.9324(17)	4284.5828(4)	4180.5618(-4)	4231.8525(59)
37.5	4337.9562(23)	4231.1572(26)	4283.8868(-36)	4279.4079(12)	4172.6044(18)	4225.2753(-19)
38.5	4334.1460(-14)	4224.5683(17)	4278.6952(-10)	4274.0811(39)	4164.4924(10)	4218.5577(28)
39.5	4330.1848(-11)	4217.8272(12)	4273.3509(27)	4268.5953(12)	4156.2297(8)	4211.6798(-3)
40.5		4210.9312(-15)	4267.8468(1)	4262.9592(18)	4147.8139(-13)	4204.6527(-2)

	$A^2\Pi_{3/2}$ - $X^2\Sigma^+$ 3-1					
	R_1	P_1	Q_1	R_{12}	P_{12}	Q_{12}
3.5	8701.9689(-7)					8689.5195(-17)
4.5	8703.2271(38)	8689.4396(16)				8687.8317(-40)

TABLE I—*Continued*

	$A^2\Pi_{3/2} - X^2\Sigma^+$ 3-1					
	R_1	P_1	Q_1	R_{12}	P_{12}	Q_{12}
5.5	8704.2712(-46)	8687.7302(-38)		8694.9095(1)		8685.9495(3)
6.5	8705.1271(2)	8685.8311(21)	8694.7910(18)	8694.1970(-30)		8683.8630(13)
7.5	8705.7794(28)	8683.7218(-12)	8694.0632(20)	8693.2870(-24)	8671.2375(19)	8681.5747(14)
8.5	-	8681.4121(-40)	8693.1344(22)	8692.1769(-8)	6867.3724(38)	8679.0830(-10)
9.5	8706.4733(16)	8678.9136(53)	8691.9987(-33)	8690.8640(-9)	8663.2974(-37)	8676.3925(-13)
10.5	8706.5162(-9)	8676.2010(14)	8690.6662(-45)	8689.3531(21)	8659.0205(-125)	8673.5035(8)
11.5	8706.3621(11)	8673.2879(-21)	8689.1388(5)	8687.6351(-10)	8654.5650(5)	8670.4098(-11)
12.5	8706.0055(21)	8670.1786(-11)	8687.4065(16)	8685.7212(12)	8649.8929(-28)	8667.1200(16)
13.5	8705.4478(34)	8666.8670(17)	8685.4680(-24)	8683.6060(30)	8645.0337(71)	8663.6285(34)
14.5	8704.6850(11)	8663.3543(-27)	8683.3366(18)	8681.2828(-22)	8639.9534(-39)	8659.9341(28)
15.5	8703.7218(0)	8659.6434(-12)	8680.9987(4)	8678.7652(-8)	8634.6892(14)	8656.0359(-10)
16.5	8702.5604(21)	8655.7303(-14)	8678.4597(-11)	8676.0406(-55)	8629.2197(13)	8651.9410(-9)
17.5	8701.1929(-3)	8651.6187(4)	8675.7220(-4)	8673.1242(-11)	8623.5499(8)	8647.6408(-57)
18.5	8699.6189(-78)	8647.3067(23)	8672.7778(-53)	8670.0076(40)	8617.6725(-75)	8643.1530(23)
19.5	-	8642.7958(57)	8669.6425(-5)	8666.6848(37)	8611.6098(-13)	8638.4550(3)
20.5	8695.8879(-12)	8638.0757(2)	8666.3023(3)	8663.1574(-5)	8605.3405(-22)	8633.5558(-25)
21.5	8693.7197(16)	8633.1584(-23)	8662.7634(32)	8659.4367(28)	8598.8717(-30)	8628.4639(21)
22.5	8691.3426(-31)	8628.0444(-13)	8659.0205(27)	8655.5077(-16)	8592.2082(9)	8623.1652(0)
23.5	8688.7707(-11)	8622.7261(-45)	8655.0764(18)	8651.3832(-8)	8585.3415(8)	8617.6736(50)
24.5	8685.9965(0)	8617.2165(10)	8650.9313(4)	8647.0581(-1)	8578.2717(-32)	8611.9722(2)
25.5	8683.0194(-4)	8611.5021(17)	8646.5901(35)	8642.5339(21)	8571.0093(-8)	8606.0775(19)
26.5	8679.8437(20)	8605.5863(8)	8642.0419(2)	8637.8072(22)	8563.5514(51)	8599.9793(-2)
27.5	8676.4620(-3)	8599.4679(-30)	8637.3001(36)	8632.8763(-16)	8555.8860(23)	8593.6826(-10)
28.5	8672.8757(-59)	8593.1554(-11)	8632.3503(-5)	8627.7520(16)	8548.0206(-18)	8587.1878(-4)
29.5	8669.1005(10)	8586.6422(-4)	8627.2042(-6)	8622.4190(-36)	8539.9663(38)	8580.4887(-46)
30.5	8665.1164(1)	8579.9305(13)	8621.8591(5)	-	8531.7003(-39)	8573.5996(7)
31.5	8660.9260(-58)	8573.0143(-21)	8616.3118(-3)	8611.1702(36)	8523.2518(42)	8566.5022(-31)
32.5	8656.5416(-45)	8565.9005(-37)	8610.5635(-21)	8605.2379(-6)	-	8559.2126(2)
33.5	8651.9499(-94)	8558.5966(37)	8604.6218(29)	8599.1065(-39)		8551.7226(21)
34.5	8647.1731(17)	8551.0682(-143)	8598.4741(17)	8592.7812(-12)		8544.0314(18)
35.5		8543.3761(31)	8592.1250(-9)	8586.2565(19)		8536.1397(0)
36.5		8535.4657(10)	8585.5820(24)	8579.5224(-47)		
37.5		8527.3621(45)	8578.8346(11)	8572.5991(-8)		
38.5		8519.0489(-29)	8571.8850(-28)			
39.5		8510.5519(44)	8564.7437(12)			

Note. The numbers in parentheses correspond to the observed minus calculated line positions (in 10^{-4} cm^{-1}) using the spectroscopic constants of Tables II and III.

