STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 74 (2018)

Supporting information for article:

Theory of order–disorder phase transitions of *B*-cations in $AB'_{1/2}B''_{1/2}O_3$ perovskites

V. P. Sakhnenko and N. V. Ter-Oganessian

Supporting information for the article "Theory of order – disorder phase transitions of B-cations in $AB'_{1/2}B''_{1/2}O_3$ perovskites"

V. P. Sakhnenko, N. V. Ter-Oganessian

The following tables give A-O and B-O unstrained elastic cation-anion bond lengths for most commonly occurring chemical elements in the perovskite structure, as determined in V. P. Sakhnenko, E. G. Fesenko, A. T. Shuvaev, E. T. Shuvaeva, and G. A. Geguzina, *Sov. Phys. Crystallogr.* **17**, 268 (1972). Several values were corrected or added after the original publication.

Element	Bond lengths, Å	
	A – O	B – O
Valence 1		
Na	2.41	
Ag	2.51	
K	2.85	
Tl	2.98	
Rb	3.00	
Cs	3.18	
Valence 2		
Cr		2.05
Ni		2.12
Cu		2.13
Mg		2.14
Fe		2.14
Zn		2.15
Co		2.15
Mn		2.22
Cd	2.45	2.38
Ca	2.55	2.39
Eu	2.72	
Sr	2.73	2.52
Pb	2.83	2.52
Ba	2.91	2.54

Element	Bond lengths, Å	
	A – O	B – O
Valence 3		
Al		1.87
Ga		1.97
Cr		1.98
V		2.00
Fe		2.00
Co		2.01
Ti		2.02
Mn		2.03
Rh		2.03
Ni		2.08
Sc		2.11
In	2.45	2.15
Sb		2.26
Lu	2.54	2.20
Yb	2.54	2.21
Tu	2.57	2.22
Er	2.57	2.23
Y	2.60	2.24
Ho	2.58	2.24
Dy	2.60	2.25
Tl		2.26
Tb	2.61	2.27
Gd	2.62	2.29
Eu	2.64	2.30
Sm	2.66	2.31
Nd	2.67	2.33
Pr	2.69	2.35
Ce		2.38
La	2.72	2.40
Bi	2.77	2.41
Pu	2.69	
Am	2.65	

Element	Bond lengths, Å	
	A – O	B – O
	Valence 4	
Ge		1.89
Cr		1.90
Mn		1.90
Co		1.93
V		1.93
Ir		1.93
Re		1.94
Ru		1.96
Ti		1.97
Fe		1.99
Mo		2.01
Tc		2.00
Sn		2.06
Hf		2.09
Zr		2.11
Pb		2.17
Pr		2.24
Pu		2.24
Ce		2.25
U		2.26
Np		2.26
Th		2.33
Pa		2.31

Element	Bond lengths, Å	
	A – O	B – O
	Valence 5	
Ru		1.96
Os		1.97
Re		1.99
Sb		2.00
Mo		2.00
Nb		2.01
Ta		2.02
Pu		2.12
Bi		2.12
U		2.20
Pa		2.21
	Valence 6	
Te		1.85
Ir		1.86
Mo		1.86
Os		1.86
Re		1.87
W		1.89
U		2.10