Supplementary material to accompany:

Adsorption and diffusion in zeolites: The pitfall of isotypic crystal structures

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1. METHODOLOGY

Henry coefficients, K_{H}, are calculated by Monte Carlo (MC) simulations in the canonical ensemble (NVT) at infinite dilution. By sampling the Rosenbluth weigths of the gas molecule in the adsorbed phase, $\langle W \rangle$, and in the ideal gas phase $\langle W_{\mathrm{ig}} \rangle$, the Henry coefficient follows [1]

$$K_{\mathrm{H}} = \frac{1}{RT} \frac{\langle W \rangle}{\langle W_{\mathrm{ig}} \rangle}, \tag{1}$$

where R denotes the ideal gas constant and T the temperature. Since methane is modeled as a single united-atom bead, the Rosenbluth weight in the gas phase equals unity.

Adsorption isotherms are obtained by means of Grand-Canonical Monte Carlo (GCMC) simulations, including translational and regrow moves. More details of GCMC can, for example, be found in reference 1.

Self-diffusivities on the basis of transition-state theory (TST), D, are determined by NVT-MC simulations, sampling residence histograms, $P(q)$, of the tagged molecule along the reaction coordinate, i.e. along the pore(s)

$$D = \sqrt{\frac{k_{\mathrm{B}}T}{2\pi m}} \frac{P(q^{\ddagger})}{\int\limits_{\text{cage A}} P(q)\,\mathrm{d}q} \lambda^2. \tag{2}$$

k_{B} is Boltzmann's constant, m the mass of the diffusing molecule, λ the site-to-site distance and $q^{\ddagger}$ denotes the dividing surface, i.e. location of the zeolite windows; note that $\exp[-F(q)/(k_{\mathrm{B}}T)] \propto P(q)$. Furthermore, diffusion coeffcients, D_U, on the basis of the mean potential-energy profiles along the pore(s), $U(q)$, are calculated

$$D_U = \sqrt{\frac{k_{\mathrm{B}}T}{2\pi m}} \frac{\exp\left[-\frac{U(q^{\ddagger})}{k_{\mathrm{B}}T}\right]}{\int\limits_{\text{cage A}} \exp\left[-\frac{U(q)}{k_{\mathrm{B}}T}\right] \mathrm{d}q} \lambda^2. \tag{3}$$

All diffusivities reported here are averaged over all three Cartesian directions

$$D = \frac{D_x + D_y + D_z}{3} \tag{4}$$

The pore system of LTA is three-dimensional and isotropic such that $D_x = D_y = D_z$. By constrast, SAS and ITE exhibit one-dimensional pores wherefore two of the three one-dimensional diffusivities equal zero.

Transmission coefficients, κ, are computed by a common two-step procedure. First, NVT-MC simulations are performed, restricting moves of the tagged molecule to the dividing

surface. Second, the configurations of step one serve as starting configurations for molecular dynamics (MD) simulations in which the reactive flux correlation function (RFCF) is sampled

$$\kappa(t) = \frac{\left\langle \dot{q}(0) \cdot \mathrm{H}[q(t) - q^{\ddagger}] \cdot \delta[q(0) - q^{\ddagger}] \right\rangle}{\left\langle 0.5 \cdot |\dot{q}(0)| \right\rangle}, \tag{5}$$

where $\dot{q}(0)$ represents the initial velocity of the molecule projected onto the reaction coordinate, H the Heaviside function, δ the Dirac pulse and angular brackets indicate an ensemble average. The transmission coefficients are then identified as the plateau of the RFCF, finally yielding the fraction of hopping attempts that are successful. For more details of the diffusion methodology, the reader is referred to reference 2 and references therein.

Methane is modeled as a single united atom. Interactions between guest and host atoms are assumed to be dominated by the methane-oxygen interactions and the host atoms are held rigid at their crystallographic positions. The force field has been specifically developed to reproduce inflection points of alkane isotherms [3]. A Nosé–Hoover chain thermostat is used in the MD part of the RFCF simulations to impose a constant temperature of 300 K.

2. LTA RESULTS AT FINITE LOADINGS

Figures 1 and 2 show relative differences of adsorption (loading, θ, vs. pressure, p) and diffusion quantities (TST self-diffusivity and transmission coefficient, respectively, vs. loading) of methane in different LTA-type zeolites. While the adsorption differences between the structure by Corma *et al.* and the IZA structure are rather small, those between Pluth and Smith and IZA structure can be quite large – especially at low p ($\leq$ 0.3 bar) and T (200 K), see Figure 1. The smaller the cages (Corma *et al.* < IZA < Pluth and Smith), the stronger is the adsorption at low pressures. This is likely due to a denser and thus more attractive potential-energy field inside the smaller cages (compare to main text). The larger a cage however, the stronger is the adsorption at high pressures because the cages are simply geometrically larger and can thus accommodate more methane molecules (larger saturation loading).

