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+           +
+ Program BVC for Bond Valence Calculation +
+   by  Hongwei Ma           +
+   Inst. Chem, CAS         +
+   Oct. 10 2006           +
+           +
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Bond Valence Calculation for Sanderite, Kieserite
 Starkyite, Pentahydrate, Hexahydrate, and Episomite
 O of H₂O molecules are not included.

BVC PARAMETERS

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Mg-O  R0=1.693  B= .37
S-O   R0=1.624  B= .37
H-O   R0= .569  B= .94

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Atom(i)-Atom(j) Rij&Ravg Vij&Vi Bondtype

Sanderite

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Mg(1)-O(1)#1      2.044(4) .387    1
Mg(1)-O(4)#2      2.096(4) .336    1
Mg(1)-O(5)        2.067(4) .364    1
Mg(1)-O(7)#3      2.023(3) .410    1
Mg(1)-O(1w)       2.116(4) .319    1
Mg(1)-O(2w)       2.099(4) .334    1
Mg(1)-O           2.074000 2.150    0

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Mg(2)-O(2)        2.060(4) .371    1
Mg(2)-O(3)#4      2.058(3) .373    1
Mg(2)-O(6)#5      2.058(3) .373    1
Mg(2)-O(8)        2.049(4) .382    1
Mg(2)-O(3w)       2.101(4) .332    1
Mg(2)-O(4w)       2.109(4) .325    1
Mg(2)-O           2.072000 2.156    0

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S(1)-O(1)         1.475(3) 1.496    2
S(1)-O(2)         1.498(4) 1.406    2
S(1)-O(3)         1.496(4) 1.413    2
S(1)-O(4)         1.493(4) 1.425    2
S(1)-O            1.490000 5.740    0

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S(2)-O(5)         1.509(4) 1.365    2
S(2)-O(6)         1.466(4) 1.533    2
S(2)-O(7)         1.463(3) 1.545    2
S(2)-O(8)         1.473(4) 1.504    2
S(2)-O            1.478000 5.946    0

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O(1)-Mg(1)#6      2.044(4) .387    1
O(1)-S(1)         1.475(3) 1.496    2

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O(1)-MgS	1.760000	1.883	0

O(2)-Mg(2)	2.060(4)	.371	1
O(2)-S(1)	1.498(4)	1.406	2
O(2)-MgS	1.779000	1.777	0

O(3)-Mg(2)#7	2.058(3)	.373	1
O(3)-S(1)	1.496(4)	1.413	2
O(3)-MgS	1.777000	1.786	0

O(4)-Mg(1)#8	2.096(4)	.336	1
O(4)-S(1)	1.493(4)	1.425	2
O(4)-MgS	1.794000	1.761	0

O(5)-Mg(1)	2.067(4)	.364	1
O(5)-S(2)	1.509(4)	1.365	2
O(5)-MgS	1.788000	1.728	0

O(6)-Mg(2)#9	2.058(3)	.373	1
O(6)-S(2)	1.466(4)	1.533	2
O(6)-MgS	1.762000	1.906	0

O(7)-Mg(1)#10	2.023(3)	.410	1
O(7)-S(2)	1.463(3)	1.545	2
O(7)-MgS	1.743000	1.955	0

O(8)-Mg(2)	2.049(4)	.382	1
O(8)-S(2)	1.473(4)	1.504	2
O(8)-MgS	1.7610000	1.886	0

O(1w)-Mg(1)	2.116(46)	.319	1
O(1w)-Mg	2.1160000	.319	0

O(2w)-Mg(1)	2.099(44)	.334	1
O(2w)-Mg	2.0990000	.334	0

O(3w)-Mg(2)	2.101(45)	.332	1
O(3w)-Mg	2.1010000	.332	0

O(4w)-Mg(2)	2.109(43)	.325	1
O(4w)-Mg	2.1090000	.325	0

Kieserite			
Mg1-O1	2.038	.394	1
Mg1-O1	2.038	.394	1
Mg1-O2	2.068	.363	1
Mg1-O2	2.068	.363	1
Mg1-O3	2.154	.288	1
Mg1-O3	2.154	.288	1
Mg-O	2.087	2.088	0

S1-O1	1.469	1.520	2
S1-O1	1.469	1.520	2
S1-O2	1.433	1.676	2

S1-O2	1.433	1.676	2
S1-O	1.451	6.392	0

O1-Mg1	2.038	.394	1
O1-S1	1.469	1.520	2
O1-MgS	1.753	1.914	0

O2-Mg1	2.068	.363	1
O2-S1	1.433	1.676	2
O2-MgS	1.750	2.039	0

Starkeyite			
Mg1-O1	2.083	.349	1
Mg1-O2	2.083	.349	1
Mg1-O5	2.052	.379	1
Mg1-O6	2.087	.345	1
Mg1-O7	2.054	.377	1
Mg1-O8	2.073	.358	1
Mg1-O	2.072	2.156	0

