UNIVERSITY OF STOCKHOLM
INSTITUTE OF PHYSICS

REPORT

Spectroscopic Studies of

the Diatomic Molecules HfO and ThO

Spectroscopic Studies of the Diatomic Molecules HfO and ThO

Inaugural Dissertation

by

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By due permission
of the faculty of Mathematics and Natural Science
of the University of Stockholm, to be publicly discussed
in the main auditorium, Institute of Physics
on December 18, 1971, at 10 A.M.,
for the degree of doctor of philosophy.

CONTENTS

INTRODUCTION

When the investigations in this thesis were started, no rotational analyses of the HfO or ThO spectra had been published. For the first two members of the TiO family, TiO and ZrO, several analyses of singlet and triplet states had been performed [1] - [13]. Gatterer et al. [14] give reproductions of the HfO and ThO spectra in their beautiful atlas "Molecular Spectra of Metallic Oxides". For HfO they also give a vibrational analysis of nine band systems but no molecular constants were derived.

The aim of the investigations constituting this thesis was to enlarge our knowledge of the TiO family through rotational analyses of high resolution spectra of HfO and ThO. The TiO family is of special interest because these diatomic oxides represent simple systems in which the effect of d electrons on molecular bonding can be studied.

SUMMARY OF THE INVESTIGATIONS

The experimental investigations which constitute this thesis have been published in the following four papers.

A. G. Edvinsson and Ch. Nylén, "On the band spectrum of HfO," Physica Scripta (1971).

B. G. Edvinsson, L.-E. Selin and N. Åslund, "On the band spectrum of ThO," Arkiv för Fysik $\underline{30}$, 283 (1965).

C. G. Edvinsson, A. v. Bornstedt and P. Nylén, "Rotational analysis for a perturbed $^1\Pi$ state in ThO," Arkiv för Fysik $\underline{38}$, 193 (1968).

D. A. v. Bornstedt and G. Edvinsson, "Rotational analysis of two mutually interacting electronic states of $^1\Pi$ character in ThO," Physica Scripa $\underline{2}$, 205 (1970).

The electronic states of HfO and ThO which have been treated in these investigations are given in Fig. 1. A short description of the contents in the four papers A - D will be given below.

A. 31 HfO bands belonging to nine band systems identified by Gatterer et al. [14] were rotationally analysed. The electronic states involved in these nine transitions are given in Fig. 1. Homogeneous perturbations between the D $^1\Pi$ and E $^1\Pi$ states were studied. The perturbations occur between the vibrational levels D_2/E_0, D_3/E_1, D_4/E_2. The difference $\Delta v = 2$ between the interacting vibrational levels gives rise to an irregular isotopic effect in the bands. In the perturbed vibrational levels, the Λ-type doubling changes sign for high J numbers. This is due to the fact that the Λ-type doubling of the unperturbed D $^1\Pi$ state is opposite to that of the unperturbed E $^1\Pi$ state.

Perturbations in the H', J' and G states have also been observed. The analysis deals only with the $Hf^{180}O^{16}$ isotopic molecule.

B. 20 bands in transitions involving the states X, A B, ..., H in ThO were rotationally analysed. The two states A and B were observed for the first time. In this paper, the light source (electrodeless microwave discharge) used in all these experiments is described.

C. The 0-0, 1-1 and 2-2 bands of the I $^1\Pi \rightarrow X$ $^1\Sigma$ transition in ThO were rotationally analysed. It was found that the I $^1\Pi$ state is perturbed by a $\Omega = 2$ state and that this perturbing state is the upper state of the previously analysed G - H transition. The analysis of the G - H transition is extended to the 2-2 band. The perturbations occur between the vibrational levels I_0/G_2, I_1/G_3 and I_2/G_4. The analysis of the perturbation makes it possible to determine the positions of the G and H state relative to the other analysed states of ThO.

D.   8 bands belonging to the transitions $K\,^1\Pi \to X\,^1\Sigma$ and $M\,^1\Pi \to X\,^1\Sigma$ were analysed. Homogeneous perturbations between the vibrational levels K_0/M_1 and K_1/M_2 were studied. It was found that, in addition to the interaction with the K state, the M state must interact strongly with other states.

In Table I, the molecular constants which have been determined for HfO and ThO are given. For Π-states the notation c and d is used in the following sense: The Λ-type doubling component which has the same symmetry properties as the rotational levels of a $^1\Sigma^+$ state is called c, the other d.

Except for the 0-0 bands of the C, H and J systems of HfO, all molecular constants have been determined by fitting energy formulae to term values using a computer. The data processing system which has been utilized is that given by Åslund [15].

