Supporting Information

Volume-Based Thermoelasticity:

Compressibility of Mineral-Structured Materials

Leslie Glasser*

E-mail: l.glasser@curtin.edu.au

Nanochemistry Research Institute, Department of Applied Chemistry

Curtin University of Technology, GPO Box U1987, Perth, WA 6845, Australia

5 Supplementary Tables

4 Supplementary Figures

*Corresponding author

L. Glasser: Telephone: + 61 8 9266-3126 Fax: + 61 8 9266-4699

Table S1: Experimental ion-pair volumes, V_{pr} / nm^3 (= $2V_m/10$) and compressibilities, β / GPa^{-1}, of silicate clinopyroxenes I and II.[a]

Clinopyroxene	(2V/n) / nm^3	β / GPa^{-1}
I		
$LiAlSi_2O_6$	0.0194	0.0068
$NaAlSi_2O_6$	0.0201	0.0074
$NaCrSi_2O_6$	0.0209	0.0078
$NaFeSi_2O_6$	0.0214	0.0085
$CaNiSi_2O_6$	0.0218	0.0081
$CaMgSi_2O_6$	0.0219	0.0089
$CaFeSi_2O_6$	0.0225	0.0092
$NaVSi_2O_6$	0.0214	0.0087
$LiFeGe_2O_6$	0.0208	0.0068
II		
$LiAlSi_2O_6$	0.0193	0.0083
$LiFeSi_2O_6$	0.0207	0.0106
$ZnZnSi_2O_6$	0.0220	0.0145
$LiScSi_2O_6$	0.0220	0.0118
$ZnZnSi_2O_6$	0.0221	0.0135

[a] McCarthy, A. C.; Downs, R. T.; Thompson, R. M. *Am. Mineral.*, **2008**, *93*, 198-209.

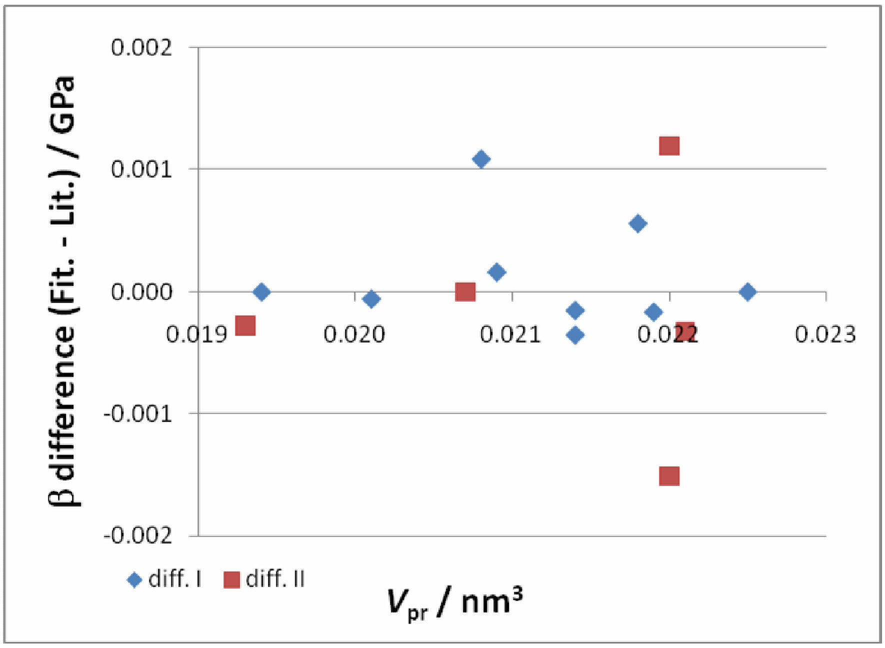

Figure S1: Difference in compressibilities, β / GPa, between linear least squares fit and literature values for silicate clinopyroxenes I (blue diamonds) and II (red squares). Mean Absolute Difference (MAD) for clinopyroxene I is 0.0003 GPa and 0.0008 GPa for clinopyroxene II.