Let us now turn to the diffusion data compiled for 300 K and low loadings, see Figure 2. The largest diffusion discrepancies (-65%) are observed between the structure by Corma *et al.* and the IZA. Over the loading range studied here, this difference is practically constant,

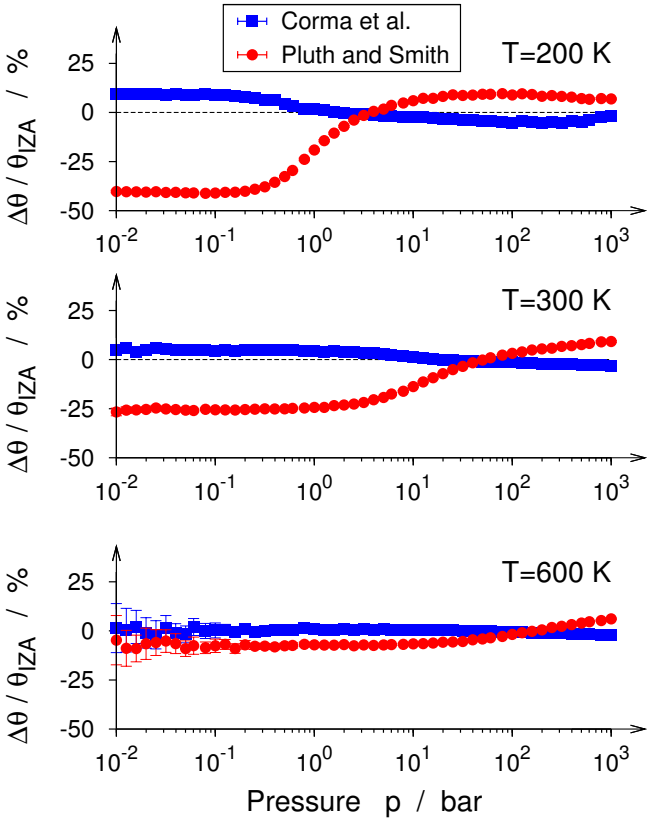

Figure 1. Structure influence on adsorption of methane in LTA-type zeolites. The values obtained from the IZA structure are taken as face values, i.e. $\Delta\theta_{\mathrm{Corma}} = \theta_{\mathrm{Corma}} - \theta_{\mathrm{IZA}}$.

indicating that the qualitative trend of D over loading is the same, see top of Figure 2. Although the absolute value of D_U (diffusivity calculated from a potential-energy profile) is, for a given structure and state point, consistently larger by a factor of approximately 100 than D (diffusivity calculated from a residence histogram, i.e. from a free-energy profile), the relative difference of D and D_U between two structures is the same. This supports the statement that the entropic barriers of different structures are equal; only the potential-energy barrier changes significantly between two structures.

The obvious insensitivity of the zeolite crystal structure on the transmission coefficient, see bottom of Figure 2, stems, most likely, from the fact that this coefficient is mainly influenced by guest molecules adsorbed in neighboring cages [6]. An analysis of the cage occupancy distributions reveals that these are, for a given average loading, the same for all three structures, see Figure 3. Hence the transmission coefficients are the same.

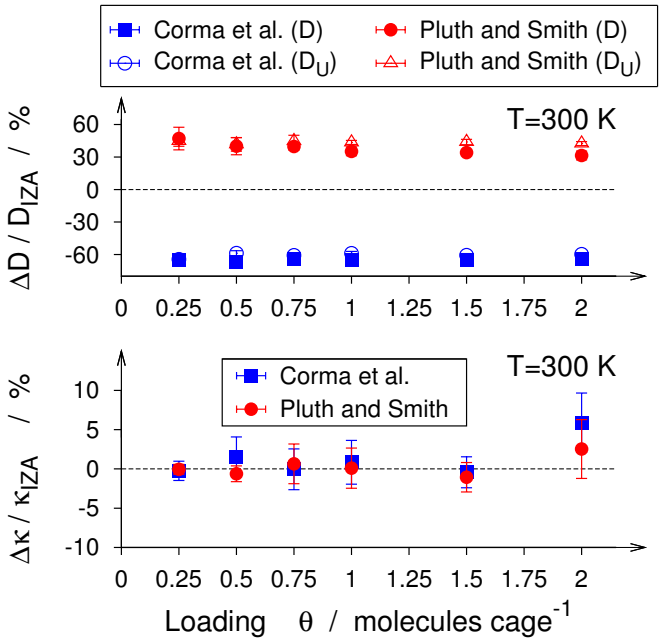

Figure 2. Structure influence on self-diffusion of methane in LTA-type zeolites.

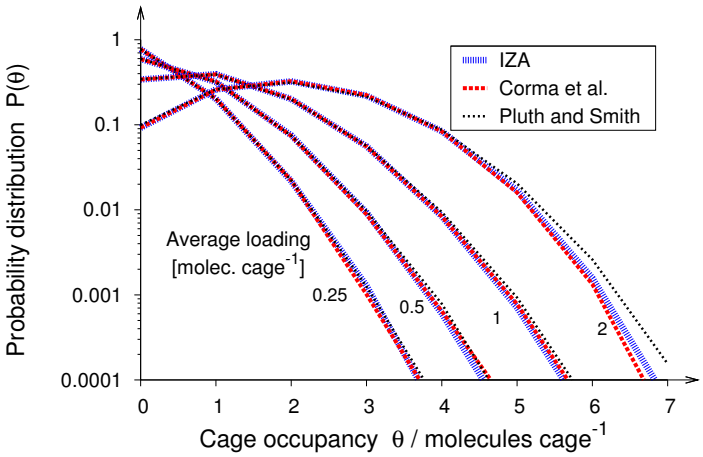

Figure 3. Probability distributions of cage occupancies; methane in three different LTA-type zeolites, various loadings.