When fitting formulae of the type $T(J) = T_0 + BJ(J+1) - DJ^2(J+1)^2$ to the term values, the constant D is obtained with a much higher accuracy than is usually obtained by graphical methods. This has made it possible to test the valitity of Kratzer's relation $\omega_e = 2\,B_e^{3/2}\,D_e^{-1/2}$. For the ground states $X\,^1\Sigma$ of both HfO and ThO, the discrepancy between the experimental ω_e value and that obtained by Kratzer's relation is less than 0.07 %.
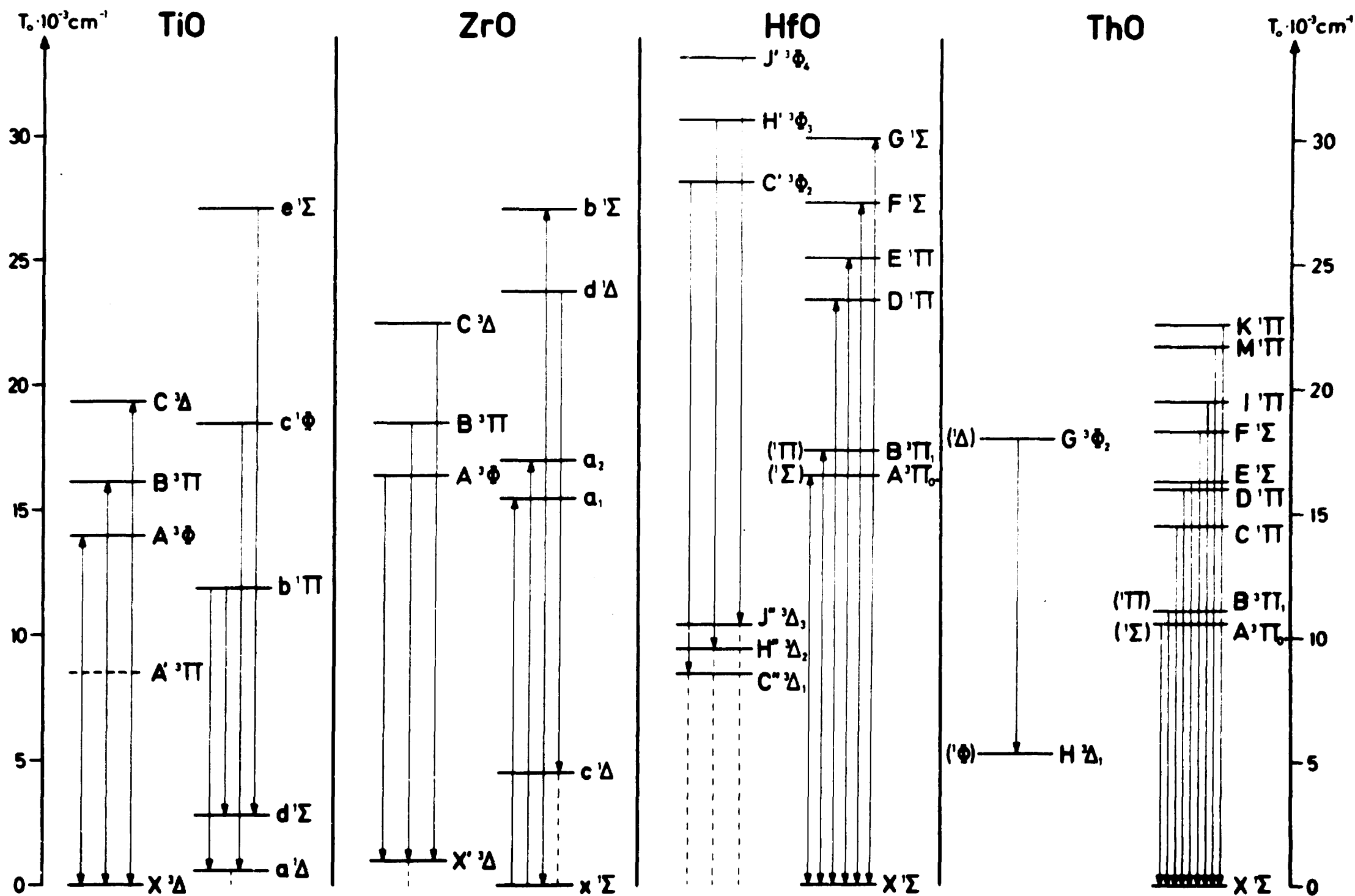
Fig. 1 Known electronic states in the TiO family. The positions of those states which are connected to the zero-level using broken lines are unknown. The absorption transitions indicated are those obtained by Weltner and McLeod for molecules trapped in solid neon and argon matrices. For TiO and ZrO only the lowest sublevels of the triplet states are given.