Table S2: Experimental ion-pair volumes, V_{pr} / nm^3 (= $2V_m/4$) and compressibilities, β / GPa^{-1}, of chalcopyrites I-III and I-IV.[a]

Chalcopyrite	(2V/n) / nm^3	β / GPa^{-1}
I: I-III		
$CuAlS_2$	0.0371	0.0106
$CuGaS_2$	0.0375	0.0112
$CuGaSe_2$	0.0433	0.0131
$CuGaTe_2$	0.0535	0.0156

$CuInSe_2$	0.0485	0.0146
$AgGaS_2$	0.0426	0.0129
$AgGaSe_2$	0.0485	0.0145
$AgGaTe_2$	0.0590	0.0206
$AgInS_2$	0.0475	0.0140
$AgInSe_2$	0.0541	0.0172
$AgInTe_2$	0.0644	0.0227
$CuInS_2$	0.0416	0.0118
$CuInTe_2$	0.0586	0.0190
II: II-IV		
$ZnSiP_2$	0.0380	0.0127
$CdSiP_2$	0.0420	0.0139
$CdGeP_2$	0.0438	0.0148
$ZnSnP_2$	0.0450	0.0148
$ZnSiAs_2$	0.0428	0.0144
$ZnGeAs_2$	0.0448	0.0149
$CdGeAs_2$	0.0495	0.0143
$ZnSnAs_2$	0.0500	0.0177
$CdSnAs_2$	0.0505	0.0182
$ZnGeP_2$	0.0400	0.0116

[a] Reddy, R. R.; Ahammed, Y. N.; Gopal, K. R.; Azeem, P. A.; Rao, T. V. R. *Opt. Matls.*, **2000**, *14,* 355-358.

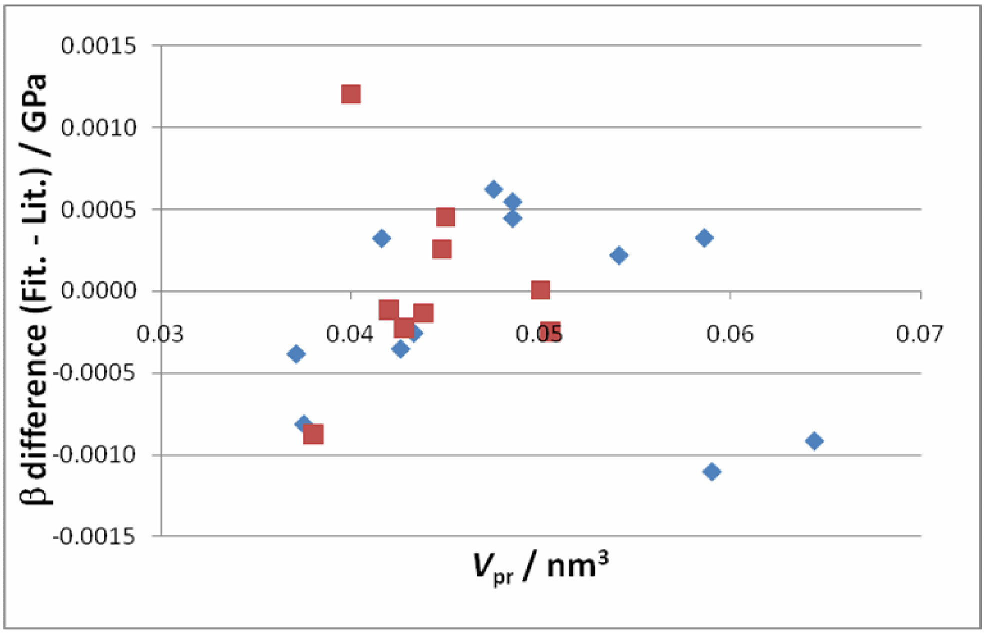

Figure S2: Difference in compressibilities, β / GPa, between linear least squares fit and literature values for chalcopyrites I (blue diamonds) and II (red squares). Mean Absolute Difference (MAD) for chalcopyrite I is 0.0006 GPa and 0.0004 GPa for chalcopyrite II.

Table S3: Experimental ion-pair volumes, V_{pr} / nm^3 (= $2V_m/4$) and compressibilities, β / GPa^{-1}, of perovskites. Data listed are from Liebermann, et al.,[a] unless otherwise indicated.

Perovskite	(2V/n) / nm^3	β / GPa^{-1}
$MgSiO_3$[b]	0.0162	0.0040
$FeSiO_3$[b]	0.0169	0.0036
$SrSiO_3$[c]	0.0297	0.0059
$CaGeO_3$[d,e]	0.0206	0.0051
$ScAlO_3$[a,f]	0.0185	0.0043
$YAlO_3$	0.0203	0.0049
$BiAlO_3$[g]	0.0196	0.0046
$SmAlO_3$	0.0209	0.0056
$EuAlO_3$	0.0208	0.0049
$GdAlO_3$	0.0207	0.0056
$FeTiO_3$[d]	0.0210	0.0059
$CdTiO_3$	0.0219	0.0047
$CaTiO_3$[a,d]	0.0223	0.0056
$SrTiO_3$	0.0238	0.0057
$BaTiO_3$	0.0256	0.0056
$CaSnO_3$[d]	0.0246	0.0062
$CdSnO_3$[h]	0.0243	0.0054
$CaZrO_3$[d]	0.0258	0.0065
$SrZrO_3$[i]	0.0277	0.0068
$BaHfO_3$[j]	0.0315	0.0068

[a] Liebermann, R. C.; Jones, L. E. A.; Ringwood, A. E. *Phys. Earth Planet. Int.*, **1977**, *14*, 165-178.