3. CRYSTAL STRUCTURE DATA

In the following, we provide the crystal structure data that are used for the molecular simulations along with plots of the fractional coordinates of the oxygen atoms in *a*-*b* and, if necessary, *a*-*c* projection. The plots include the per-atom deviation in fractional atomic

positions, δr, of the experimental structures from the IZA structure

$$\delta r_{\mathrm{exp}} = \frac{1}{N_{\mathrm{atoms}}} \cdot \sum_{i=1}^{N_{\mathrm{atoms}}} \sqrt{\left(a_i^{\mathrm{exp}} - a_i^{\mathrm{IZA}}\right)^2 + \left(b_i^{\mathrm{exp}} - b_i^{\mathrm{IZA}}\right)^2 + \left(c_i^{\mathrm{exp}} - c_i^{\mathrm{IZA}}\right)^2}, \qquad (6)$$

where the sum runs over all N_{atoms} in the unit cell and a_i, b_i and c_i represent the position of atom i in the unit cell (fractional coordinates).

The structures published by the International Zeolite Association (IZA) represent "hypothetical" all-silica zeolites on the basis of the framework type definition and a refinement of the atomic positions that uses weighted atomic distances between nearest Si–O, O–O and Si–Si atoms. The structures by Corma *et al.*, Wragg *et al.*, and Camblor *et al.* are experimentally determined all-silica LTA, SAS, and ITE-type zeolites [4, 7, 8], whereas those published by Pluth and Smith (LTA) and Patinec *et al.* (SAS) are, in fact, aluminosilicates [5] and magnesioaluminophosphates [9], respectively, that, for the simulations, are converted to purely siliceous structures.