Table I. Molecular constants for $Hf^{180}O^{166}$ and $Th^{232}O^{16}$. The figures in brackets after the values are the error limits and should always be referred to the last preceeding figure. Error limits are given only for those constants which have been derived from an overdetermined system of equations. If the whole value of a constant is given in brackets it represents a $\Delta G_{1/2}$, B_0 or D_0-value.

$Hf^{180}O^{16}$

State	T_0	ω_e	$\omega_e x_e$	B_e	$\alpha_e \times 10^2$	$D_e \times 10^6$	r_e Å	Remarks
J' $^3\Phi_4$	22655.82 + c	-	-	(0.3719)	-	-	1.76	Perturbation in v = 0
H' $^3\Phi_3$	21239.87 + b	-	-	(0.3699)	-	-	1.76	Perturbation in v = 0
C' $^3\Phi_2$	19682.94 + a	(845)	-	(0.3696)	-	(0.30)	1.76	
J" $^3\Delta_3$	c	-	-	(0.3788)	-	(0.26)	1.74	
H" $^3\Delta_2$	b	-	-	(0.3781)	-	(0.26)	1.74	
C" $^3\Delta_1$	a	(918)		(0.3776)	-	(0.28)	1.74	
G $^1\Sigma$	30032.706(8)	(852.29)	-	0.370106	0.2071	(0.2764(3))	1.761	Perturbation in v = 1
F $^1\Sigma$	27351.136(8)	849.40	3.67	0.36563 (2)	0.188 (1)	0.2702(2)	1.772	
E $^1\Pi$ (c) (d)	25177.246(7)	866.93	3.68	0.36868 (2) 0.36928 (2)	0.197 (2) 0.198 (2)	0.267 (2) 0.269 (2)	1.764	Perturbations between D_2/E_0, D_3/E_1, $D_4/E2$
D $^1\Pi$ (c) (d)	23503.648(5)	872.60(9)	3.31 (2)	0.36912 (2) 0.36837 (2)	0.182 (1) 0.1800(9)	0.2624(8) 0.2631(4)	1.764	
B $^3\Pi_1$ (c) (d)	17528.645(7)	907.01	3.38	0.378060(7) 0.377537(5)	0.1852(5) 0.1848(4)	0.263 (1) 0.2618(4)	1.743	
A $^3\Pi_{0^+}$	16586.955(9)	914.24	3.38	0.377985(4)	0.1827(3)	0.2587(5)	1.742	
X $^1\Sigma^+$	0.000(7)	974.09(3)	3.228(6)	0.386537(7)	0.1724(3)	0.2438(3)	1.723	

Table I   continued

$$\text{Th}^{232}\text{O}^{16}$$

State	T_0	ω_e	$\omega_e x_e$	B_e	$\alpha_e \times 10^2$	$D_0 \times 10^6$	r_e Å	Remarks
K $^1\Pi$ (c) (d)	22.635.65(2)	(795.5)	-	0.318636 / 0.318642	0.124 / 0.133	0.2007(3) / 0.2025(3)	1.880	Perturbations between K_0/M_1, K_1/M_2
M $^1\Pi$ (c) (d)	21734.32(2)	(850.87)	-	0.325857 / 0.325754	0.1390 / 0.1398	0.2059(3) / 0.2051(3)	1.860	
I $^1\Pi$ (c) (d)	19539.06(2)	800.85	1.47	0.330434(7) / 0.328921(7)	0.183 (1) / 0.191 (1)	0.2390(4) / 0.2211(4)	1.849	Perturbations between I_0/G_2, I_1/G_3, I_2/G_4
F $^1\Sigma$	18337.56(1)	(757.36)	-	(0.321397(3))	-	0.2042(3)	1.870	Perturbation in v = 1
G $^3\Phi_2$	17998 (5)	816	2.4*	0.318192	0.128	0.1936(2)	1.882	
E $^1\Sigma$	16320.37(1)	829.26(4)	2.30(1)	0.323090(4)	0.1303(3)	0.1996(2)		
D $^1\Pi$ (c) (d)	15946.22(1)	839.2*	2.50*	0.321550 / 0.325691	0.130 / 0.1357	0.1850(3) / 0.1997(2)	1.866	Large Λ-type doubling
C $^1\Pi$ (c) (d)	14490.02(1)	835.1*	2.39*	0.322455 / 0.321618	0.1280 / 0.129	0.1931(2) / 0.1873(3)	1.870	
B $^3\Pi_1$ (c) (d)	11129.14(2)	842.80	2.18	0.324973(5) / 0.32364 (2)	0.1299(4) / 0.129 (1)	0.1942(3) / 0.1882(6)	1.864	
A $^3\Pi_{0^+}$	10600.82(1)	846.4*	2.44*	0.323044	0.1294	0.1866(3)	1.867	
H $^3\Delta_1$	5305 (5)	864*	2.4*	0.326427	0.126	0.1864(2)	1.858	
X $^1\Sigma^+$	0.00(1)	895.77	2.39	0.332644(4)	0.1302(3)	0.1833(3)	1.840	

* This value have been obtained using Pekeris formula.

