DISSOCIATION ENERGIES OF HfO AND ThO

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ABSTRACT

The RKR potential energy curves are constructed for the ground states of diatomic hafnium oxide and thorium oxide. Using Lippincott and Hulburt-Hirschfelder potential function the dissociation energies are estimated by curve fitting method. The H-H potential function was found to give a better fit in both cases. The dissociation energies of hafnium oxide and thorium oxide are estimated as 9.04 ± 0.02 eV and 10.34 ± 0.01 eV respectively.

INTRODUCTION

THE HfO and ThO molecules belong to an iso-electronic (in valence electrons) series made up of ScF, TiO, ZrO, HfO and ThO. The potential energy curves and dissociation energies of TiO and ZrO were reported earlier[1, 2]. The potential energy curves of ZrO have also been reported[3].

Recent kinetic studies of chemi-ionization[4] reaction involving thorium have permitted the consideration of ThO as a laser material. These facts tempted us to undertake the calculations of dissociation energies of HfO and ThO.

Molecular constants

The spectra of HfO and ThO have been studied earlier[5-9] and the spectra of those molecules belonging to an iso-electronic series have been reviewed[10]. The Franck-Condon factors and *r*-centroids of twelve electronic states of HfO and ThO have also been reported[11]. Behere *et al*[11] suggested the possibility of a low lying triplet state of ThO. Molecular constants were taken from the work of Edvinsson *et al* and listed in table 1.

Potential energy curves

The RKR[12] potential energy curves of the ground states of HfO and ThO are constructed and the turning points are calculated using experimental $G(v)$ values for $v = 0$ to 10. Few potential functions like Steele *et al*[13], Hulburt and Hirschfelder[14] and the one which was suggested by Birajdar *et al*[15] were tried but the H–H function was found to give the best fit. Recently Navati and Korwar[16] suggested the modification in Morse potential named as Morse-Korwar-Navati model in which Morse constant α is not a constant but a function of internuclear separation. Besides the complexity involved in this MKN model the H–H function has proved to be equally or even more satisfactory in the study of the potential energy curves of GeO and SiO molecules.

CONCLUSIONS

The RKR turning points and the U calculated values along with U experimental values are listed in table 2. It is clear that the D_e values $73400\ cm^{-1}$ and $83900\ cm^{-1}$ show minimum average percentage deviation for HfO and ThO respectively. The D_0^0 values

Table 1 *Molecular constants* (ground state)*

Molecule	w_e	$w_e x_e$	α_e	r_e	B_e
HfO	974.09	3.228	0.001724	1.7234	0.386537
ThO	895.77	2.39	0.001302	1.8403	0.332644

*All constants in cm^{-1} except r_e which is in Å unit.

Table 2 *RKR turning points and energy values from H–H function*

HfO

v	RKR (Å)	$G(v)$ (cm^{-1})	$U(r)$ in cm^{-1} $D_e = 73300$	$D_e = 73400$	$D_e = 73500$
0	1.6764	486.238	486.286	486.949	487.613
1	1.6445	1453.872	1454.132	1456.116	1458.100
2	1.6236	2415.050	2414.974	2418.268	2421.563
3	1.6072	3369.772	3370.257	3374.854	3379.452
4	1.5934	4318.038	4322.242	4328.138	4334.035
5	1.5815	5259.848	5258.923	5266.097	5273.272
6	1.5708	6195.202	6197.750	6206.205	6214.660
7	1.5611	7124.100	7134.724	7141.454	7151.183
8	1.5522	8046.542	8061.041	8072.038	8083.036
9	1.5440	8962.528	8980.998	8993.250	9005.502
10	1.5363	9872.058	9902.534	9916.043	9929.553
0	1.7736	486.238	483.596	484.256	484.916
1	1.8133	1453.872	1445.841	1447.813	1449.786
2	1.8422	2415.050	2405.476	2408.758	2412.039
3	1.8666	3369.772	3357.725	3362.306	3366.887
4	1.8884	4318.038	4302.940	4308.810	4314.680
5	1.9084	5259.848	5238.166	5245.312	5252.458
6	1.9273	6195.202	6174.180	6182.603	6191.026
7	1.9451	7124.100	7096.291	7105.972	7115.854
8	1.9622	8046.542	8014.532	8025.466	8036.400
9	1.9787	8962.528	8926.797	8938.975	8951.154
10	1.9947	9872.058	9832.793	9846.207	9859.622
Average percentage deviation			+0.162	+0.0324	−0.112

ThO

v	RKR (Å)	$G(v)$ (cm^{-1})	$U(r)$ in cm^{-1} $D_e = 83800$	$D_e = 83900$	$D_e = 84000$
0	1.7919	447.287	448.057	448.592	449.127
1	1.7588	1338.277	1336.715	1338.309	1339.905
2	1.7369	2224.487	2226.045	2228.710	2231.358
3	1.7198	3105.917	3105.209	3108.914	3112.62
4	1.7054	3982.567	3981.002	3985.753	3990.504
5	1.6928	4854.437	4855.358	4861.152	4866.946
6	1.6816	5721.527	5721.830	5728.658	5735.486
7	1.6714	6583.837	6587.562	6595.423	6603.284
8	1.6621	7441.367	7443.321	7452.203	7461.085
9	1.6535	8294.117	8293.269	8303.166	8313.062
10	1.6454	9142.087	9147.169	9158.085	9169.000
0	1.8923	447.287	445.009	445.541	446.072
1	1.9331	1338.277	1335.409	1337.003	1338.596
2	1.9625	2224.487	2219.571	2222.219	2224.868
3	1.9873	3105.917	3100.222	3103.922	3107.622
4	2.0093	3982.567	3971.984	3976.724	3981.469
5	2.0296	4854.437	4843.343	4849.123	4854.902
6	2.0486	5721.527	5710.864	5717.679	5724.494
7	2.0666	6583.837	6574.226	6582.071	6589.916
8	2.0837	7441.367	7427.974	7436.838	7445.702
9	2.1002	8294.117	8279.880	8289.468	8299.348
10	2.1162	9142.087	9128.809	9139.703	9150.597
Average percentage deviation			+0.101	−0.0176	−0.096

correspond to 9.04 ± 0.02 eV and 10.34 ± 0.01 eV. The thermochemical value[17] of D_0^0 for HfO is 8.19 eV. In the case of ThO it is 9.00 eV.

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ANNOUNCEMENTS

WORKSHOP ON ENVIRONMENTAL MANAGEMENT

The International Society for Environmental Education (ISEE) and Committee on Science and Technology for Developing Countries (COSTED) are organising a workshop on Environmental Management. The workshop will be held during **May 26–31, 1986** at Hotel President Merlin, Singapore.

Pollution has been recognised as one of the major problems in industrialised nations. Sophisticated legislation, controls and techniques have been developed to contain and cope with it. Many developing countries are now faced with similar problems as their manufacturing industries develop and the population moves towards the cities, often at frightening and uncontrolled rate.

The following topics will be discussed during the workshop: (a) Industrial Pollution, (b) Management of Toxic substances, (c) Environment Impacts and Management, (d) Solid Waste disposal and Management, (e) Human Settlements, (f) Information Systems, (g) Environmental Law.

For further details please contact: Dr. Desh Bandhu, President, ISEE, B. M. 150 (West), Shalimar Bagh, Delhi 110 052 (India).

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