

# ThO Levels and Spectroscopy

F [ $^1\Sigma^+ ?^*$ ] (545/767)

E [55%  $^1\Sigma^+$ , 35%  $^3\Sigma^-$ ] (613/908)

A [95%  $^3\Pi$ , 5%  $^1\Sigma^+$ ] (944/1892)

X [100%  $^1\Sigma^+$ ]

G [95%  $^3\Phi$ ] (555/787)

D [75%  $^3\Sigma^+$ , 15%  $^3\Phi$ ] (627/940)

C [75%  $^1\Pi$ , 20%  $^3\Pi$ ] (690/1090)

B [75%  $^3\Pi$ , 20%  $^1\Pi$ ] (898/1720)

H [100%  $^3\Delta$ ] (1880)

Q [95%  $^3\Delta$ , 5%  $^1\Delta$ ] (1632/12326)

$\Omega = 0^+$

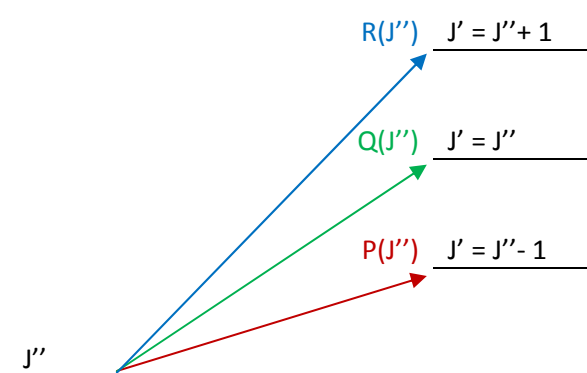
$\Omega = 1$

$\Omega = 2$

[Square brackets] give  $\Lambda S$  states rounded to the nearest multiple of 5.  
 (Round brackets) give the wavelength in nm for the transition to the ground state/H state.

State	$\Omega$	$^{2S+1}\Lambda$ , three leading terms	$T_0$ [ $\text{cm}^{-1}$ ]	$\omega_e$ [ $\text{cm}^{-1}$ ]	$B_e$ [ $\text{cm}^{-1}$ ] <sup>†</sup>	$r_e$ [ $\text{\AA}$ ]	$\mu_{\text{elec}}$ [D]
X	0	99.9% $^1\Sigma^+$	0	895.77	0.33326	1.840	3.9
H	1	98.4% $^3\Delta$ , 1.1% $^3\Pi$ , 0.5% $^1\Pi$	5316.60	857.2	0.32638	1.858	5.4
A	0	95.3% $^3\Pi$ , 4.7% $^1\Sigma^+$	10600.82	846.4	0.32304	1.867	
B	1	76.5% $^3\Pi$ , 17.8% $^1\Pi$ , 5.2% $^3\Sigma^+$	11129.14	842.80	0.32497 0.32364	1.864	
C	1	76.6% $^1\Pi$ , 19.5% $^3\Pi$ , 1.5% $^3\Delta$	14490.02	825.1	0.32246 0.32162	1.870	
D	1	74.5% $^3\Sigma^+$ , 14.6% $^3\Phi$ , 6.5% $^1\Pi$	15946.22	839.2	0.32155 0.32569	1.866	
E	0	53.1% $^1\Sigma^+$ , 35.1% $^3\Sigma^-$ , 9.9% $^3\Phi$	16320.37	829.26	0.32309	1.867	
F	0	$^1\Sigma^+ ?^*$	18337.56	757.36	0.32140	1.870	
G	2	94.9% $^3\Phi$ , 3.0% $^1\Delta$ , 2.0% $^3\Delta$	18009.93	809.1	0.31814	1.882	
Q	2	94.1% $^3\Delta$ , 4.0% $^1\Delta$ , 1.9% $^3\Pi$	6127.92	858.42	0.32703	1.856	

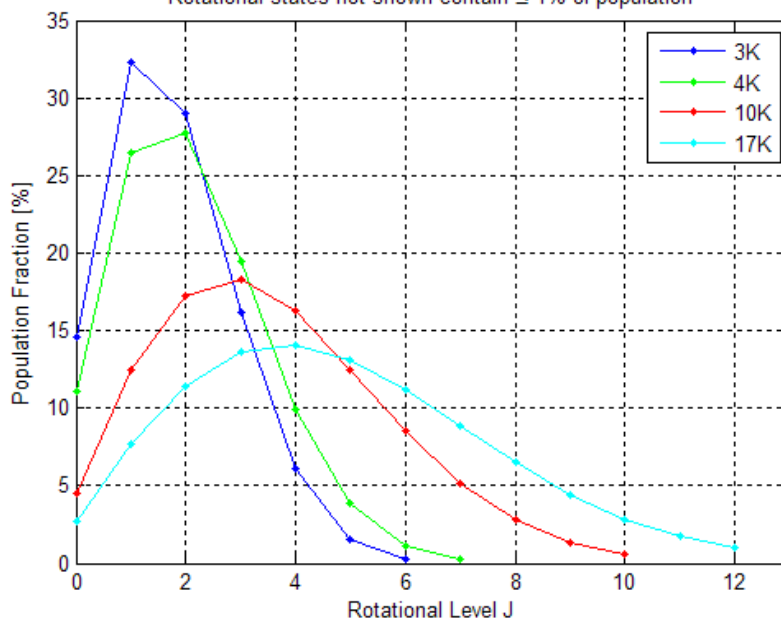
<sup>†</sup>When two values of  $B_e$  are shown, they correspond to the upper and lower  $\Omega$  doublet components



## Other electronic transitions [nm]

	I	M	K	O	L	N
X	511	460	441	432	402	360
H	703	609	577	561	511	446?

Rotational Population in a Case (c) Molecule with  $B=0.33\text{cm}^{-1}$  and  $\Omega=0$   
 Rotational states not shown contain  $\leq 1\%$  of population



## X - C (690 nm)

R(1)	14490.64
Q(1)	14489.98
Q(2)	14489.93
Q(3)	14489.86
Q(4)	14489.77
Q(5)	14489.67
Q(6)	14489.53

## H - E (908 nm)

P(1)	11003.12
P(2)	11002.46
Q(1)	11003.76
Q(2)	11003.75
R(1)	11005.06
R(2)	11005.69

## H - G (787 nm)

R(1)	12694.58
R(2)	12695.18
R(3)	12695.78
R(4)	12696.34
Q(2)	12693.29
Q(3)	12693.24
P(3)	12691.34
P(4)	12690.63

## X - A (944 nm)

P(1)	10600.15
P(2)	10599.47
P(3)	10598.77
R(1)	10601.47
R(2)	10602.09
R(3)	10602.70

## References

Marian et al, Journal of Molecular Structure (Theochem), 169 (1988) 339-354  
 Paulovic et al, Journal of Chemical Physics, Volume 119 Number 2, (2003)

\*Edvinsson et al, Ark. Fys. Band 30 nr. 22, 1965  
 Edvinsson et al, Journal of Molecular Spectroscopy 113, 93-104 (1985)