COMPARISON BETWEEN HfO and ThO

It is to be expected that the spectra of HfO and ThO should show similarities since the metal atoms belong to the same group in the periodic system and have the same number of valence electrons. In the HfO spectrum, 9 band systems can be easily identified in the visible and ultraviolet region (3 000 Å – 7 000 Å). In the ThO spectrum, there are many more band systems in the same wavelength region and the spectrum looks quite unlike that of HfO. The difference between the spectra is very apparent if they are compared in the atlas published by Gatterer et al. [14]. In spite of the difference in appearance of the two spectra, it is possible to find counterparts in ThO for most of the electronic states found for HfO. In Fig. 2 the electronic states analysed for the two molecules are given in different energy scales. The position of the C'' state for HfO is not known experimentally but has been put to the same height as the H state for ThO.

As indicated in Fig. 2, a one-to-one correspondence has been established between the electronic states. For the connected states the relative energy is approximately the same, the Ω-values are the same and if there is Λ-type doubling, it has the same sign. Also the ω_e values show a similar variation for the connected states. This similarity between the term schemes of the two molecules probably reflects a similar electronic structure in the corresponding states.

For the I, K and M states of ThO, no counterparts have been found in HfO. There are also strong bands, not analysed, in the ThO spectrum which seem to have no correspondence in the HfO spectrum. The strongest of these ThO bands are those at 7288.9, 7159.0, 6405.9 and 5599.8 A. I have photographed these bands in high resolution but so far all attempts to analyse the bands have failed. The transitions giving rise to these bands do not seem to involve the X $^1\Sigma$ state.
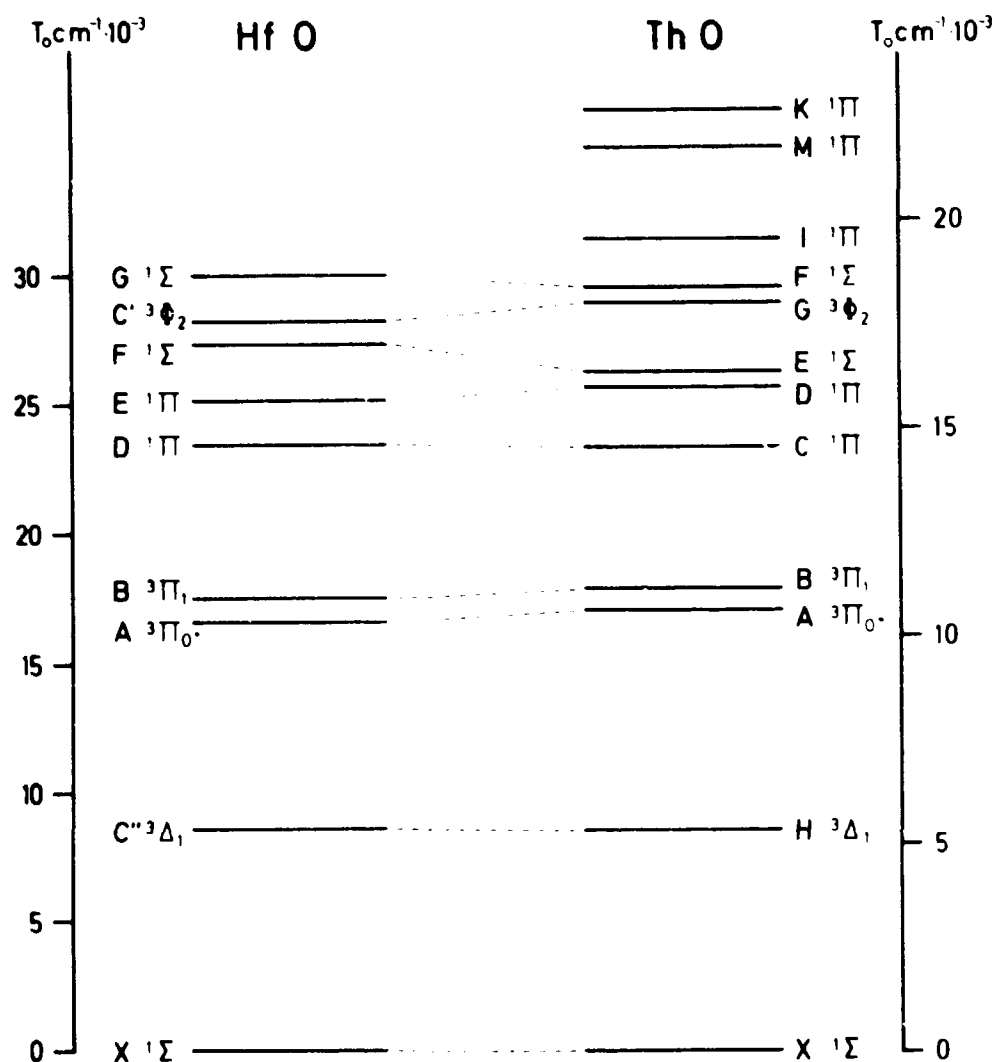
Fig. 2   Comparison between electronic states of HfO and ThO. The
energy scale is not the same for the two molecules.

