

Supplementary Information

Structure and relaxation of network units and crystallization of lithium silicate based glasses doped with oxides of Al and B

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S1. Derivation of the model

The solution given by eq. (11) is obtained from the Lagrange function $\mathcal{L}(P_n^m)$ with the Lagrange multipliers $\alpha, \beta, \gamma, \{\gamma_f\}$ and $\{\gamma_{ij}\}$ corresponding to the following constraints,

$$\sum_{n,m} P_n^m = 1 \quad ; \quad \sum_{n,m} E_n^m P_n^m = \langle E \rangle \quad ; \quad \sum_{n,m} r_n^m P_n^m = \langle 2x \rangle \quad ;$$

$$\sum_{n,m} f_n^m P_n^m = \langle f \rangle \quad , f \in \{f_{Si}, f_{Al}, f_B \dots\} \quad ; \quad \sum_{n,m} (i,j)_n^m P_n^m = k_{ij}$$

$$\begin{aligned} L(P_n^m) &= k_B \sum_{n,m} (P_n^m \ln P_n^m) + \alpha \left[\sum_{n,m} P_n^m - 1 \right] + \beta \left[\sum_{n,m} E_n^m P_n^m \right. \\ &\quad \left. + \sum_{i,j} \gamma_{ij} \left[\sum_{n,m} (i,j)_n^m P_n^m - k_{ij} \right] \right] \end{aligned} \quad (A1)$$

Differentiating $\mathcal{L}(P_n^m)$ with respect to P_n^m would equal zero,

$$\frac{\partial L(P_n^m)}{\partial P_n^m} = k_B (1 + \ln P_n^m) + \alpha + \beta E_n^m + \gamma r_n^m + \sum_f \gamma_f f_n^m + \sum_{j>i} \gamma_{ij} (i,j)_n^m = 0$$

Rearranging,

$$\ln P_n^m = -\ln Z_{gr} - \frac{\beta E_n^m}{k_B} - \frac{r_n^m \gamma}{k_B} - \frac{\sum_{ij} f_n^m \gamma_f}{k_B} - \frac{\sum_{ij} (ij)_n^m \gamma_{ij}}{k_B} \quad (\text{A2})$$

Where, $\ln Z_{gr} = \frac{(\alpha + k_B)}{k_B}$ and substituting eq. (A2) in eq. (10)

$$S = -k_B \sum_{n,m} \left(-P_n^m \ln Z_{gr} - P_n^m \frac{\beta E_n^m}{k_B} - P_n^m \frac{r_n^m \gamma}{k_B} - P_n^m \frac{\sum_f f_n^m \gamma_f}{k_B} - P_n^m \frac{\sum_{j>i} (ij)_n^m \gamma_{ij}}{k_B} \right)$$

Solving using the constraint equations,

$$S = k_B \ln Z_{gr} + \beta \langle E \rangle + \gamma \langle 2x \rangle + \sum_f \gamma_f \langle f \rangle + \sum_{j>i} \gamma_{ij} \langle k_{ij} \rangle$$

Rearranging,

$$\langle E \rangle = \frac{1}{\beta} S - \frac{k_B}{\beta} \ln Z_{gr} - \frac{\gamma}{\beta} \langle 2x \rangle - \sum_f \frac{\gamma_f}{\beta} \langle f \rangle - \sum_{j>i} \frac{\gamma_{ij}}{\beta} \langle k_{ij} \rangle$$

Differentiating,

$$d\langle E \rangle = \frac{1}{\beta} dS - \frac{k_B}{\beta} d\ln Z_{gr} - \frac{\gamma}{\beta} d\langle 2x \rangle - \sum_f \frac{\gamma_f}{\beta} d\langle f \rangle - \sum_{j>i} \frac{\gamma_{ij}}{\beta} dk_{ij}$$

Comparing the above equation with the *fundamental thermodynamic relation* (A3),[S1]

$$dE = TdS - PdV + \sum \mu_i dn_i \quad (\text{A3})$$

Would yield,

$$\beta = \frac{1}{T} \quad (\text{A4})$$

$$\gamma = -\frac{\mu}{T} \quad (\text{A5})$$

$$\gamma_f = -\frac{\mu_f}{T}$$

$$\gamma_{ij} = -\frac{\mu_{ij}}{T}$$

Therefore, substituting eq. (A4) and eq. (A5) into eq. (A2) and rearranging gives,

$$P_n^m = \frac{1}{Z_{gr}} e^{\frac{\sum_{j>i}^{(i,j)} m \mu_{ij} + \sum_f m \mu_f + r_n^m \mu_r - E_n^m}{k_B T}} \quad (\text{A17})$$

