Supplemental Materials, Wander et al. American Mineralogist Jan 2015

Table S1. Spin States used for calculations. Wherever possible spin states were taken from NIST's Computational Chemistry Comparison and Benchmark DataBase. The remaining few were decided from molecular orbital considerations.

Atom1	Atom2	Spin
H	H	1
H	Li	1
H	Be	2
H	B	1
H	C	2
H	N	3
H	O	2
H	F	1
Li	Li	1
Li	Be	2
Li	B	1
Li	C	2
Li	N	3
Li	O	2
Li	F	1
Be	Be	1
Be	B	2
Be	C	3
Be	N	4
Be	O	1
Be	F	2
B	B	3
B	C	2
B	N	3

B	O	2
B	F	1
C	C	1
C	N	2
C	O	1
C	F	2
N	N	0
N	O	2
N	F	3
O	O	3
O	F	2
F	F	1
Al	H	1
Al	O	2
Si	H	2
Si	O	1
Al	Si	2
Si	Si	3
Al	Al	3