Weltner and McLeod [16] have made a comparison between some of the elec-
tronic states of ZrO and HfO. According to their interpretation the D $^1\Pi$.
E $^1\Pi$ and F $^1\Sigma$ states of HfO correspond to the a_1, a_2 and b $^1\Sigma$ states of ZrO
and the states should arise from the same electron configurations. The Ω-
values of the two states a_1 and a_2 have so far not been determined experi-
mentally.

ELECTRONIC STATES AND ELECTRONIC CONFIGURATIONS
IN THE TiO FAMILY

The known electronic states of the TiO family are given in Fig. 1. All rota-
tional analyses have been performed on emission sp ctra. The absorption
spectra indicated in the figure are those obtained by Weltner and McLeod [16]
from molecules trapped in neon and argon matrices at low temperature. The

absorption spectra obtained by Weltner and McLeod show that the ground state of TiO is a $^3\Delta$ state and, for ZrO and HfO, the ground states are $^1\Sigma$ states. Weltner and McLeod did not include ThO in their investigations but the similarity between HfO and ThO indicates that the ground state of ThO is also a $^1\Sigma$ state.

TiO: In 1959 Pettersson [5] found the lowlying d $^1\Sigma$ state for TiO. The identification of this state made it clear that in TiO there are three low-lying states $^3\Delta$, $^1\Delta$ and $^1\Sigma$ in order of increasing energy and that these states ought to be derived from $\delta\sigma$ and σ^2 electron configurations outside closed shells.

Carlson et al. [17] - [20] have made Hartree-Fock calculations on the low-lying states of TiO. For the low-lying d $^1\Sigma$ state, they give the following configuration for the 30 electrons:

$$(1\sigma^2 2\sigma^2 3\sigma^2 1\pi^4 4\sigma^2 5\sigma^2 6\sigma^2 2\pi^4)_{core} 7\sigma^2 8\sigma^2 3\pi^4 9\sigma^2 \ .$$
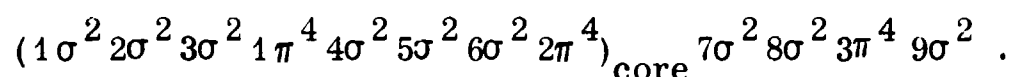
The core consists of slightly perturbed atomic orbitals and can be written $KK(L3s^2 3p^6)_{Ti}$. The 7σ, 8σ and 3π are bonding M.O's and 9σ is a nonbonding orbital mainly of $4s\sigma$ (Ti) character. From the configuration for the d $^1\Sigma$ state, the configuration .... $3\pi^4 1\delta 9\sigma$ was derived for the ground state X $^3\Delta$ and the a $^1\Delta$ state. The 1δ orbital corresponds to the $3d\delta$ (Ti) atomic orbital.