S1-O1	1.479	1.480	2
S1-O2	1.468	1.524	2
S1-O3	1.478	1.484	2
S1-O4	1.466	1.533	2
S1-O	1.473	6.021	0

O1-Mg1	2.083	.349	1
O1-S1	1.479	1.480	2
O1-MgS	1.781	1.828	0

O2-Mg1	2.083	.349	1
O2-S1	1.468	1.524	2
O2-MgS	1.776	1.873	0

O3-S1	1.478	1.484	2
O3-S	1.478	1.484	0

O4-S1	1.466	1.533	2
O4-S	1.466	1.533	0

Pentahydrate			
Mg1-O1	2.097	.336	1
Mg1-O1	2.097	.336	1
Mg1-O5	2.062	.369	1
Mg1-O5	2.062	.369	1
Mg1-O6	2.051	.380	1
Mg1-O6	2.051	.380	1
Mg1-O	2.070	2.169	0

Mg2-O2	2.105	.328	1
Mg2-O2	2.105	.328	1
Mg2-O7	2.048	.383	1
Mg2-O7	2.048	.383	1
Mg2-O8	2.042	.389	1

Mg2-O8	2.042	.389	1
Mg2-O	2.065	2.202	0

S1-O1	1.478	1.484	2
S1-O2	1.477	1.488	2
S1-O3	1.465	1.537	2
S1-O4	1.535	1.272	2
S1-O	1.489	5.780	0

O1-Mg1	2.097	.336	1
O1-S1	1.477	1.488	2
O1-MgS	1.787	1.823	0

O2-Mg2	2.105	.328	1
O2-S1	1.477	1.488	2
O2-MgS	1.791	1.816	0

O3-S1	1.465	1.537	2
O3-S	1.465	1.537	0

O4-S1	1.535	1.272	2
O4-S	1.535	1.272	0

Hexahydrate			
Mg1-O5	2.046	.385	1
Mg1-O5	2.046	.385	1
Mg1-O6	2.044	.387	1
Mg1-O6	2.044	.387	1
Mg1-O7	2.080	.351	1
Mg1-O7	2.080	.351	1
Mg1-O	2.057	2.248	0

Mg2-O8	2.083	.349	1
Mg2-O8	2.083	.349	1
Mg2-O9	2.054	.377	1
Mg2-O9	2.054	.377	1
Mg2-O10	2.058	.373	1
Mg2-O10	2.058	.373	1
Mg2-O	2.065	2.197	0

S1-O1	1.476	1.492	2
S1-O2	1.459	1.562	2
S1-O3	1.494	1.421	2
S1-O4	1.476	1.492	2
S1-O	1.476	5.967	0

O1-S1	1.476	1.492	2
O1-S	1.476	1.492	0

O2-S1	1.459	1.562	2
O2-S	1.459	1.562	0

O3-S1	1.494	1.421	2
O3-S	1.494	1.421	0

O4-S1	1.476	1.492	2
O4-S	1.476	1.492	0

Epsomite			
Mg1-O5	2.058	.373	1
Mg1-O6	2.103	.330	1
Mg1-O7	2.052	.379	1
Mg1-O8	2.050	.381	1
Mg1-O9	2.099	.334	1
Mg1-O10	2.057	.374	1
Mg1-O	2.070	2.171	0

S1-O1	1.462	1.549	2
S1-O2	1.474	1.500	2
S1-O3	1.471	1.512	2
S1-O4	1.485	1.456	2
S1-O	1.473	6.017	0

O1-S1	1.462	1.549	2
O1-S	1.462	1.549	0

O2-S1	1.474	1.500	2
O2-S	1.474	1.500	0

O3-S1	1.471	1.512	2
O3-S	1.471	1.512	0

O4-S1	1.485	1.456	2
O4-S	1.485	1.456	0

SYMMETRY CODE

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Symmetry transformations used
to generate equivalent atoms:

- #1 -x+1,y-1/2,-z+1/2
- #2 x+1,y,z
- #3 -x+3/2,-y+1,z-1/2
- #4 -x+1/2,-y+1,z+1/2
- #5 x-1/2,-y+3/2,-z+1
- #6 -x+1,y+1/2,-z+1/2
- #7 -x+1/2,-y+1,z-1/2
- #8 x-1,y,z
- #9 x+1/2,-y+3/2,-z+1
- #10 -x+3/2,-y+1,z+1/2