

Noritake et al., (2012, *J. Non-Cryst. Sol.*)

in Paper (**wrong**)

Atomic	q	a(nm)	b(nm)	c(kJ/mol·nm <sup>3</sup> )
O		0.099759	0.008300	0.000000
Si		0.181819	0.015390	27400.0
Na	1.000000	0.139500	0.011500	10000.0
Pair	D <sub>1</sub> (MJ/mol)	b <sub>1</sub> (1/nm)	D <sub>1</sub> (MJ/mol)	b <sub>2</sub> (1/nm)
Si-O	668.428	59.6360	-105.335	45.514
3-body	f(kJ/mol)	t <sub>0</sub> (deg.)	r <sub>m</sub> (nm)	g <sub>r</sub> (1/nm)
Si-O-Si	0.0006	147.000	0.170000	168.000

forNa<sub>X</sub>Si<sub>Y</sub>O<sub>Z</sub>

$$1) q_{Si}q_O = -2.5$$

$$2) Xq_{Na} + Yq_{Si} + Zq_O = 0$$

Correct

Atomic	q	a(nm)	b(nm)	c(kcal <sup>1/2</sup> /mol·nm <sup>3</sup> )
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forNa<sub>X</sub>Si<sub>Y</sub>O<sub>Z</sub>

$$1) q_{Si}q_O = -2.5$$

$$2) Xq_{Na} + Yq_{Si} + Zq_O = 0$$

$$3) q_O < 0$$

Noritake & Kawamura (2014, *Prog. Earth Planet. Sci.*)

in Paper (**wrong**)

Atomic	q	a(Å)	b(Å)	c(kJ/mol·Å <sup>3</sup> )
O	2.23607	0.99759	0.08300	0.000000
Si	-1.11803	1.81819	0.15390	27.400
Mg	1.11803	1.09881	0.04700	40.000
Pair	D <sub>1</sub> (MJ/mol)	b <sub>1</sub> (1/Å)	D <sub>1</sub> (MJ/mol)	b <sub>2</sub> (1/Å)
Si-O	668.428	59.6360	-105.335	45.514
Mg-O	28.960	5.0	-1.5568	2.24
3-body	f(kJ/mol)	t <sub>0</sub> (deg.)	r <sub>m</sub> (nm)	g <sub>r</sub> (1/nm)
Si-O-Si	0.0006	147.000	0.170000	168.000

Correct

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Si	-1.11803	1.81819	0.15390	27.400
Mg	1.11803	1.09881	0.04700	40.000
Pair	D <sub>1</sub> (Mcal/mol)	b <sub>1</sub> (1/Å)	D <sub>1</sub> (Mcal/mol)	b <sub>2</sub> (1/Å)
Si-O	668.428	<b>5.96360</b>	-105.335	<b>4.5514</b>
	28.960	5.0	-1.5568	2.24
3-body	f( <b>fJ</b> )	t <sub>0</sub> (deg.)	r <sub>m</sub> (nm)	g <sub>r</sub> (1/nm)
Si-O-Si	0.0006	147.000	0.170000	168.000

Noritake et al., (2015, *Phys. Earth Planet. Int.*)

same with Sakuma & Kawamura (2011, *Geochim. Cosmochim. Act.*)