Carlson and Nesbet [18], Cheetham and Barrow [21] and others have given electron configurations for the excited states of TiO. The configurations given in Fig. 3 are from Cheetham and Barrow and are identical to those given by Carlson and Nesbet except for the b $^1\Pi$ state. Electrons in the 9σ orbital are on excitation mainly 3d(Ti) atomic orbitals of δ, π and σ symmetry. Only two of the predicted electronic states are unobserved. The e $^1\Sigma$ state recently discovered by Phillips [8] may arise from configuration .... $\pi^4\sigma\sigma^*$.
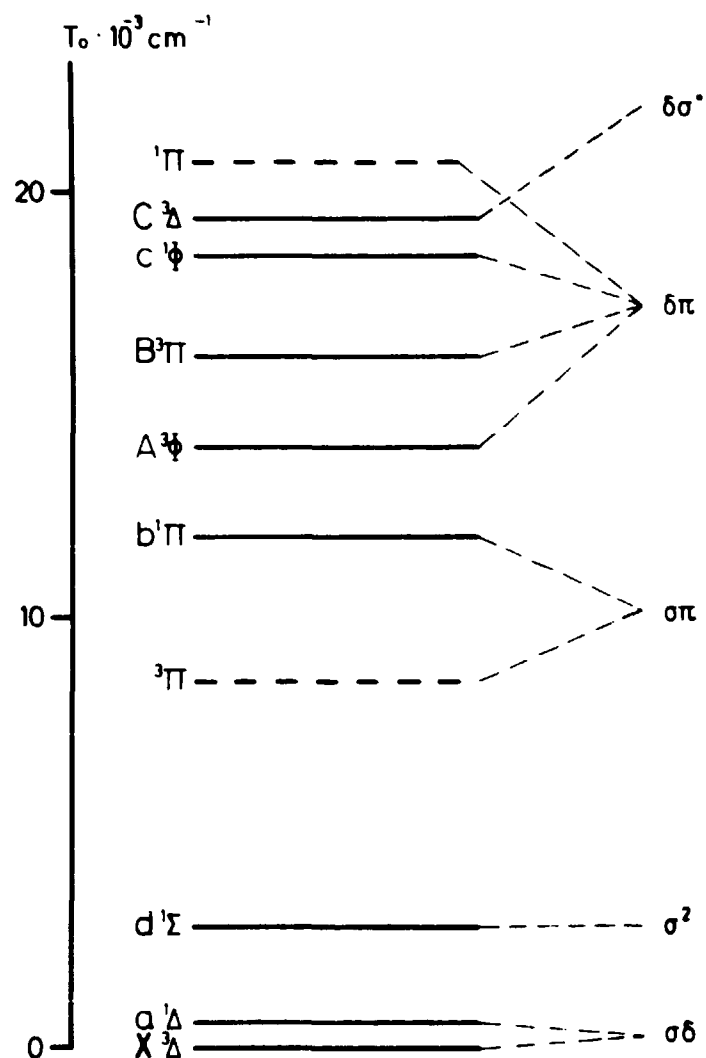
Fig. 3   Electron configurations and electronic states for TiO. Predicted
but unobserved states are indicated by broken lines.

ZrO: Electron configurations for ZrO have been given by Weltner and McLeod
and by Brewer and Green [22]. These authors give the following electron
configurations outside closed shells for the five lowest electronic states
of ZrO:

$$\sigma^2(^1\Sigma), \sigma\delta(^3\Delta, \,^1\Delta) \text{ and } \sigma\pi(^3\Pi, \,^1\Pi).$$

HfO: The spectra of TiO and ZrO are dominated by the strong triplet-triplet
transitions and the subbands of these transitions form easily recognized
groups in the spectrum. No such groups are found in HfO. Now HfO has
32 electrons more than ZrO and therefore a much larger splitting for
the triplet states of HfO is expected. For such a heavy molecule as HfO,

triplet-singlet transitions may well be allowed. These properties of the heavy HfO molecule make it difficult to distinguish singlet electronic states from sublevels of triplet states. For instance there is no difference between a $^3\Pi_{0^+} - {}^1\Sigma$ and a $^1\Sigma - {}^1\Sigma$ transition.

The lower electronic states of HfO probably have the same electron configurations outside closed shells as in TiO and ZrO. The ground state $X\ ^1\Sigma$ of HfO then has the configuration $\dots \pi^4\sigma^2$.

The lower states of the C, H and J transitions have the properties expected for the sublevels of a $(\sigma\delta)^3\Delta$. The B values are nearly equal and vary in a regular way and, as in the case for TiO and ZrO, no Λ-type doubling can be detected. The C, H and J band systems are therefore interpreted as being due to the transitions $^3\Phi_2 \rightarrow {}^3\Delta_1$, $^3\Phi_3 \rightarrow {}^3\Delta_2$ and $^3\Phi_4 \rightarrow {}^3\Delta_3$ respectively. In Table II some molecular constants for the 0-0 bands of the $^3\Phi \rightarrow {}^3\Delta$ transitions in TiO, ZrO and HfO are given. The differences, $\Delta\nu_{00}$, between the ν_{00} values of the subbands increase when going from TiO to HfO as expected when the metal atom becomes heavier. For all of the three molecules the two $\Delta\nu_{00}$ values are unequal. This indicate that in no case can both the $^3\Phi$ state and the $^3\Delta$ state be described as pure coupling cases a.

The position of the $^3\Delta$ state relative to the $X\ ^1\Sigma$ state in HfO is not known and the $^1\Delta$ state which can also be derived from the $\sigma\delta$ configuration is so far unobserved.

The A and B states of HfO have now to be considered. The transitions $A \rightarrow X\ ^1\Sigma$ and $B \rightarrow X\ ^1\Sigma$ have the typical properties of $^1\Sigma - {}^1\Sigma$ and $^1\Pi - {}^1\Sigma$ transitions and on these grounds the A and B states have been interpreted as $^1\Sigma$ and $^1\Pi$ states in paper A. However, the first excited states above the $\sigma\delta(^3\Delta, {}^1\Delta)$ states are expected to be $\sigma\pi(^3\Pi, {}^1\Pi)$. Therefore the A and B states are reinterpreted as the $^3\Pi_{0^+}$ and $^3\Pi_1$ levels of this

Table II. Data on the 0-0 bands of the $^3\Phi - {}^3\Delta$ transitions in TiO, ZrO and HfO.

