**SUPPLEMENTARY MATERIAL FOR:**

**CRYSTAL CHEMISTRY OF THE SERANDITE-SCHIZOLITE-PECTOLITE SERIES**

Lussier, A.J., Grice, J.D., Friis, H. & Poirier, G. G.

|  |
| --- |
| TABLE S1. CALCULATED THERMODYNAMIC PARAMETERS FOR SERANDITE-PECTOLITE SOLID SOLUTION SERIES (*K* = 20.0(5)), AS IN NAVROTSKY (1971) |
| ∑Mn | ∑Ca | *N* | *X* | *a*ΔHex | xΔH | *b*TΔSex | *c*ΔGex |
| kcal  | kcal  | kcal  | kcal  |
| 0.10 | 1.90 | 0.050 | 0.04 | -1.77 | -0.08 | -0.03 | -0.05 |
| 0.25 | 1.75 | 0.125 | 0.11 | -1.77 | -0.19 | -0.08 | -0.12 |
| 0.50 | 1.50 | 0.250 | 0.21 | -1.77 | -0.37 | -0.16 | -0.21 |
| 0.75 | 1.25 | 0.375 | 0.29 | -1.77 | -0.51 | -0.23 | -0.28 |
| 1.00 | 1.00 | 0.500 | 0.32 | -1.77 | -0.56 | -0.26 | -0.30 |
| 1.25 | 0.75 | 0.625 | 0.29 | -1.77 | -0.51 | -0.23 | -0.28 |
| 1.50 | 0.50 | 0.750 | 0.21 | -1.77 | -0.37 | -0.16 | -0.21 |
| 1.75 | 0.25 | 0.875 | 0.11 | -1.77 | -0.19 | -0.08 | -0.12 |
| 1.99 | 0.01 | 0.995 | 0.00 | -1.77 | -0.01 | 0.00 | -0.01 |
| *a,* with$(∂G/∂x)\_{I} = 0$, and thus (∂G/∂x)*N* = 0 (at equilibrium), ∆*H*ex = RTln*K* (*R* = 1.987 x 10 -3 kcal K-1 mol-1; *T* = 298 K); *b*, *T*∆*S*ex = *RT* [(*N* + *x*)ln(*N* + *x*)+(1 - *N* - *x*)ln(1 - *N* - *x*) + (*N* – *x*)ln(*N* – x) + (1 - *N* + *x*)ln(1 - *N* + *x*) + (*N* – *x*)ln(*N* – *x*) + (1 - *N* + *x*)ln(1 - *N* + *x*) – (2*N*ln*N*) – 2(1-*N*)ln(1-*N*)]; *c*, Gex = ∆Hex - T∆Sex; |



|  |
| --- |
| TABLE S2. BOND VALENCE TABLE FOR SERANDITE-SCHIZOLITE-PECTOLITE TOPOLOGY |
|  | *A* | *M*1 | *M*2 | *Si*1 | *Si*2 | *Si*3 | H | CN |
| *O*1 |  | *g*1x→,1x↓ | *l*1x→,1x↓ |  |  | *y*1x→,1x↓ |  | 3 |
| *O*2 | *a*1x→,1x↓ | *h*1x→,1x↓ | *m*1x→,1x↓ |  |  | *z*1x→,1x↓ |  | 4 |
| *O*3 | *b*1x→,1x↓ | *i*1x→,1x↓ |  | *q*1x→,1x↓ |  |  | *a*1x→,1x↓ | 4 |
| *O*4 | *c*1x→,1x↓ |  | *n*1x→,1x↓ |  | *u*1x→,1x↓ |  | (*1-a*)1x→,1x↓ | 3 |
| *O*5 |  | *j*2x→,2x↓ | *o*1x→,2x↓ | *r*1x→,1x↓ |  |  |  | 4 |
| *O*6 |  | *k*1x→,1x↓ | *p*2x→,1x↓ |  | *v*1x→,1x↓ |  |  | 4 |
| *O*7 | *d*2x→,2x↓ |  |  | *w*1x→,1x↓ |  | *a*'1x→,1x↓ |  | 4 |
| *O*8 | *e*2x→,2x↓ |  |  |  | *w*1x→,1x↓ | *b*’ 1x→,1x↓ |  | 4 |
| *O*9 | *f*1x→,1x↓ |  |  | *t*1x→,1x↓ | *x*1x→,1x↓ |  |  | 3 |
| CN | 8 | 6 | 6 | 4 | 4 | 4 |  |  |