3.1. LTA – IZA [10]

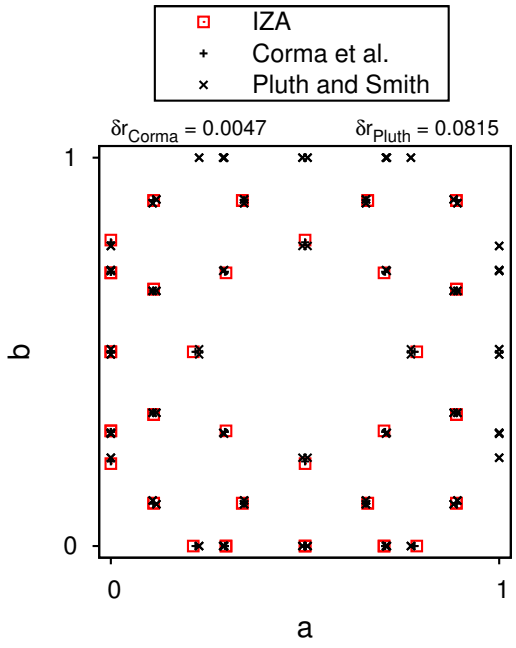

Figure 4. Plot of the fractional coordinates (a vs. b) of the unit-cell oxygen atoms of the three different LTA materials studied. Projections a–c and b–c are identical.

```
                                    11.919 11.919 11.919
                        90.000  90.000  90.000    SPGR =  1 P 1         OPT = 1
  72   0
     0 LTA          : LTA
  1 O1    0.0000   0.2122   0.5000     0 0 0 0 0 0 0 0 0.000
  2 O1    0.0000   0.5000   0.2122     0 0 0 0 0 0 0 0 0.000
  3 O1    0.0000   0.5000   0.7878     0 0 0 0 0 0 0 0 0.000
  4 O1    0.5000   0.2122   0.0000     0 0 0 0 0 0 0 0 0.000
  5 O1    0.7878   0.0000   0.5000     0 0 0 0 0 0 0 0 0.000
  6 O1    0.2122   0.0000   0.5000     0 0 0 0 0 0 0 0 0.000
  7 O1    0.5000   0.0000   0.2122     0 0 0 0 0 0 0 0 0.000
  8 O1    0.2122   0.5000   0.0000     0 0 0 0 0 0 0 0 0.000
  9 O1    0.7878   0.5000   0.0000     0 0 0 0 0 0 0 0 0.000
 10 O1    0.5000   0.0000   0.7878     0 0 0 0 0 0 0 0 0.000
 11 O1    0.0000   0.7878   0.5000     0 0 0 0 0 0 0 0 0.000
 12 O1    0.5000   0.7878   0.0000     0 0 0 0 0 0 0 0 0.000
 13 O2    0.1103   0.1103   0.3384     0 0 0 0 0 0 0 0 0.000
 14 O2    0.1103   0.6616   0.1103     0 0 0 0 0 0 0 0 0.000
 15 O2    0.1103   0.3384   0.8897     0 0 0 0 0 0 0 0 0.000
 16 O2    0.3384   0.1103   0.8897     0 0 0 0 0 0 0 0 0.000
 17 O2    0.6616   0.1103   0.1103     0 0 0 0 0 0 0 0 0.000
 18 O2    0.8897   0.1103   0.3384     0 0 0 0 0 0 0 0 0.000
 19 O2    0.1103   0.8897   0.3384     0 0 0 0 0 0 0 0 0.000
 20 O2    0.3384   0.1103   0.1103     0 0 0 0 0 0 0 0 0.000
 21 O2    0.1103   0.3384   0.1103     0 0 0 0 0 0 0 0 0.000
 22 O2    0.8897   0.6616   0.1103     0 0 0 0 0 0 0 0 0.000
 23 O2    0.3384   0.8897   0.8897     0 0 0 0 0 0 0 0 0.000
 24 O2    0.8897   0.3384   0.8897     0 0 0 0 0 0 0 0 0.000
 25 O2    0.6616   0.8897   0.1103     0 0 0 0 0 0 0 0 0.000
 26 O2    0.6616   0.1103   0.8897     0 0 0 0 0 0 0 0 0.000
 27 O2    0.1103   0.6616   0.8897     0 0 0 0 0 0 0 0 0.000
 28 O2    0.1103   0.8897   0.6616     0 0 0 0 0 0 0 0 0.000
 29 O2    0.8897   0.1103   0.6616     0 0 0 0 0 0 0 0 0.000
 30 O2    0.8897   0.8897   0.3384     0 0 0 0 0 0 0 0 0.000
 31 O2    0.1103   0.1103   0.6616     0 0 0 0 0 0 0 0 0.000
 32 O2    0.8897   0.8897   0.6616     0 0 0 0 0 0 0 0 0.000
 33 O2    0.3384   0.8897   0.1103     0 0 0 0 0 0 0 0 0.000
 34 O2    0.6616   0.8897   0.8897     0 0 0 0 0 0 0 0 0.000
 35 O2    0.8897   0.3384   0.1103     0 0 0 0 0 0 0 0 0.000
 36 O2    0.8897   0.6616   0.8897     0 0 0 0 0 0 0 0 0.000
 37 O3    0.0000   0.2967   0.2967     0 0 0 0 0 0 0 0 0.000
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 42 O3    0.7033   0.0000   0.2967     0 0 0 0 0 0 0 0 0.000
 43 O3    0.2967   0.0000   0.2967     0 0 0 0 0 0 0 0 0.000
```

```
44 O3    0.7033   0.7033   0.0000     0 0 0 0 0 0 0 0 0.000
45 O3    0.2967   0.0000   0.7033     0 0 0 0 0 0 0 0 0.000
46 O3    0.7033   0.0000   0.7033     0 0 0 0 0 0 0 0 0.000
47 O3    0.2967   0.7033   0.0000     0 0 0 0 0 0 0 0 0.000
48 O3    0.0000   0.7033   0.7033     0 0 0 0 0 0 0 0 0.000
49 Si1   0.0000   0.1823   0.3684     0 0 0 0 0 0 0 0 0.000
50 Si1   0.0000   0.6316   0.1823     0 0 0 0 0 0 0 0 0.000
51 Si1   0.0000   0.3684   0.8177     0 0 0 0 0 0 0 0 0.000
52 Si1   0.3684   0.1823   0.0000     0 0 0 0 0 0 0 0 0.000
53 Si1   0.6316   0.1823   0.0000     0 0 0 0 0 0 0 0 0.000
54 Si1   0.8177   0.0000   0.3684     0 0 0 0 0 0 0 0 0.000
55 Si1   0.1823   0.0000   0.3684     0 0 0 0 0 0 0 0 0.000
56 Si1   0.3684   0.0000   0.1823     0 0 0 0 0 0 0 0 0.000
57 Si1   0.1823   0.3684   0.0000     0 0 0 0 0 0 0 0 0.000
58 Si1   0.8177   0.6316   0.0000     0 0 0 0 0 0 0 0 0.000
59 Si1   0.3684   0.0000   0.8177     0 0 0 0 0 0 0 0 0.000
60 Si1   0.8177   0.3684   0.0000     0 0 0 0 0 0 0 0 0.000
61 Si1   0.6316   0.0000   0.1823     0 0 0 0 0 0 0 0 0.000
62 Si1   0.6316   0.0000   0.8177     0 0 0 0 0 0 0 0 0.000
63 Si1   0.1823   0.6316   0.0000     0 0 0 0 0 0 0 0 0.000
64 Si1   0.0000   0.8177   0.6316     0 0 0 0 0 0 0 0 0.000
65 Si1   0.0000   0.1823   0.6316     0 0 0 0 0 0 0 0 0.000
66 Si1   0.0000   0.8177   0.3684     0 0 0 0 0 0 0 0 0.000
67 Si1   0.1823   0.0000   0.6316     0 0 0 0 0 0 0 0 0.000
68 Si1   0.8177   0.0000   0.6316     0 0 0 0 0 0 0 0 0.000
69 Si1   0.3684   0.8177   0.0000     0 0 0 0 0 0 0 0 0.000
70 Si1   0.6316   0.8177   0.0000     0 0 0 0 0 0 0 0 0.000
71 Si1   0.0000   0.3684   0.1823     0 0 0 0 0 0 0 0 0.000
72 Si1   0.0000   0.6316   0.8177     0 0 0 0 0 0 0 0 0.000
```