The B_0'' values for the individual sublevels of the $^3\Delta$ state of TiO have been determined from the wave numbers published by Phillips[3].

Transition	ν_{00}	$\Delta\nu_{00}$	B_0''	$\Delta B_0''$
$^3\Phi_4-{}^3\Delta_3$	14612.96		0.5392	
		67.11		0.0049
TiO $\quad{}^3\Phi_3-{}^3\Delta_2$	14095.85		0.5343	
		76.11		0.0060
$^3\Phi_2-{}^3\Delta_1$	14019.74		0.5283	
$^3\Phi_4-{}^3\Delta_3$	16033.85		0.4156	
		292.49		0.0008
ZrO $\quad{}^3\Phi_3-{}^3\Delta_2$	15741.36		0.4148	
		314.58		0.0014
$^3\Phi_2-{}^3\Delta_1$	15426.78		0.4134	
$^3\Phi_4-{}^3\Delta_3$	22655.82		0.3788	
		1415.95		0.0007
HfO $\quad{}^3\Phi_3-{}^3\Delta_2$	21239.87		0.3781	
		1556.93		0.0005
$^3\Phi_2-{}^3\Delta_1$	19682.94		0.3776	

$\sigma\pi(^3\Pi)$ state. This reinterpretation is not in conflict with the rotational analyses of the A and B systems. The $\sigma\pi(^1\Pi)$ state could then be the D $^1\Pi$ state.

It is difficult to give any electron configurations for the remaining observed states in HfO because one must also consider the possibility of exciting electrons from the π^4 shell and the number of predictable states becomes very large. Weltner and McLeod have given such electron configurations for the remaining observed states in HfO.

The $\sigma\pi(^3\Pi)$ state has not been observed for TiO and ZrO. The energy of this $^3\Pi$ state may be too low for these molecules to permit a photographic recording of the expected transition $\sigma\pi(^3\Pi) \rightarrow \sigma\delta(^3\Delta)$. In HfO

however, the energy of the $\sigma\pi$ ($^3\Pi$) state is about 17 000 cm^{-1} and the energy of the $\sigma\delta$ ($^3\Delta$) state is probably also higher than for TiO and ZrO. A similar displacement towards higher energies for HfO compared to TiO and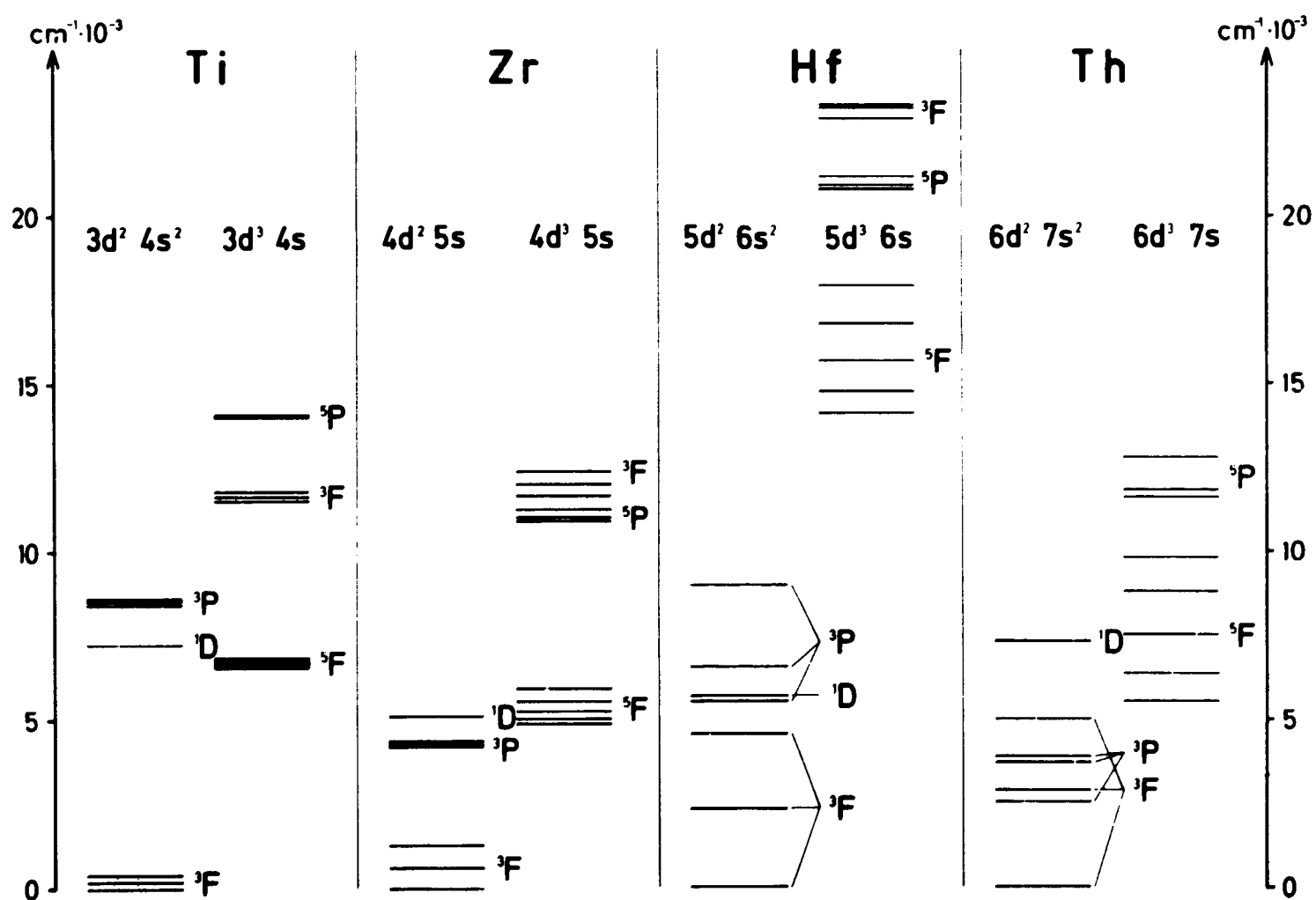 ZrO can be found for the atomic energy levels of the isolated metal atoms. In Fig. 4, the lowest atomic energy levels for the Ti group corresponding to the configurations d^2s^2 and d^3s are given. The data on atomic energy levels have been obtained from Moore [23] and Zalubas [24]. As can be seen from Fig. 4 the lower energy levels corresponding to the d^3s configuration lie considerably higher in Hf than for the other atoms.