**= = = = = = = = = = = = = = = = = =**

(Eq. S1)

**[A]s** = **V =**

$$\left[\begin{matrix}1&1&1&2&2&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&1&1&1&2&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&1&1&1&1&2&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&1&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&1&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&1\\0&0&0&0&0&0&1&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0\\1&0&0&0&0&0&0&1&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0\\0&1&0&0&0&0&0&0&1&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0\\0&0&1&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&1&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&2&0&0&0&0&1&0&0&1&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&2&0&0&0&0&0&1&0&0&0&0&0&0\\0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&1&0\\0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&1\\0&0&0&0&0&0&1&\overbar{1}&0&0&0&\overbar{1}&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&1&\overbar{1}&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&\overbar{1}&1&0&0\\1&\overbar{1}&0&0&0&0&0&\overbar{1}&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\0&1&0&\overbar{1}&0&0&0&0&0&0&0&0&0&0&0&0&\overbar{1}&0&1&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&1&\overbar{1}&0&0&0&0&0&0&\overbar{1}&1&0&0&0&0&0&0&0&0&0&0\\0&0&1&0&\overbar{1}&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&\overbar{1}&0&1&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&\overbar{1}&0&0&0&0&\overbar{1}&1&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&1&\overbar{1}&0&0&0&\overbar{1}&1&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&1&0&\overbar{1}&0&0&0&0&0&0&0&0&0&0&0&0&\overbar{1}&1&0&0&0&0&0&0&0&0\\0&0&0&1&\overbar{1}&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&\overbar{1}&1\\0&0&0&0&1&\overbar{1}&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&\overbar{1}&1&0&0&0&0\\0&0&0&0&0&0&0&1&0&0&\overbar{1}&0&\overbar{1}&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&\overbar{1}&0&\overbar{1}&0&0&0&0&0&0&0&1&\overbar{1}&0&0&0&0&0&0&\overbar{1}&1&0\\1&0&\overbar{1}&0&0&0&0&0&0&0&0&0&\overbar{1}&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0\end{matrix}\right]\left[\begin{matrix}a\\b\\c\\d\\e\\f\\g\\h\\i\\j\\k\\l\\m\\n\\o\\p\\q\\r\\s\\t\\u\\v\\w\\x\\y\\z\\a'\\b'\end{matrix}\right]=\left[\begin{matrix}1\\2\\2\\4\\4\\4\\2\\2\\1.3\\1.7\\2\\2\\2\\2\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\end{matrix}\right]$$

|  |
| --- |
| TABLE S3. *A PRIORI* BOND LENGTHS (Å) FOR SERANDITE-SCHIZOLITE-PECTOLITE CRYSTALS LISTED IN TABLES 6-7  |
| SAMPLE | <*A*-*Φ*> | <*M*1-*Φ*> | <*M*2-*Φ*> | <*Si*1-*Φ*> | <*Si*2-*Φ*> | <*Si*3-*Φ*> |
| TK01 | 2.623 | 2.365 | 2.359 | 1.624 | 1.625 | 1.626 |
| NAG01 | 2.623 | 2.365 | 2.359 | 1.624 | 1.625 | 1.626 |
| NAG02 | 2.623 | 2.365 | 2.359 | 1.624 | 1.625 | 1.626 |
| ROZ01 | 2.623 | 2.365 | 2.357 | 1.624 | 1.625 | 1.626 |
| ROZ02 | 2.623 | 2.365 | 2.341 | 1.624 | 1.625 | 1.626 |
| ARA01 | 2.623 | 2.365 | 2.323 | 1.624 | 1.625 | 1.626 |
| ROZ3 | 2.623 | 2.359 | 2.313 | 1.624 | 1.625 | 1.626 |
| KNR95 | 2.623 | 2.348 | 2.306 | 1.624 | 1.625 | 1.626 |
| ROZ4 | 2.623 | 2.329 | 2.221 | 1.624 | 1.625 | 1.626 |
| OF02 | 2.623 | 2.348 | 2.265 | 1.624 | 1.625 | 1.626 |
| KNR96 | 2.623 | 2.342 | 2.227 | 1.624 | 1.625 | 1.626 |
| NDMH01 | 2.623 | 2.330 | 2.226 | 1.624 | 1.625 | 1.626 |
| NAG03 | 2.623 | 2.333 | 2.219 | 1.624 | 1.625 | 1.626 |
| NDMH02 | 2.623 | 2.329 | 2.235 | 1.624 | 1.625 | 1.626 |
| CMN01 | 2.623 | 2.300 | 2.212 | 1.624 | 1.625 | 1.626 |
| OF01 | 2.623 | 2.269 | 2.201 | 1.624 | 1.625 | 1.626 |
| NAG04 | 2.623 | 2.252 | 2.201 | 1.624 | 1.625 | 1.626 |
| TKY01 | 2.623 | 2.237 | 2.205 | 1.624 | 1.625 | 1.626 |
| CMN2 | 2.623 | 2.219 | 2.207 | 1.624 | 1.625 | 1.626 |
| WW01 | 2.623 | 2.207 | 2.604 | 1.624 | 1.625 | 1.626 |
| Note: Names and references as given in Table 6.  |

