

Additional Rotationally Assigned Subbands

Q branch intensities imply perpendicular. Lack Q(.5) suggests

$P'' = -0.5$ $P' = P'' - 1$.

J''

0.5			2952.3379
1.5		2949.5920	2953.6238
2.5	2945.0076	2949.0439	2955.0330
3.5	2942.6296	2948.6208	2956.4836
4.5	2940.3755	2948.2383	2958.0667
5.5	2938.1592	2947.9871	
6.5	2936.0776		

fits poorly to a quadratic in $J'(J'+1)$ & not better to J'

E_0 2958.6755

B 0.81064 bizarrely low B value

D -0.00145

σ 0.06

$P'' = -0.5$ Q branch intensities imply $P' \neq P''$. Lack of Q(.5) suggests $P' = P'' - 1$
But weak P implies $P' = P'' + 1$

J''

P	Q	R
0.5		2970.3887
1.5		2972.3227
2.5	2963.0486	2974.2911
3.5		2976.2659
4.5		2978.2716
5.5		
6.5		
7.5		
8.5	2952.9392	

fits well to a quadratic in $J'(J'+1)$

E_0 2976.3173

B 0.93707

D 0.00009

σ 0.007

$P'' = 0.5$

P Obs.

Q Obs.

R Obs.

0.5		2929.7461
1.5		2931.4622

2.5				2933.2317
3.5	2920.4575			2934.9985
4.5	2918.5564	2926.7480		2936.8062
5.5	2916.6626	2926.7178		2938.5344
6.5				
7.5	2912.8547			
Fit Parameters				
E0	2926.323343			
B	0.904012372			
D	-0.000105363			
s.d.	0.04			

P''=0.5

	P Obs.	Q Obs.	R Obs.
0.5			2929.8639
1.5			2931.9504
2.5		2927.3660	2934.0056
3.5	2920.9504	2927.5896	2936.0547
4.5	2919.3347	2927.8000	2938.1260
5.5		2928.0422	2940.2214
6.5		2928.2996	
7.5			
Fit Parameters			
E0	2926.320188		
B	0.956154407		
D	0.000265938		
s.d.	0.04		

Note:

The above two bands have the same $J'=0$ energy. Generally the sums of the omc for the two bands for the same J' are much smaller than the individual. This is the kind of behavior expected for parity splittings, but these levels are of E symmetry.

P''=1.5 Very fragmentary band. Upper state levels all e symmetry

	P	Q	R
1.5			
2.5			2933.2317
3.5		2926.8025	2934.9985
4.5	2918.5564		2936.7532
5.5	2916.6626		
6.5	2914.7473		

2.5	2944.2090	2949.3362	2956.4004
3.5	2942.9082	2949.9841	2958.9587
4.5	2941.7122	2950.7151	2961.5896
5.5	2940.5977	2951.5203	2964.2793
6.5	2939.5552	2952.4358	
7.5	2938.6145		

Upper state energies fit very poorly to a quadratic in $J'(J'+1)$

Upper state energies fit very well to a quadratic in J'

E0 2946.6000

linear in J' 1.27210

square of J' 0.96335

Since $P'=0.5$ $\sigma=0.5$ mixes with $P'=-0.5$, $\sigma=-.5$ for $\lambda+I=0$,
 tried fit with $E=E_0+B(J+1)+\sqrt{\Delta E+(JT^2+B(J+.5))^2}$

	Value	std error of parameter
E0	2938.9	1.9403
B	0.93316	0.0039397
ΔE	7.4394	1.787
JT^2	1.8941	0.73953
Chisq	0.00029909	

Strangely $J'=5.5$ has by far largest residual (-0.015 cm^{-1})

Clearly these parameters are highly correlated.

$P''=1.5$ Perpendicular selection rules. Upper state levels all f symmetry. Probably F

J''	P	Q	R
1.5			2963.0730
2.5		2958.4902	2965.4053
3.5		2958.9849	2967.7913
4.5	2950.7151		2970.1652
5.5	2949.4294		2972.5450
6.5	2948.1292		
7.5	2946.8386		
8.5			

Upper state energy fit quadratic in $J'(J'+1)$

E0 2956.2827

B 0.9975

D 0.00046

σ 0.017

Upper state energy fit quadratic in J

E0 2955.70829

linear in J' 1.38889

square of J' 0.92501

Q e<-f	R e<-e	R
	2976.1418	2976.1418
2971.5541	2978.1408	2978.1408
2971.7140	2980.1636	2980.1636
2971.8946	2982.2012	2982.2012

sigma	0.015	Most error (-.016) in J'=3.5	2972.0889	2984.2415
			2972.2787	

P''=1.5 Selection rules unclear probably perpendicular with P'=P''+1

	P e<-e	P f<-f	Q f<-e
1.5			
2.5			2971.5556
3.5	2965.1299	2965.1299	2971.7223
4.5		2963.4541	2971.9112
5.5	2961.8254	2961.7955	2972.1118
6.5	2960.1858	2960.1372	2972.3219
7.5			

There is no discernible splitting of the upper state so that average upper energies were

Fit E vs J'(J'+1)

E0	2969.7916
B	0.94345
D	0.00013
sigma	0.003