S2. Reduced number of units

a. Composition G

For composition G, the only units are Q_2 , Q_3 and Q_4 . The number of combinations of neighbouring units for each is calculated by,

$$Q_2: \binom{\binom{3}{2}}{\binom{2}{2}} = \binom{3+2-1}{2} = \binom{4}{2} = 6$$

$$Q_3: \binom{\binom{3}{3}}{\binom{3}{3}} = \binom{3+3-1}{3} = \binom{5}{3} = 10$$

$$Q_4: \binom{\binom{3}{4}}{\binom{4}{4}} = \binom{3+4-1}{4} = \binom{6}{4} = 15$$

Total number of units is 31. Number of constraint equations is equal to number types of BOs O_{ij} . Calculated by,

$$O_{ij}: \binom{\binom{3}{2}}{\binom{2}{2}} - 3 = \binom{3+2-1}{2} - 3 = \binom{4}{2} - 3 = 6 - 3 = 3$$

Total number of network connectivity constraint equations is 3.

b. Composition G_{Al}

For composition G_{Al} , the only units are Q_2 , Q_3 , Q_4 and Al^{IV} . The number of combinations of neighbouring units for each is calculated by,

$$Q_2: \binom{4}{2} = \binom{4+2-1}{2} = \binom{5}{2} = 10$$

$$Q_3: \binom{4}{3} = \binom{4+3-1}{3} = \binom{6}{3} = 20$$

$$Q_4: \binom{4}{4} = \binom{4+4-1}{4} = \binom{7}{4} = 35$$

$$A^{IV}: \binom{3}{4} = \binom{3+4-1}{4} = \binom{6}{4} = 15$$

Total number of units is 80. Number of constraint equations is equal to number types of BOs O_{ij} . Calculated by,

$$O_{ij}: \binom{3}{2} - 3 + 3 = \binom{3+2-1}{2} = \binom{4}{2} = 6$$

Total number of network connectivity constraint equations is 6.

c. Composition G_B

For composition G_B , the only units are Q_2 , Q_3 , Q_4 , B^{IV} and B^{III} . The number of combinations of neighbouring units for each is calculated by,

$$Q_2: \binom{5}{2} = \binom{5+2-1}{2} = \binom{6}{2} = 15$$

$$Q_3: \binom{5}{3} = \binom{5+3-1}{3} = \binom{7}{3} = 35$$

$$Q_4: \binom{5}{4} = \binom{5+4-1}{4} = \binom{8}{4} = 70$$

$$B^{IV}: \binom{3}{4} = \binom{3+4-1}{4} = \binom{6}{4} = 15$$

$$B^{III}: \binom{3}{2} = \binom{3+2-1}{2} = \binom{4}{2} = 6$$

Total number of units is 141. Number of constraint equations is equal to number types of BOs O_{ij} . Calculated by,

$$\mathbf{O}_{ij}: \binom{3}{2} - 3 + 3 + 3 = \binom{3+2-1}{2} + 3 = \binom{4}{2} + 3 = 6 + 3 = 9$$

Total number of network connectivity constraint equations is 9.

S3. Network volume for binary lithium silicate

The variation of NV for binary lithium silicate glass; the density data was taken from Shelby [S2].

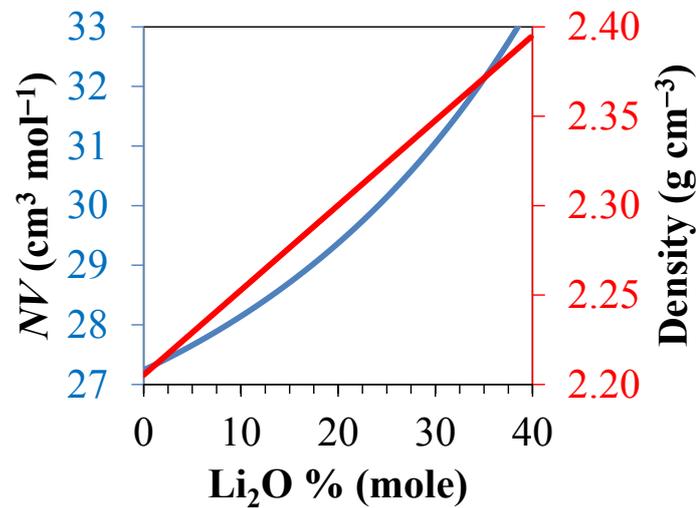


Figure S1. Variation of density and network volume with composition.