3.2. LTA – Corma *et al.* [4]

```
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    0 LTA         : LTA
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2   0     0.00000  0.50000  0.21790      0 0 0 0 0 0 0 0 0.00
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4   0     0.50000  0.21790  0.00000      0 0 0 0 0 0 0 0 0.00
5   0     0.78210  0.00000  0.50000      0 0 0 0 0 0 0 0 0.00
6   0     0.21790  0.00000  0.50000      0 0 0 0 0 0 0 0 0.00
7   0     0.50000  0.00000  0.21790      0 0 0 0 0 0 0 0 0.00
8   0     0.21790  0.50000  0.00000      0 0 0 0 0 0 0 0 0.00
9   0     0.78210  0.50000  0.00000      0 0 0 0 0 0 0 0 0.00
```

```
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14   O     0.10980  0.65710  0.10980     0 0 0 0 0 0 0 0 0.00
15   O     0.10980  0.34290  0.89020     0 0 0 0 0 0 0 0 0.00
16   O     0.34290  0.10980  0.89020     0 0 0 0 0 0 0 0 0.00
17   O     0.65710  0.10980  0.10980     0 0 0 0 0 0 0 0 0.00
18   O     0.89020  0.10980  0.34290     0 0 0 0 0 0 0 0 0.00
19   O     0.10980  0.89020  0.34290     0 0 0 0 0 0 0 0 0.00
20   O     0.34290  0.10980  0.10980     0 0 0 0 0 0 0 0 0.00
21   O     0.10980  0.34290  0.10980     0 0 0 0 0 0 0 0 0.00
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25   O     0.65710  0.89020  0.10980     0 0 0 0 0 0 0 0 0.00
26   O     0.65710  0.10980  0.89020     0 0 0 0 0 0 0 0 0.00
27   O     0.10980  0.65710  0.89020     0 0 0 0 0 0 0 0 0.00
28   O     0.10980  0.89020  0.65710     0 0 0 0 0 0 0 0 0.00
29   O     0.89020  0.10980  0.65710     0 0 0 0 0 0 0 0 0.00
30   O     0.89020  0.89020  0.34290     0 0 0 0 0 0 0 0 0.00
31   O     0.10980  0.10980  0.65710     0 0 0 0 0 0 0 0 0.00
32   O     0.89020  0.89020  0.65710     0 0 0 0 0 0 0 0 0.00
33   O     0.34290  0.89020  0.10980     0 0 0 0 0 0 0 0 0.00
34   O     0.65710  0.89020  0.89020     0 0 0 0 0 0 0 0 0.00
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44   O     0.70610  0.70610  0.00000     0 0 0 0 0 0 0 0 0.00
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52   Si1   0.36830  0.18470  0.00000     0 0 0 0 0 0 0 0 0.00
53   Si1   0.63170  0.18470  0.00000     0 0 0 0 0 0 0 0 0.00
54   Si1   0.81530  0.00000  0.36830     0 0 0 0 0 0 0 0 0.00
55   Si1   0.18470  0.00000  0.36830     0 0 0 0 0 0 0 0 0.00
56   Si1   0.36830  0.00000  0.18470     0 0 0 0 0 0 0 0 0.00
```

```
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59  Si1    0.36830  0.00000  0.81530      0 0 0 0 0 0 0 0 0.00
60  Si1    0.81530  0.36830  0.00000      0 0 0 0 0 0 0 0 0.00
61  Si1    0.63170  0.00000  0.18470      0 0 0 0 0 0 0 0 0.00
62  Si1    0.63170  0.00000  0.81530      0 0 0 0 0 0 0 0 0.00
63  Si1    0.18470  0.63170  0.00000      0 0 0 0 0 0 0 0 0.00
64  Si1    0.00000  0.81530  0.63170      0 0 0 0 0 0 0 0 0.00
65  Si1    0.00000  0.18470  0.63170      0 0 0 0 0 0 0 0 0.00
66  Si1    0.00000  0.81530  0.36830      0 0 0 0 0 0 0 0 0.00
67  Si1    0.18470  0.00000  0.63170      0 0 0 0 0 0 0 0 0.00
68  Si1    0.81530  0.00000  0.63170      0 0 0 0 0 0 0 0 0.00
69  Si1    0.36830  0.81530  0.00000      0 0 0 0 0 0 0 0 0.00
70  Si1    0.63170  0.81530  0.00000      0 0 0 0 0 0 0 0 0.00
71  Si1    0.00000  0.36830  0.18470      0 0 0 0 0 0 0 0 0.00
72  Si1    0.00000  0.63170  0.81530      0 0 0 0 0 0 0 0 0.00
```