The rotational assignments of the five bands was straightforward using combination differences and the previous estimates of the molecular constants (*2–4*). There are 12 branches in each band and the notation appropriate for a $^2\Pi$–$^2\Sigma$ transition is given by Herzberg (*15*). The observed line positions are listed in Table I.

TABLE II

Rotational Constants for the $X^2\Sigma^+$ State of CP (in cm^{-1}; 1 SD in Parentheses)

Constant	v = 0	v = 1	v = 2
T_v	0.0	1 226.1273(2)	2 438.5743(3)
B_v	0.7958816(22)	0.7898955(22)	0.7838944(23)
10^6x D_v	1.32736(83)	1.33083(84)	1.33611(90)
10^2x γ_v	1.85439(51)	1.85006(69)	1.84549(77)

TABLE III

Rotational Constants for the $A^2\Pi$ State of CP (in cm^{-1}; 1 SD in Parentheses)

Constant	v = 0	v = 1	v = 3
T_v	6 884.0056(2)	7 934.4145(2)	9 999.0066(4)
A_v	-156.2437(2)	-156.1269(3)	-155.8933[a]
10^5x A_{Dv}	4.856(18)	4.323(35)	3.257[a]
B_v	0.7092769(22)	0.7036497(22)	0.6923644(27)
10^6x D_v	1.27986(82)	1.28239(86)	1.2864(13)
10^3x p_v	9.411(14)	9.438(22)	9.492[a]
10^5x q_v	-4.839(47)	-4.89(11)	-5.19(15)
10^7x p_{Dv}	-1.20(11)	-0.98(18)	-0.54[a]

[a] Fixed by extrapolation from $v = 0$ and 1. See text.

Band-by-band fits of the line positions of Table I were made utilizing the effective Hamiltonian of Brown *et al.* (*16*). An explicit listing of the matrix elements for a $^2\Pi$ and a $^2\Sigma^+$ state are given, for example, in a paper by Amiot *et al.* (*17*). For the final fit all of the line positions of all of the bands (except 3–1 for which a special fit was made) were fitted simultaneously to provide the molecular constants of Tables II and III. Since only the $^2\Pi_{3/2}$ spin component was observed in the 3–1 band, the values of A_3, A_{D3}, p_3 and p_{D3} were estimated by extrapolation from $v = 0$ and 1 and fixed.

Equilibrium molecular constants were derived from the data of Tables II and III and are displayed in Table IV. Since only three vibrational levels are available for the $A^2\Pi$ and $X^2\Sigma^+$ states, the vibrational and rotational constants of Table IV are an exact fit to the data. The quoted errors are derived by simple propagation of errors and are not proper statistical errors. The neglect of $\omega_e y_e$ almost certainly causes systematic errors in ω_e and $\omega_e x_e$ far exceeding the quoted errors. From the B'_e and B''_e values the equilibrium bond distances of 1.561977(7) Å for the $X^2\Sigma^+$ state and 1.654421(7) Å for $A^2\Pi$ are computed.

TABLE IV

Equilibrium Molecular Constants for CP (in cm^{-1})

Constant	$X^2\Sigma^+$	$A^2\Pi$
ω_e	1 239.8076(5)	1 062.4841(5)
$\omega_e x_e$	6.8402(3)	6.0376(2)
B_e	0.7988690(36)	0.7120866(28)
α_e	0.0059711(55)	0.0056169(35)
γ_e	-0.0000075(23)	-0.00000515(78)
r_e (Å)	1.561977(7)	1.654421(7)

The Kratzer relationship (*15*) predicts $D''_e = 1.3267 \times 10^{-6}$ cm^{-1} and $D'_e = 1.2794 \times 10^{-6}$ cm^{-1} compared to the experimental values of 1.3256×10^{-6} and 1.2786×10^{-6} cm^{-1} for the $X^2\Sigma^+$ and $A^2\Pi$ states, respectively. The Pekeris relationship (*15*) predicts $\alpha''_e = 0.005949$ cm^{-1} and $\alpha'_e = 0.005474$ compared to the observed values of 0.005971 and 0.005617 cm^{-1}.

The constants of Tables II–IV are in reasonable agreement with, but much more accurate and extensive than, those of Tripathi *et al.* (*4*) for the $A^2\Pi$ state. The agreement with the $X^2\Sigma^+$ constants of Bärwald *et al.* (*1*) is also good except for the sign of γ, the phenomenological spin–rotation constant. We concur with Tripathi *et al.* (*4*) that γ'' is positive. The signs and magnitudes of the Λ-doubling constants in the $A^2\Pi$ state and the spin–rotation constant in the $X^2\Sigma^+$ are similar to the values for the isostructural molecules CN (*18*) and SiN (*19*).

CONCLUSION

The $A^2\Pi$–$X^2\Sigma^+$ transition of CP was observed with a high-resolution Fourier transform spectrometer. This infrared electronic transition is the analog of the red system of CN. The molecular constants may prove useful in the extraterrestrial detection of phosphorus-containing molecules.

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