ThO Useful Information

Compiled by: ACME Collaboration

1 Level diagram

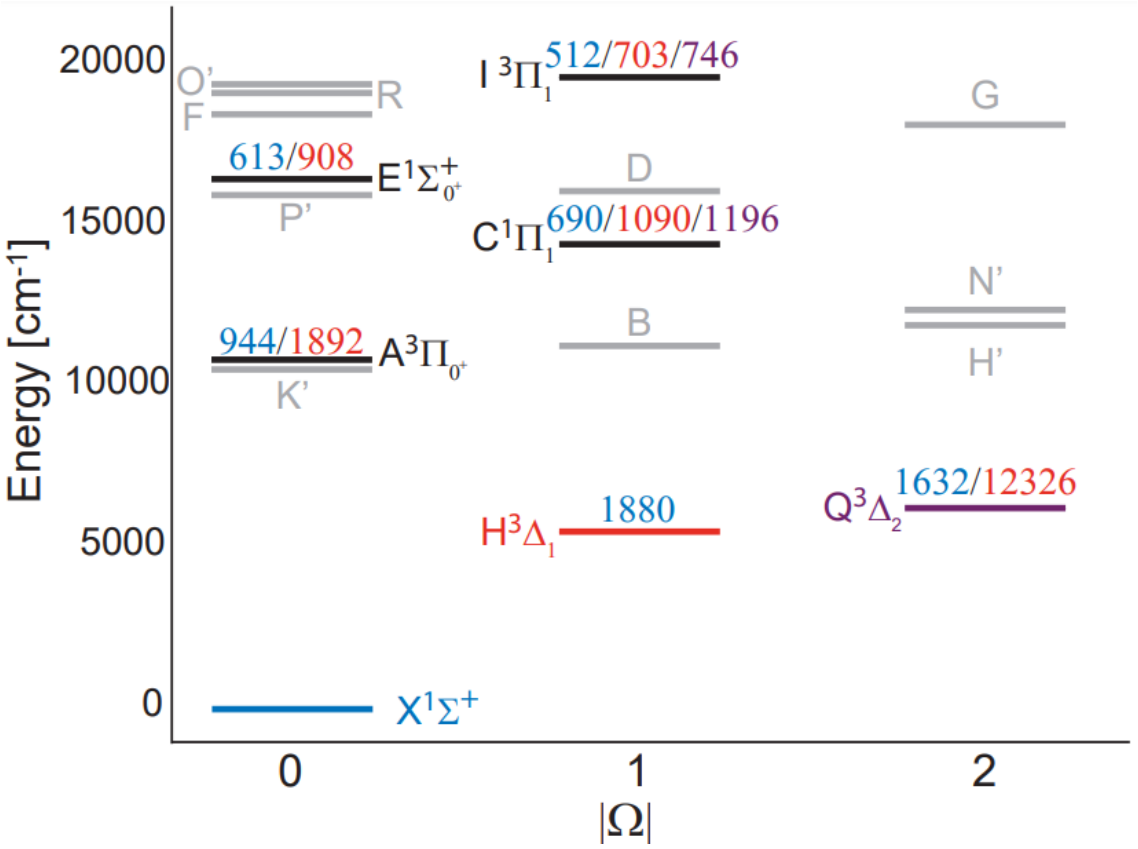


Figure 1: Energy level diagrams of ThO. Grey lines indicate levels less likely to be useful for ACME III. Lowest three levels X, H, Q colored with blue, red, purple. Transition wavelengths are given in corresponding colors in nm.

For more energy level details [1]. References for the next page:

- 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)
- Original ThO cheat sheet

2 Electronic state general information

State	Ω	$^{2S+1}\Lambda$	T_0[cm^{-1}]	ω_e [cm^{-1}]	B_e [cm^{-1}]	r_e[Å]	μ_E[D]
X	0	99.9% $^1\Sigma^+$	0	895.77	0.33264	1.84	2.8
H	1	98.4%$^3\Delta$, 1.1%$^3\Pi$, 0.5%$^1\Pi$	5316.6	857.2	0.32638	1.858	4.2
Q	2	94.1%$^3\Delta$, 4.0%$^1\Delta$, 1.9%$^3\Pi$	6127.92	858.42	0.32703	1.856	4.1
A	0	95.3%$^3\Pi$, 4.7%$^1\Sigma^+$	10600.82	846.4	0.32304	1.867	
C	1	76.6%$^1\Pi$, 19.5%$^3\Pi$, 1.5$^3\Delta$	14490.02	825.1	0.32246 0.32162	1.870	2.6
E	0	53.1%$^1\Sigma^+$, 35.1%$^3\Sigma^-$, 9.9%$^3\Phi$	16320.37	829.26	0.32309	1.867	
I	1	$\sim$ 20%$^3\Pi_1/^1\Pi_1$	19538.99		0.32869 0.00154		4.2

Table 1: The rotational constants are given for both the upper and lower Ω doublets in the C state. For the I state, the Λ doublet is given instead.

