Appendices

Appendix A

Calculation of the Configurational Entropy Term

Configurational entropy:

$$S = k \ln \Omega \tag{A.1}$$

where S is the configuration entropy, k is Boltzmann's constant and Ω is the configurational term taking account the number of ways it is possible to arrange the ions on the site(s). This is calculated as in

$$\Omega = \frac{N!}{n!(N-n)!} \tag{A.2}$$

Using the structural information regarding the δ-phase (see table A.1). There is 1 Sc ion and 2 Hf ions on the 3a cation site and 11 Sc ions and 7 Hf ions on the 18f cation site.

Table A.1: Structural information for $Sc_4Hf_3O_{12}$ from [1]

Atom	Site	a	b	c	Occupancy
Hf	3a	0	0	0	$\frac{2}{3}$
Sc	3a	0	0	0	$\frac{1}{3}$
Hf	18f	0.2894	0.4084	0.0179	0.4
Sc	18f	0.2894	0.4084	0.0179	0.6
O	18f	0.306	0.459	-0.224	1.0
O	18f	0.309	0.441	0.269	1.0

Therefore for the 3a site

$$\Omega = \frac{3!}{1!2!} = 3 \tag{A.3}$$

and for the 18f site

$$\Omega = \frac{18!}{7!11!} = 31824 \tag{A.4}$$

In total

$$S = k \ln(31824 \times 3) = 9.88 \times 10^{-4}\text{eV/K} \tag{A.5}$$

This is for the full unit cell so the value of S for one formula unit is 3.29×10^{-4}eV/K.