3.3. LTA – Pluth and Smith [5]

```
                                    24.555  24.555  24.555
                    90.000  90.000  90.000    SPGR =  1 P 1         OPT = 1
576   0 Created by Cota-0.6
    0 LTA5A          : LTA5A
  1 Si       0.00000   0.09316   0.18499    0   0   0   0   0   0   0   0   0.000
  2 Si       0.00000   0.18715   0.09042    0   0   0   0   0   0   0   0   0.000
  3 O        0.00000   0.11367   0.24663    0   0   0   0   0   0   0   0   0.000
  4 O        0.00000   0.14459   0.14591    0   0   0   0   0   0   0   0   0.000
  5 O        0.05379   0.05865   0.17152    0   0   0   0   0   0   0   0   0.000
  6 Si       0.00000   0.90684   0.18499    0   0   0   0   0   0   0   0   0.000
  7 Si       0.00000   0.81285   0.09042    0   0   0   0   0   0   0   0   0.000
  8 O        0.00000   0.88633   0.24663    0   0   0   0   0   0   0   0   0.000
  9 O        0.00000   0.85541   0.14591    0   0   0   0   0   0   0   0   0.000
 10 O        0.94621   0.94135   0.17152    0   0   0   0   0   0   0   0   0.000
 11 Si       0.00000   0.09316   0.81501    0   0   0   0   0   0   0   0   0.000
 12 Si       0.00000   0.18715   0.90958    0   0   0   0   0   0   0   0   0.000
 13 O        0.00000   0.11367   0.75337    0   0   0   0   0   0   0   0   0.000
 14 O        0.00000   0.14459   0.85409    0   0   0   0   0   0   0   0   0.000
 15 O        0.94621   0.05865   0.82848    0   0   0   0   0   0   0   0   0.000
 16 Si       0.00000   0.90684   0.81501    0   0   0   0   0   0   0   0   0.000
 17 Si       0.00000   0.81285   0.90958    0   0   0   0   0   0   0   0   0.000
 18 O        0.00000   0.88633   0.75337    0   0   0   0   0   0   0   0   0.000
 19 O        0.00000   0.85541   0.85409    0   0   0   0   0   0   0   0   0.000
 20 O        0.05379   0.94135   0.82848    0   0   0   0   0   0   0   0   0.000
 21 Si       0.18499   0.00000   0.09316    0   0   0   0   0   0   0   0   0.000
 22 Si       0.09042   0.00000   0.18715    0   0   0   0   0   0   0   0   0.000
```

23	O	0.24663	0.00000	0.11367	0	0	0	0	0	0	0	0.000
24	O	0.14591	0.00000	0.14459	0	0	0	0	0	0	0	0.000
25	O	0.17152	0.05379	0.05865	0	0	0	0	0	0	0	0.000
26	Si	0.18499	0.00000	0.90684	0	0	0	0	0	0	0	0.000
27	Si	0.09042	0.00000	0.81285	0	0	0	0	0	0	0	0.000
28	O	0.24663	0.00000	0.88633	0	0	0	0	0	0	0	0.000
29	O	0.14591	0.00000	0.85541	0	0	0	0	0	0	0	0.000
30	O	0.17152	0.94621	0.94135	0	0	0	0	0	0	0	0.000
31	Si	0.81501	0.00000	0.09316	0	0	0	0	0	0	0	0.000
32	Si	0.90958	0.00000	0.18715	0	0	0	0	0	0	0	0.000
33	O	0.75337	0.00000	0.11367	0	0	0	0	0	0	0	0.000
34	O	0.85409	0.00000	0.14459	0	0	0	0	0	0	0	0.000
35	O	0.82848	0.94621	0.05865	0	0	0	0	0	0	0	0.000
36	Si	0.81501	0.00000	0.90684	0	0	0	0	0	0	0	0.000
37	Si	0.90958	0.00000	0.81285	0	0	0	0	0	0	0	0.000
38	O	0.75337	0.00000	0.88633	0	0	0	0	0	0	0	0.000
39	O	0.85409	0.00000	0.85541	0	0	0	0	0	0	0	0.000
40	O	0.82848	0.05379	0.94135	0	0	0	0	0	0	0	0.000
41	Si	0.09316	0.18499	0.00000	0	0	0	0	0	0	0	0.000
42	Si	0.18715	0.09042	0.00000	0	0	0	0	0	0	0	0.000
43	O	0.11367	0.24663	0.00000	0	0	0	0	0	0	0	0.000
44	O	0.14459	0.14591	0.00000	0	0	0	0	0	0	0	0.000
45	O	0.05865	0.17152	0.05379	0	0	0	0	0	0	0	0.000
46	Si	0.90684	0.18499	0.00000	0	0	0	0	0	0	0	0.000
47	Si	0.81285	0.09042	0.00000	0	0	0	0	0	0	0	0.000
48	O	0.88633	0.24663	0.00000	0	0	0	0	0	0	0	0.000
49	O	0.85541	0.14591	0.00000	0	0	0	0	0	0	0	0.000
50	O	0.94135	0.17152	0.94621	0	0	0	0	0	0	0	0.000
51	Si	0.09316	0.81501	0.00000	0	0	0	0	0	0	0	0.000
52	Si	0.18715	0.90958	0.00000	0	0	0	0	0	0	0	0.000
53	O	0.11367	0.75337	0.00000	0	0	0	0	0	0	0	0.000
54	O	0.14459	0.85409	0.00000	0	0	0	0	0	0	0	0.000
55	O	0.05865	0.82848	0.94621	0	0	0	0	0	0	0	0.000
56	Si	0.90684	0.81501	0.00000	0	0	0	0	0	0	0	0.000
57	Si	0.81285	0.90958	0.00000	0	0	0	0	0	0	0	0.000
58	O	0.88633	0.75337	0.00000	0	0	0	0	0	0	0	0.000
59	O	0.85541	0.85409	0.00000	0	0	0	0	0	0	0	0.000
60	O	0.94135	0.82848	0.05379	0	0	0	0	0	0	0	0.000
61	Si	0.59316	0.50000	0.31501	0	0	0	0	0	0	0	0.000
62	Si	0.68715	0.50000	0.40958	0	0	0	0	0	0	0	0.000
63	O	0.61367	0.50000	0.25337	0	0	0	0	0	0	0	0.000
64	O	0.64459	0.50000	0.35409	0	0	0	0	0	0	0	0.000
65	O	0.55865	0.55379	0.32848	0	0	0	0	0	0	0	0.000
66	Si	0.40684	0.50000	0.31501	0	0	0	0	0	0	0	0.000
67	Si	0.31285	0.50000	0.40958	0	0	0	0	0	0	0	0.000
68	O	0.38633	0.50000	0.25337	0	0	0	0	0	0	0	0.000
69	O	0.35541	0.50000	0.35409	0	0	0	0	0	0	0	0.000