S4. Differential thermal analysis

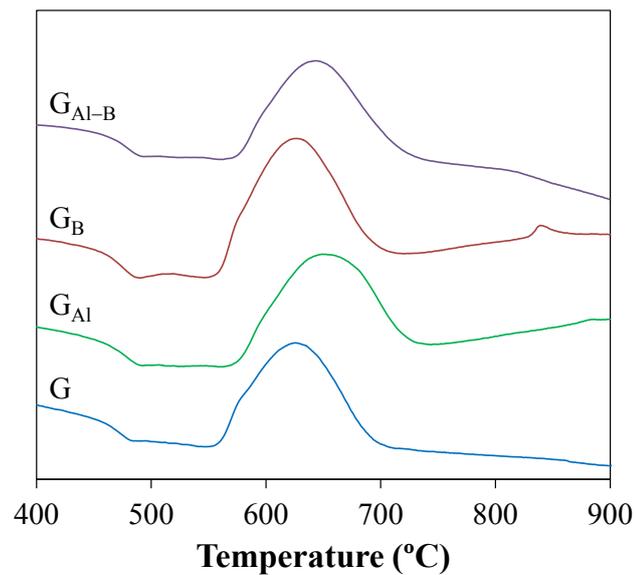


Figure S2. DTA of experimental glasses

S5. Values of energies (in Joules) used for simulations

Q_n^{ijkl}	G	G_{AI}	G_B	Q_n^{ijkl}	G	G_{AI}	G_B	Q_n^{ijkl}	G	G_{AI}	G_B
S_4^{4444}	6.43E-19	6.43E-19	6.43E-19	$S_4^{33\alpha\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{23\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{3444}	6.43E-19	6.43E-19	6.43E-19	$S_4^{24\alpha\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{22\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{3344}	6.43E-19	6.43E-19	6.43E-19	$S_4^{23\alpha\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{4\alpha\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{3334}	6.43E-19	6.43E-19	6.43E-19	$S_4^{22\alpha\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{3\alpha\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{3333}	6.43E-19	6.43E-19	6.43E-19	$S_4^{4\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{2\alpha\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{2444}	6.43E-19	6.43E-19	6.43E-19	$S_4^{34\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{4\beta\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{2344}	6.43E-19	6.43E-19	6.43E-19	$S_4^{33\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{3\beta\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{2334}	6.43E-19	6.43E-19	6.43E-19	$S_4^{24\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{2\beta\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{2333}	6.43E-19	6.43E-19	6.43E-19	$S_4^{23\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{\alpha\alpha\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{2244}	6.43E-19	6.43E-19	6.43E-19	$S_4^{22\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{\alpha\beta\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{2234}	6.43E-19	6.43E-19	6.43E-19	$S_4^{4\alpha\alpha\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{\beta\beta\beta}$	3.50E-19	3.50E-19	3.50E-19
S_4^{2233}	6.43E-19	6.43E-19	6.43E-19	$S_4^{3\alpha\alpha\beta}$	6.30E-19	6.30E-19	6.30E-19	S_2^{44}	2.00E-19	2.10E-19	2.10E-19
S_4^{2224}	6.43E-19	6.43E-19	6.43E-19	$S_4^{2\alpha\alpha\beta}$	6.30E-19	6.30E-19	6.30E-19	S_2^{34}	2.00E-19	2.10E-19	2.10E-19
S_4^{2223}	6.43E-19	6.43E-19	6.43E-19	$S_4^{4\alpha\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	S_2^{33}	2.00E-19	2.10E-19	2.10E-19
S_4^{2222}	6.43E-19	6.43E-19	6.43E-19	$S_4^{3\alpha\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	S_2^{24}	2.00E-19	2.10E-19	2.10E-19
