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RESEARCH NOTE

The electronic partition functions of lanthanide atoms and ions between 1500 and 8000 K

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THEORY

DE GALAN *et al.* [1] have calculated partition functions for the atoms and first ions of 73 elements over the temperature 1500–7000 K, fitted the resulting values to a fifth-order polynomial, and reported the regression coefficients in tabular form. The partition functions for the lanthanides and actinides were not published because energy level data for these species were not available in the tables of MOORE [2]. Atomic energy levels for the lanthanides have been published by MARTIN *et al.* [3] in 1978. In this manuscript, the electronic partition functions of the atoms and first ions of the lanthanides are compiled in the manner of DE GALAN *et al.* [1].

The electronic partition function is given by:

$$B(T) = \sum_{s=0}^{n} g_s \exp(-E_s/kT) \tag{1}$$

where $B(T)$ is the electronic partition function, k is the Boltzmann constant, g_s and E_s are the statistical weight and

Table 1. Values of polynomial coefficients for lanthanide atoms and first ions

	a	*b*	*c*	*d*	*e*	*f*
Ce I	7.8011	1.4065	8.1361	−0.6081	0.1011	−0.0055
Ce II	13.5043	−14.7240	17.8475	−2.1319	0.1291	−0.0032
Pr I	5.2754	10.3983	−6.1586	2.6715	−0.2427	0.0077
Pr II	10.2006	6.3863	−0.0177	1.4075	−0.1819	0.0073
Nd I	−1.1347	18.3341	−8.0333	2.0424	−0.0887	
Nd II	4.9385	11.3564	−1.1460	0.8744	−0.0425	
Pm I	5.8296	1.0052	3.6891	−0.9673	0.1140	−0.0045
Pm II	5.0631	2.1378	5.4968	−0.7121	0.0334	
Sm I	−5.5519	13.2757	−2.8727	0.3076	0.0275	−0.0024
Sm II	−3.9213	12.4250	−0.7073	0.1704	−0.0043	
Eu I	7.6246	0.6951	−0.4167	0.0824	−4.223E-4	
Eu II	6.9612	3.4806	−1.1061	0.2463	−0.0229	−8.404E-4
Gd I	5.9750	16.2554	−4.6555	1.0023	−0.0684	0.0020
Gd II	7.3830	10.5601	1.3468	−0.1286	0.0112	−3.522E-4
Tb I	23.3855	18.8008	−0.3665	0.5702	−0.0229	
Tb II	15.7730	−0.6403	6.1190	−0.6973	0.0300	
Dy I	15.0835	2.6642	−1.3069	0.3604		
Dy II	15.9055	8.7037	−2.0395	0.3750	0.0022	−8.947E-4
Ho I	14.5902	2.2345	−1.4541	0.4372	−0.0156	
Ho II	19.9010	4.0575	−0.4455	0.0965	−0.0042	
Er I	13.1758	−0.2926	−0.1141	0.1765	0.0024	
Er II	18.2590	3.1786	−0.8387	0.2893	−0.0116	
Tm I	7.9400	−0.0049	0.1044	−0.0767	0.0191	−7.508E-4
Tm II	12.9226	1.7210	−0.5073	0.0717		
Yb I	0.9763	0.0162	0.0052	−0.0053	9.139E-4	
Yb II	2.0043	−0.0182	0.0178	−0.0064	7.764E-4	
Lu I	2.9553	1.2346	0.1398	−0.0730	0.0105	−4.154E-4
Lu II	0.8525	0.2597	−0.1631	0.0424	−0.0038	1.273E-4

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energy for level s respectively, and T is the temperature. The calculation included all energy levels listed in Ref. [3] and were carried out on a IBM-AT compatible computer (Telex Model 1280, Tulsa, OK). Values of $B(T)$ were calculated at intervals of 500 K. The $B(T)$ values were fitted with third-, fourth-, and fifth-order polynomials using the software package Cricket Graph®(Cricket Software, Philadelphia, PA) on a Macintosh-Plus (Apple Computers, Cupritino, CA) personal computer. The results for each of these fits were compared to the original data at temperatures of 1500, 5000 and 8000 K and the fit which provided the lowest total error was selected. In keeping with the format used by DE GALAN *et al.*, values are presented in Table 1 for the polynomial coefficients for the fifth-order polynomial equation below:

$$B(T) = a + b\left(\frac{T}{10^3}\right) + c\left(\frac{T}{10^3}\right)^2 + d\left(\frac{T}{10^3}\right)^3 + e\left(\frac{T}{10^3}\right)^4 + f\left(\frac{T}{10^3}\right)^5. \quad (2)$$

We have found these polynomials to be a very rapid and convenient means of estimating the electronic partition function with an error of less than 1%.

Summary

Electronic partition functions for the lanthanide atoms and ions have been calculated over the temperature range 1500–8000 K. The results are presented in the form of a fifth order polynomial expression which has been fitted to the data by the method of least squares.

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