|  |
| --- |
| TABLE S4. STRAIN AT INDIVIDUAL SITES (*A*, *M1*, *M2*, *Si1*, *Si2*, and *Si3*) AND BOND STRAIN INDEX (BSI) FOR SERANDITE-SCHZOLITE-PECTOLITE CRYSTALS IN TABLES 6-7 |
| SAMPLE | ∑Ca | ΔBL<*A*-*Φ*> | ΔBL<*M*1-*Φ*> | ΔBL<*M*2-*Φ*> | ΔBL<*Si*1-*Φ*> | ΔBL<*Si*2-*Φ*> | ΔBL<*Si*3-*Φ*> | BSI |
| (*apfu*) | |-------------------------------------------(Å)------------------------------------------| |
| TK01 | 2.00 | 0.049 | 0.000 | 0.008 | -0.001 | -0.001 | -0.012 | 0.060 |
| NAG01 | 2.00 | 0.047 | 0.001 | 0.001 | -0.001 | -0.001 | -0.010 | 0.060 |
| NAG02 | 2.00 | 0.040 | 0.001 | 0.010 | 0.000 | 0.001 | -0.008 | 0.063 |
| ROZ1 | 1.98 | 0.046 | -0.002 | 0.002 | -0.001 | 0.000 | -0.010 | 0.059 |
| ROZ2 | 1.86 | 0.049 | -0.001 | -0.001 | -0.003 | 0.000 | -0.010 | 0.061 |
| ARA01 | 1.73 | 0.053 | -0.006 | -0.005 | -0.004 | -0.004 | -0.013 | 0.064 |
| ARA02 | 1.73 | 0.053 | -0.006 | -0.005 | -0.004 | -0.004 | -0.013 | 0.064 |
| ROZ3 | 1.61 | 0.057 | -0.009 | -0.008 | -0.002 | -0.002 | -0.011 | 0.062 |
| KNR95 | 1.48 | 0.060 | -0.020 | -0.004 | -0.001 | 0.000 | -0.010 | 0.065 |
| ROZ4 | 0.83 | 0.088 | -0.026 | -0.019 | 0.006 | 0.002 | -0.007 | 0.073 |
| OF02 | 1.22 | 0.067 | -0.028 | 0.002 | 0.003 | 0.003 | -0.002 | 0.072 |
| KNR96 | 0.96 | 0.078 | -0.028 | -0.017 | -0.001 | -0.001 | -0.011 | 0.076 |
| NHMD01 | 0.87 | 0.075 | -0.041 | -0.024 | -0.001 | -0.001 | -0.010 | 0.073 |
| NAG03 | 0.85 | 0.155 | -0.016 | -0.012 | 0.003 | 0.002 | -0.008 | 0.082 |
| NHMD2 | 0.91 | 0.074 | -0.044 | -0.015 | -0.002 | -0.002 | -0.011 | 0.073 |
| CMN01 | 0.59 | 0.145 | -0.010 | -0.022 | 0.008 | 0.002 | -0.007 | 0.069 |
| OF01 | 0.34 | 0.118 | -0.017 | -0.033 | 0.006 | 0.006 | -0.003 | 0.065 |
| NAG04 | 0.24 | 0.123 | -0.020 | -0.033 | 0.003 | 0.003 | -0.007 | 0.065 |
| TKY01 | 0.18 | 0.138 | -0.013 | -0.026 | 0.005 | 0.006 | -0.003 | 0.064 |
| CMN2 | 0.09 | 0.135 | -0.020 | -0.026 | 0.004 | 0.005 | -0.006 | 0.066 |
| a, ΔBL = BL*a priori* – Blobs; b, $BSI = \left〈\left(S\_{ij} - s\_{ij}\right)^{2}\right〉^{1/2}$ |