$S_4^{444\alpha}$	6.30E-19	6.30E-19	6.30E-19	$S_4^{2\alpha\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	S_2^{23}	2.00E-19	2.10E-19	2.10E-19
$S_4^{344\alpha}$	6.30E-19	6.30E-19	6.30E-19	$S_4^{4\beta\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	S_2^{22}	2.00E-19	2.10E-19	2.10E-19
$S_4^{334\alpha}$	6.30E-19	6.30E-19	6.30E-19	$S_4^{3\beta\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_2^{4\alpha}$	3.00E-19	3.00E-19	3.00E-19
$S_4^{333\alpha}$	6.30E-19	6.30E-19	6.30E-19	$S_4^{2\beta\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_2^{3\alpha}$	3.00E-19	3.00E-19	3.00E-19
$S_4^{244\alpha}$	6.30E-19	6.30E-19	6.30E-19	$S_4^{\alpha\alpha\alpha\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_2^{2\alpha}$	3.00E-19	3.00E-19	3.00E-19
$S_4^{234\alpha}$	6.30E-19	6.30E-19	6.30E-19	$S_4^{\alpha\alpha\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_2^{\alpha\alpha}$	3.00E-19	3.00E-19	3.00E-19
$S_4^{233\alpha}$	6.30E-19	6.30E-19	6.30E-19	$S_4^{\alpha\beta\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_2^{4\beta}$	3.00E-19	3.00E-19	3.00E-19
$S_4^{224\alpha}$	6.30E-19	6.30E-19	6.30E-19	$S_4^{\beta\beta\beta\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_2^{3\beta}$	3.00E-19	3.00E-19	3.00E-19
$S_4^{223\alpha}$	6.30E-19	6.30E-19	6.30E-19	S_3^{444}	3.61E-19	3.60E-19	3.60E-19	$S_2^{2\beta}$	3.00E-19	3.00E-19	3.00E-19
$S_4^{222\alpha}$	6.30E-19	6.30E-19	6.30E-19	S_3^{344}	3.61E-19	3.60E-19	3.60E-19	$S_2^{\alpha\beta}$	3.00E-19	3.00E-19	3.00E-19
$S_4^{44\alpha\alpha}$	6.30E-19	6.30E-19	6.30E-19	S_3^{334}	3.61E-19	3.60E-19	3.60E-19	$S_2^{\beta\beta}$	3.00E-19	3.00E-19	3.00E-19
$S_4^{34\alpha\alpha}$	6.30E-19	6.30E-19	6.30E-19	S_3^{333}	3.61E-19	3.60E-19	3.60E-19	A_4^{4444}	---	4.00E-19	3.86E-19
$S_4^{33\alpha\alpha}$	6.30E-19	6.30E-19	6.30E-19	S_3^{244}	3.61E-19	3.60E-19	3.60E-19	A_4^{3444}	---	4.00E-19	3.86E-19
$S_4^{24\alpha\alpha}$	6.30E-19	6.30E-19	6.30E-19	S_3^{234}	3.61E-19	3.60E-19	3.60E-19	A_4^{3344}	---	4.00E-19	3.86E-19
$S_4^{23\alpha\alpha}$	6.30E-19	6.30E-19	6.30E-19	S_3^{233}	3.61E-19	3.60E-19	3.60E-19	A_4^{3334}	---	4.00E-19	3.86E-19
$S_4^{22\alpha\alpha}$	6.30E-19	6.30E-19	6.30E-19	S_3^{224}	3.61E-19	3.60E-19	3.60E-19	A_4^{3333}	---	4.00E-19	3.86E-19
$S_4^{4\alpha\alpha\alpha}$	6.30E-19	6.30E-19	6.30E-19	S_3^{223}	3.61E-19	3.60E-19	3.60E-19	A_4^{2444}	---	4.00E-19	3.86E-19
$S_4^{3\alpha\alpha\alpha}$	6.30E-19	6.30E-19	6.30E-19	S_3^{222}	3.61E-19	3.60E-19	3.60E-19	A_4^{2344}	---	4.00E-19	3.86E-19