[b] Stixrude, L.; Lithgow-Bertelloni, C. *Geophys. J. Int.*, **2005**, *162*, 610-632.

[c] Hofmeister, ; Mao, *Geochim. Cosmochim. Acta*, **2003B,** *67*, 1207-1227.

[d] Ross, N. L.; Chaplin, T. D. *J. Solid State Chem.*, **2003**,*172*, 123-126.

[e]Liu, W.; Kung, J.; Wang, L.; Li, B. *Am. Miner.* **2008**,*93*, 745-750

[f] Ross, N. L. *Phys. Chem. Minerals*, **1998**, *25*, 597-602.

[g] Bouhemadou, A.; Khenata, R.; Amrani, B. *Physica B*, **2009**, *404*, 3534-3538.

[h] Kung, J.; Angel, R. J.; Ross, N. L. *Phys. Chem. Minerals*, **2001**, *28*, 35-43.

[i] McKnight, R. E. A.; Kennedy, B. J.; Zhou, Q.; Carpenter, M. A. *J. Phys.: Condens. Matter*, **2009**, *21*, 015902 (12 pp).

[j] Zhao, H.; Chang, A.; Wang, Y. *Physica B*, **2009**, *404*, 2192-2196.

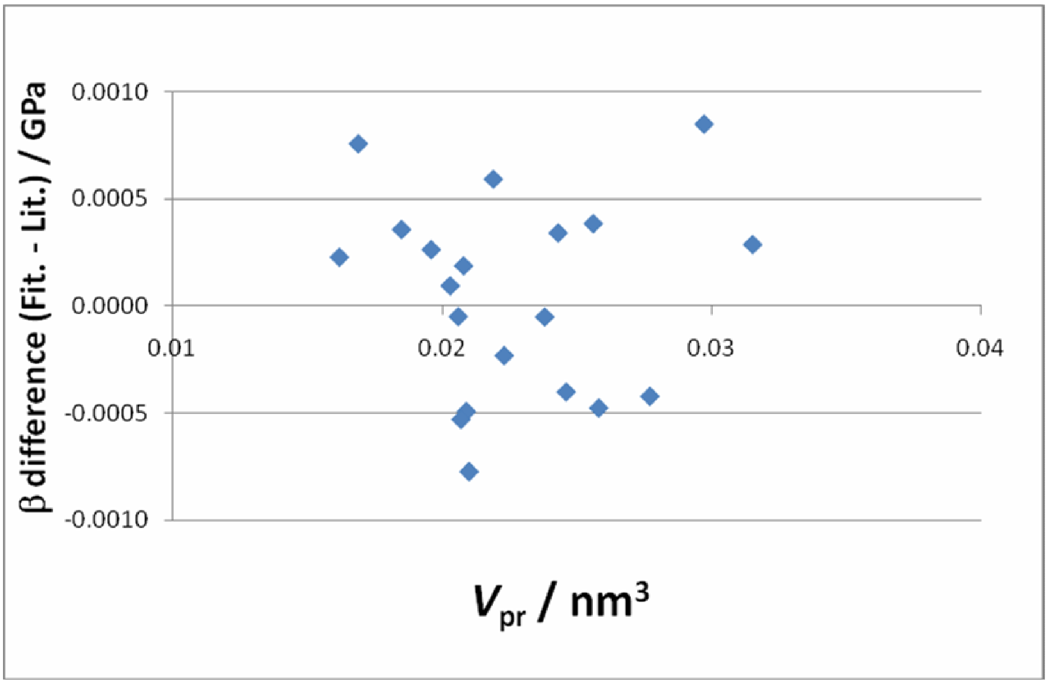

Figure S3: Difference in compressibilities, β / GPa, between linear least squares fit and literature values for perovskites. Mean Absolute Difference (MAD) is 0.0004 GPa.