Fig. 4   The lowest atomic energy levels for the Ti group corresponding to the configurations d^2s^2 and d^3s.

ThO: The similarity between the term schemes for the observed states of ThO and HfO suggests that the electron configurations given for the lower states of HfO can also be adopted for ThO. The G → H transition has been interpreted as a G $^1\Delta$ → H $^1\Phi$ transition in paper C. A low-lying $^1\Phi$ state, however, is not expected from any simple electron configuration. The similarity between the term schemes of HfO and ThO suggests that the G → H transition in ThO is a $^3\Phi_2$ → $^3\Delta_1$ transition. With this reinterpretation, the G state still has $\Omega = 2$ but the H state now has $\Omega = 1$ instead of $\Omega = 3$ (H $^1\Phi$). As long as the first lines in the bands cannot be observed with certainty, this reinterpretation is not in conflict with the rotational analyses performed for the G → H transition.

The A and B states of ThO were interpreted as $^1\Sigma$ and $^1\Pi$ states in paper B. For the same reasons as for HfO these two states are reinterpreted as the $^3\Pi_{0^+}$ and $^3\Pi_1$ sublevels of a $\sigma\pi$ ($^3\Pi$) state.

As already mentioned there are several strong bands in ThO which have not been analysed. In a paper on the atomic energy levels of Th, Zalubas [24] has pointed out that excitation of one 6 s electron to the 5 f shell gives rather low-lying energy levels. If similar excitation takes place in ThO, the number of low-lying valence states can be very large.

The three lowest electron configurations for the TiO family and the corresponding electronic states are given in Table III.

Table III. The three lowest electron configurations for the TiO family and the corresponding electronic states. Predicted but unobserved states are indicated by broken lines.

Config	States	TiO	ZrO	HfO	ThO
$\sigma\pi$	$^1\Pi$	b $^1\Pi$	(a$_1$ $^1\Pi$)	D $^1\Pi$	C $^1\Pi$
	$^3\Pi$	----	-----	A $^3\Pi_{0^+}$, B $^3\Pi_1$, ...	A $^3\Pi_{0^+}$, B $^3\Pi_1$, ...
$\sigma\delta$	$^1\Delta$	a $^1\Delta$	c $^1\Delta$	----	----
	$^3\Delta$	X $^3\Delta$	X $^3\Delta$	C'' $^3\Delta_1$, H'' $^3\Delta_2$, J'' $^3\Delta_3$	H $^3\Delta_1$, ..., ...
σ^2	$^1\Sigma$	d $^1\Sigma$	x $^1\Sigma$	X $^1\Sigma$	X $^1\Sigma$

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