S_4^{2aaa}	6.30E-19	6.30E-19	6.30E-19	S_3^{44a}	3.50E-19	3.50E-19	3.50E-19	A_4^{2334}	---	4.00E-19	3.86E-19
S_4^{aaaa}	6.30E-19	6.30E-19	6.30E-19	S_3^{34a}	3.50E-19	3.50E-19	3.50E-19	A_4^{2333}	---	4.00E-19	3.86E-19
$S_4^{444\beta}$	6.30E-19	6.30E-19	6.30E-19	S_3^{33a}	3.50E-19	3.50E-19	3.50E-19	A_4^{2244}	---	4.00E-19	3.86E-19
$S_4^{344\beta}$	6.30E-19	6.30E-19	6.30E-19	S_3^{24a}	3.50E-19	3.50E-19	3.50E-19	A_4^{2234}	---	4.00E-19	3.86E-19
$S_4^{334\beta}$	6.30E-19	6.30E-19	6.30E-19	S_3^{23a}	3.50E-19	3.50E-19	3.50E-19	A_4^{2233}	---	4.00E-19	3.86E-19
$S_4^{333\beta}$	6.30E-19	6.30E-19	6.30E-19	S_3^{22a}	3.50E-19	3.50E-19	3.50E-19	A_4^{2224}	---	4.00E-19	3.86E-19
$S_4^{244\beta}$	6.30E-19	6.30E-19	6.30E-19	S_3^{4aa}	3.50E-19	3.50E-19	3.50E-19	A_4^{2223}	---	4.00E-19	3.86E-19
$S_4^{234\beta}$	6.30E-19	6.30E-19	6.30E-19	S_3^{3aa}	3.50E-19	3.50E-19	3.50E-19	A_4^{2222}	---	4.00E-19	3.86E-19
$S_4^{233\beta}$	6.30E-19	6.30E-19	6.30E-19	S_3^{2aa}	3.50E-19	3.50E-19	3.50E-19	B_2^{44}	---	---	3.48E-19
$S_4^{224\beta}$	6.30E-19	6.30E-19	6.30E-19	S_3^{aaa}	3.50E-19	3.50E-19	3.50E-19	B_2^{34}	---	---	3.48E-19
$S_4^{223\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{44\beta}$	3.50E-19	3.50E-19	3.50E-19	B_2^{33}	---	---	3.48E-19
$S_4^{222\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{34\beta}$	3.50E-19	3.50E-19	3.50E-19	B_2^{24}	---	---	3.48E-19
$S_4^{44a\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{33\beta}$	3.50E-19	3.50E-19	3.50E-19	B_2^{23}	---	---	3.48E-19
$S_4^{34a\beta}$	6.30E-19	6.30E-19	6.30E-19	$S_3^{24\beta}$	3.50E-19	3.50E-19	3.50E-19	B_2^{22}	---	---	3.48E-19

S6. States of broken phase space components

Component 1:

S_4^{4444}

Component 2:

$S_4^{3444}, S_4^{3344}, S_4^{3334}, S_4^{3333}, S_3^{444}, S_3^{344}, S_3^{334}, S_3^{333}$

Component 3:

$S_4^{2444}, S_4^{2344}, S_4^{2334}, S_4^{2333}, S_4^{2244}, S_4^{2234}, S_4^{2233}, S_4^{2224}, S_4^{2223}, S_4^{2222}, S_3^{244}, S_3^{234}, S_3^{233}, S_3^{224}, S_3^{223}, S_3^{222}, S_2^{44}, S_2^{34}, S_2^{33}, S_2^{24}, S_2^{23}, S_2^{22}$

Component 4:

$S_4^{444a}, S_4^{344a}, S_4^{334a}, S_4^{333a}, S_4^{244a}, S_4^{234a}, S_4^{233a}, S_4^{224a}, S_4^{223a}, S_4^{222a}, S_4^{44aa}, S_4^{34aa}, S_4^{33aa}, S_4^{24aa}, S_4^{23aa}, S_4^{22aa}, S_4^{4aaa}, S_4^{3aaa}, S_4^{2aaa}, S_4^{aaaa}, S_4^{444\beta}, S_4^{344\beta}, S_4^{334\beta}, S_4^{333\beta}, S_4^{244\beta}, S_4^{234\beta}, S_4^{233\beta}, S_4^{224\beta}, S_4^{223\beta}, S_4^{222\beta}, S_4^{44a\beta}, S_4^{34a\beta}, S_4^{33a\beta}, S_4^{24a\beta}, S_4^{23a\beta}, S_4^{22a\beta}, S_4^{44\beta\beta}, S_4^{34\beta\beta}, S_4^{33\beta\beta}, S_4^{24\beta\beta}, S_4^{23\beta\beta}, S_4^{22\beta\beta}, S_4^{4aa\beta}, S_4^{3aa\beta}, S_4^{2aa\beta}, S_4^{4a\beta\beta}, S_4^{3a\beta\beta}, S_4^{2a\beta\beta}, S_4^{4\beta\beta\beta}, S_4^{3\beta\beta\beta}, S_4^{2\beta\beta\beta}, S_4^{\alpha a\beta}, S_4^{\alpha a\beta\beta}, S_4^{\alpha\beta\beta\beta}, S_4^{\beta\beta\beta\beta}, S_3^{44a}, S_3^{34a}, S_3^{33a}, S_3^{24a}, S_3^{23a}, S_3^{22a}, S_3^{4aa}, S_3^{3aa}, S_3^{2aa}, S_3^{aaa}, S_3^{44\beta}, S_3^{34\beta}, S_3^{33\beta}, S_3^{24\beta}, S_3^{23\beta}, S_3^{22\beta}, S_3^{4a\beta}, S_3^{3a\beta}, S_3^{2a\beta}, S_3^{4\beta\beta}, S_3^{3\beta\beta}, S_3^{2\beta\beta}, S_3^{\alpha a\beta}, S_3^{\alpha\beta\beta}, S_3^{\beta\beta\beta}, S_2^{4a}, S_2^{3a}, S_2^{2a}, S_2^{\alpha a}, S_2^{4\beta}, S_2^{3\beta}, S_2^{2\beta}, S_2^{\alpha\beta}, S_2^{\beta\beta}, A_4^{4444}, A_4^{3444}, A_4^{3344}, A_4^{3334}, A_4^{3333}, A_4^{2444}, A_4^{2344}, A_4^{2334}, A_4^{2333}, A_4^{2244}, A_4^{2234}, A_4^{2233}, A_4^{2224}, A_4^{2223}, A_4^{2222}, B_2^{44}, B_2^{34}, B_2^{33}, B_2^{24}, B_2^{23}, B_2^{22}$

S7. Chemical shift values used for the simulation of ^{29}Si NMR spectra

Q_n^{ijkl}	δ_{iso}	Q_n^{ijkl}	δ_{iso}	Q_n^{ijkl}	δ_{iso}	Q_n^{ijkl}	δ_{iso}
S_4^{4444}	-110	S_4^{444a}	-105	S_4^{23aa}	-95	S_3^{223}	-87
S_4^{3444}	-109	S_4^{344a}	-104	S_4^{22aa}	-94	S_3^{222}	-86
S_4^{3344}	-108	S_4^{334a}	-103	S_4^{4aaa}	-95	S_3^{44a}	-90
S_4^{3334}	-106	S_4^{333a}	-101	S_4^{3aaa}	-94	S_3^{34a}	-89
S_4^{3333}	-104	S_4^{244a}	-102	S_4^{2aaa}	-92	S_3^{33a}	-88
S_4^{2444}	-107	S_4^{234a}	-100	S_4^{aaaa}	-90	S_3^{24a}	-86
S_4^{2344}	-105	S_4^{233a}	-98	S_3^{444}	-95	S_2^{44}	-82
S_4^{2334}	-103	S_4^{224a}	-99	S_3^{344}	-94	S_2^{34}	-81
S_4^{2333}	-101	S_4^{223a}	-97	S_3^{334}	-93	S_2^{33}	-80
S_4^{2244}	-104	S_4^{222a}	-93	S_3^{333}	-92	S_2^{24}	-78
S_4^{2234}	-102	S_4^{44aa}	-100	S_3^{244}	-91	S_2^{23}	-77
S_4^{2233}	-100	S_4^{34aa}	-99	S_3^{234}	-90	S_2^{22}	-75
S_4^{2224}	-98	S_4^{33aa}	-98	S_3^{233}	-89		
S_4^{2223}	-96	S_4^{24aa}	-97	S_3^{224}	-88		

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