3 Measured spectrum

X − C (690nm)	
R(0)	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
P(2)	14488.65
P(3)	14487.95

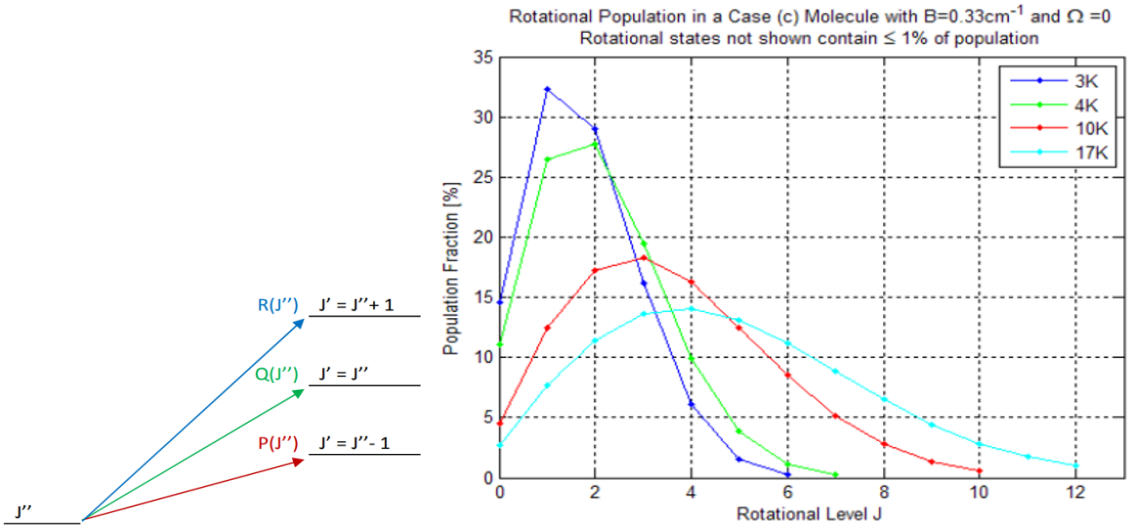
X − A (944nm)	
P(1)	10600.15
P(2)	10599.47
P(3)	10598.77
R(0)	10601.47
R(1)	10602.09
R(2)	10602.70

H − C (1090nm)	
Q(1)	9173.38

H − I (703nm)	
Q(1)	14222.43

Q − I (746nm)	
P(2)	13409.78

Q − C (1196nm)	
P(2)	8360.71
R(2)	8363.92



4 Ω doublet splitting

H($J=1$)	Q($J=2$)	C($J=1$)	I($J=1$)
360kHz [BO]	$<$ 10kHz [XW]	51MHz [BO]	91MHz [CP]

5 Lifetime

H	Q	C	I
4.2(5)ms [DGA]	$>$ 62ms [XW]	468(30)ns [TS]	115(4)ns [TS]

6 Electronic branching ratios

$\|f\rangle$	$\|\langle f \mid C\rangle\|^2$	$\omega\,(\mathrm{cm}^{-1})$	Computed branching (%)	Range (%)	Measured
X	0.77	14490	88.0	$73-95$	88(6)%
H	0.09	9174	2.7	$1-7$	
Q	0.37	8362	8.2	$3-20$	10(2)%
A	0.13	3890	0.3	$0.1-0.8$	
B	0.58	3361	0.8	$0.3-2.3$	

Table 2: Estimated and measured electronic branching ratios from C state [XW,ZL].

$\|f\rangle$	$\|\langle f \mid I\rangle\|^2$	$\omega\,(\mathrm{cm}^{-1})$	Branching (%)
$X(v=0)$	0.77	19538	91
$X(v=1)$	0.09	18648	1
$H(v=0)$	0.37	14224	5
$Q(v=0)$	0.13	13420	3

Table 3: Measured electronic branching ratios from I state [TS].

7 Vibrational branching ratios

$H, v=0$ to $X, v=0 \sim 94\%$ [CP]
$C, v=0$ to $X, v=0 \sim 84\%$ [ZL]

- Ω doublet: H(pg 11)[6]; Q(pg 2)[10]; C(pg94)[6]; I(pg 79)[7].
- Lifetime: H(pg 1)[3]; Q(pg 5)[10]; C(pg 1)[2]; I(pg 1)[2].
- Electronic branching: C(pg 63)[5]; I(pg 8)[2].
- Vibrational branching: H(pg 59)[7]; C(pg 63)[5].