Table S4: Experimental ion-pair volumes, V_{pr} / nm^3 (= 2V_m/4) and compressibilities, β / GPa^1, of transition metal diborides.[a] Mean Absolute Difference (MAD) between linear least squares fit and literature values is 0.0001 GPa.

Transition Metal Diboride	**(2V/n) / nm^3**	**β / GPa^{-1}**
TiB_2	0.0171	0.0033
ZrB_2	0.0208	0.0036
VB_2	0.0159	0.0034
NbB_2	0.0183	0.0034
WB_2	0.0161	0.0031

[a] Shein, I. R.; Ivanovskii, A. L. *J. Phys.: Condens. Matter*, **2008**, *20*, 415218 (9pp). Where a range of values is reported, the smallest compressibility has been chosen as most likely representing the least defective material.

Table S5: Experimental ion-pair volumes, V_{pr} / nm^3 (= $2V_m/7$) and compressibilities, β / GPa^{-1}, for spinels.[a]

	(2V/n) / nm^3	**β / GPa^{-1}**
$MgAl_2O_4$	0.0188	0.0052
$FeAl_2O_4$	0.0193	0.0048
$ZnAl_2O_4$	0.0189	0.0050
$FeCr_2O_4$	0.0209	0.0049
Fe_2SiO_4	0.0200	0.0048
$CuMn_2O_4$	0.0205	0.0051
$ZnCr_2O_4$	0.0206	0.0055
Fe_3O_4	0.0211	0.0051
$NiMn_2O_4$	0.0215	0.0049
$ZnMn_2O_4$	0.0217	0.0051
Ni_2SiO_4	0.0186	0.0051
$ZnFe_2O_4$	0.0215	0.0060

[a] Reichmann, H. J.; Jacobsen, S. D. *Am. Mineral.*, **2006**, *91*, 1049-1054.

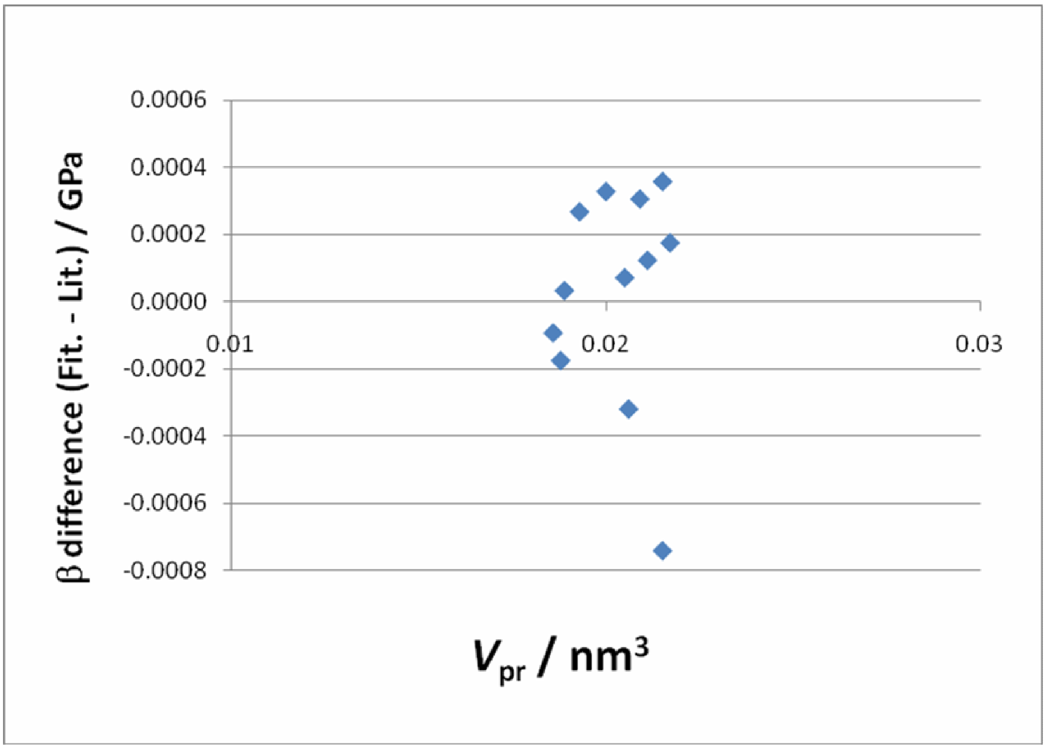

Figure S4: Difference in compressibilities, β / GPa, between linear least squares fit and literature values for spinels. Mean Absolute Difference (MAD) is 0.0003 GPa.