70	O	0.44135	0.44621	0.32848	0	0	0	0	0	0	0	0.000
71	Si	0.59316	0.50000	0.68499	0	0	0	0	0	0	0	0.000
72	Si	0.68715	0.50000	0.59042	0	0	0	0	0	0	0	0.000
73	O	0.61367	0.50000	0.74663	0	0	0	0	0	0	0	0.000
74	O	0.64459	0.50000	0.64591	0	0	0	0	0	0	0	0.000
75	O	0.55865	0.44621	0.67152	0	0	0	0	0	0	0	0.000
76	Si	0.40684	0.50000	0.68499	0	0	0	0	0	0	0	0.000
77	Si	0.31285	0.50000	0.59042	0	0	0	0	0	0	0	0.000
78	O	0.38633	0.50000	0.74663	0	0	0	0	0	0	0	0.000
79	O	0.35541	0.50000	0.64591	0	0	0	0	0	0	0	0.000
80	O	0.44135	0.55379	0.67152	0	0	0	0	0	0	0	0.000
81	Si	0.50000	0.68499	0.40684	0	0	0	0	0	0	0	0.000
82	Si	0.50000	0.59042	0.31285	0	0	0	0	0	0	0	0.000
83	O	0.50000	0.74663	0.38633	0	0	0	0	0	0	0	0.000
84	O	0.50000	0.64591	0.35541	0	0	0	0	0	0	0	0.000
85	O	0.55379	0.67152	0.44135	0	0	0	0	0	0	0	0.000
86	Si	0.50000	0.68499	0.59316	0	0	0	0	0	0	0	0.000
87	Si	0.50000	0.59042	0.68715	0	0	0	0	0	0	0	0.000
88	O	0.50000	0.74663	0.61367	0	0	0	0	0	0	0	0.000
89	O	0.50000	0.64591	0.64459	0	0	0	0	0	0	0	0.000
90	O	0.44621	0.67152	0.55865	0	0	0	0	0	0	0	0.000
91	Si	0.50000	0.31501	0.40684	0	0	0	0	0	0	0	0.000
92	Si	0.50000	0.40958	0.31285	0	0	0	0	0	0	0	0.000
93	O	0.50000	0.25337	0.38633	0	0	0	0	0	0	0	0.000
94	O	0.50000	0.35409	0.35541	0	0	0	0	0	0	0	0.000
95	O	0.44621	0.32848	0.44135	0	0	0	0	0	0	0	0.000
96	Si	0.50000	0.31501	0.59316	0	0	0	0	0	0	0	0.000
97	Si	0.50000	0.40958	0.68715	0	0	0	0	0	0	0	0.000
98	O	0.50000	0.25337	0.61367	0	0	0	0	0	0	0	0.000
99	O	0.50000	0.35409	0.64459	0	0	0	0	0	0	0	0.000
100	O	0.55379	0.32848	0.55865	0	0	0	0	0	0	0	0.000
101	Si	0.68499	0.59316	0.50000	0	0	0	0	0	0	0	0.000
102	Si	0.59042	0.68715	0.50000	0	0	0	0	0	0	0	0.000
103	O	0.74663	0.61367	0.50000	0	0	0	0	0	0	0	0.000
104	O	0.64591	0.64459	0.50000	0	0	0	0	0	0	0	0.000
105	O	0.67152	0.55865	0.44621	0	0	0	0	0	0	0	0.000
106	Si	0.68499	0.40684	0.50000	0	0	0	0	0	0	0	0.000
107	Si	0.59042	0.31285	0.50000	0	0	0	0	0	0	0	0.000
108	O	0.74663	0.38633	0.50000	0	0	0	0	0	0	0	0.000
109	O	0.64591	0.35541	0.50000	0	0	0	0	0	0	0	0.000
110	O	0.67152	0.44135	0.55379	0	0	0	0	0	0	0	0.000
111	Si	0.31501	0.59316	0.50000	0	0	0	0	0	0	0	0.000
112	Si	0.40958	0.68715	0.50000	0	0	0	0	0	0	0	0.000
113	O	0.25337	0.61367	0.50000	0	0	0	0	0	0	0	0.000
114	O	0.35409	0.64459	0.50000	0	0	0	0	0	0	0	0.000
115	O	0.32848	0.55865	0.55379	0	0	0	0	0	0	0	0.000
116	Si	0.31501	0.40684	0.50000	0	0	0	0	0	0	0	0.000