8 E1 (reduced) matrix element

	X	H	Q	A	C	E	I
X	1.09(1) [TS]			0.15(4) [DGA]	0.51(2) [XW]		0.72 [TS]
H		1.67(4) [AV]		0.31(9) [DGA]	0.02 [CP]	0.018(11) [BS]	0.27 [CP]
Q			1.60 [XW]		0.40 [XW]		0.23 [TS] 0.16 [XW]
A	0.15(4) [DGA]	0.31(9) [DGA]					
C	0.51(2) [XW]	0.02 [CP]	0.40 [XW]		1.03 [XW]		
E		0.018(11) [BS]				1.39(1) [TS]	
I	0.72 [TS]	0.27 [CP]	0.23 [TS] 0.16 [XW]				1.67(1) [TS]

Table 4: E1 reduced matrix given in ea_0 or 1.28 MHz/(V/cm) or 2.54 D. For actual matrix element, an extra factor of
$\pm\sqrt{(2J+1)\,(2J'+1)}\begin{pmatrix} J & 1 & J' \\ -\Omega & (\Omega-\Omega') & \Omega' \end{pmatrix}\begin{pmatrix} J & 1 & J' \\ -M & (M-M') & M' \end{pmatrix}$
is picked up for an E field in the Z direction. In the limit of full mixing so that the good quantum numbers are J, M, Ω, this factor reduces to $\pm\frac{\Omega M}{J(J+1)}$.

- Ang: lab log October 8, 2021
- Steimle: pg 2[9]; pg 8[2]; pg 1[4].
- Lasner: pg 32, 291[5].
- Spaun: pg 62[8].
- Panda: pg 51, 76[7].
- Wu: pg 7, 9[10].

9 M1 (reduced) matrix element

	X	H	Q	C	I
X	< 0.001 [XW]			0.9(2) [BO]	
H		$-0.0088(5)$ [XW]		0.08(3) [BO]	0.08(5) [BO]
Q			2.07(11) [XW]		
C	0.9(2) [BO]	0.08(3) [BO]		1.23(6) [XW]	
I		0.08(5) [BO]			0.5260(1) [TS]

Table 5: Directly or indirectly measured g factor. The actual Zeeman shift is given by the diagonal terms $-\mathcal{B}_Z \mu_B g \frac{M\Omega}{J(J+1)}$. For actual off diagonal terms, an extra factor like that of table 4 is picked up. Mostly only diagonal terms (g factor) are important. Off diagonal terms are useful for Stark interference systematics estimation.

- Wu: pg 3, 12[10].
- O'Leary: pg 77[6].
- Steimle: pg 4[4].

References

[1] The electronic structure of thorium monoxide: Ligand field assignment of states in the range 0–5 eV - Kaledin - 2019 - Journal of Computational Chemistry - Wiley Online Library.

[2] Phys. Rev. A 90, 062503 (2014) - Branching ratios and radiative lifetimes of the U, L, and I states of thorium oxide.

[3] D. G. Ang, C. Meisenhelder, C. D. Panda, X. Wu, D. DeMille, J. M. Doyle, and G. Gabrielse. Measurement of the H$ˆ3\Delta_1$ Radiative Lifetime in ThO, Apr. 2022. Number: arXiv:2204.05904 arXiv:2204.05904 [physics].

[4] D. L. Kokkin, T. C. Steimle, and D. DeMille. Characterization of the $I(|\ensuremath{\Omega}|=1)–X\phantom{\rule{0.16em}{0ex}}{}ˆ{1}{\ensuremath{\Sigma}}ˆ{
band of thorium oxide. *Physical Review A*, 91(4):042508, Apr. 2015. Publisher: American Physical Society.

[5] Z. Lasner. Order-of-magnitude-tighter bound on the electron electric dipole moment.

[6] B. R. O'Leary. In search of the electron's electric dipole moment in thorium monoxide: an improved upper limit, systematic error models, and apparatus upgrades.

[7] C. Panda. Order of magnitude improved limit on the electric dipole moment of the electron.

[8] B. N. Spaun. A Ten-Fold Improvement to the Limit of the Electron Electric Dipole Moment. page 229.

[9] F. Wang, A. Le, T. C. Steimle, and M. C. Heaven. Communication: The permanent electric dipole moment of thorium monoxide, ThO. *The Journal of Chemical Physics*, 134(3):031102, Jan. 2011.

[10] X. Wu, Z. Han, J. Chow, D. G. Ang, C. Meisenhelder, C. D. Panda, E. P. West, G. Gabrielse, J. M. Doyle, and D. DeMille. The metastable Q $^3\triangle_2$ state of ThO: a new resource for the ACME electron EDM search. *New Journal of Physics*, 22(2):023013, Feb. 2020.