117 Si	0.40958	0.31285	0.50000	0	0	0	0	0	0	0	0	0.000
118 O	0.25337	0.38633	0.50000	0	0	0	0	0	0	0	0	0.000
119 O	0.35409	0.35541	0.50000	0	0	0	0	0	0	0	0	0.000
120 O	0.32848	0.44135	0.44621	0	0	0	0	0	0	0	0	0.000
121 O	0.94621	0.94135	0.82848	0	0	0	0	0	0	0	0	0.000
122 O	0.05379	0.05865	0.82848	0	0	0	0	0	0	0	0	0.000
123 O	0.05379	0.94135	0.17152	0	0	0	0	0	0	0	0	0.000
124 O	0.94621	0.05865	0.17152	0	0	0	0	0	0	0	0	0.000
125 O	0.82848	0.94621	0.94135	0	0	0	0	0	0	0	0	0.000
126 O	0.82848	0.05379	0.05865	0	0	0	0	0	0	0	0	0.000
127 O	0.17152	0.05379	0.94135	0	0	0	0	0	0	0	0	0.000
128 O	0.17152	0.94621	0.05865	0	0	0	0	0	0	0	0	0.000
129 O	0.94135	0.82848	0.94621	0	0	0	0	0	0	0	0	0.000
130 O	0.05865	0.82848	0.05379	0	0	0	0	0	0	0	0	0.000
131 O	0.94135	0.17152	0.05379	0	0	0	0	0	0	0	0	0.000
132 O	0.05865	0.17152	0.94621	0	0	0	0	0	0	0	0	0.000
133 O	0.44135	0.44621	0.67152	0	0	0	0	0	0	0	0	0.000
134 O	0.55865	0.55379	0.67152	0	0	0	0	0	0	0	0	0.000
135 O	0.44135	0.55379	0.32848	0	0	0	0	0	0	0	0	0.000
136 O	0.55865	0.44621	0.32848	0	0	0	0	0	0	0	0	0.000
137 O	0.44621	0.32848	0.55865	0	0	0	0	0	0	0	0	0.000
138 O	0.55379	0.32848	0.44135	0	0	0	0	0	0	0	0	0.000
139 O	0.55379	0.67152	0.55865	0	0	0	0	0	0	0	0	0.000
140 O	0.44621	0.67152	0.44135	0	0	0	0	0	0	0	0	0.000
141 O	0.32848	0.44135	0.55379	0	0	0	0	0	0	0	0	0.000
142 O	0.32848	0.55865	0.44621	0	0	0	0	0	0	0	0	0.000
143 O	0.67152	0.44135	0.44621	0	0	0	0	0	0	0	0	0.000
144 O	0.67152	0.55865	0.55379	0	0	0	0	0	0	0	0	0.000
145 Si	0.00000	0.59316	0.68499	0	0	0	0	0	0	0	0	0.000
146 Si	0.00000	0.68715	0.59042	0	0	0	0	0	0	0	0	0.000
147 O	0.00000	0.61367	0.74663	0	0	0	0	0	0	0	0	0.000
148 O	0.00000	0.64459	0.64591	0	0	0	0	0	0	0	0	0.000
149 O	0.05379	0.55865	0.67152	0	0	0	0	0	0	0	0	0.000
150 Si	0.00000	0.40684	0.68499	0	0	0	0	0	0	0	0	0.000
151 Si	0.00000	0.31285	0.59042	0	0	0	0	0	0	0	0	0.000
152 O	0.00000	0.38633	0.74663	0	0	0	0	0	0	0	0	0.000
153 O	0.00000	0.35541	0.64591	0	0	0	0	0	0	0	0	0.000
154 O	0.94621	0.44135	0.67152	0	0	0	0	0	0	0	0	0.000
155 Si	0.00000	0.59316	0.31501	0	0	0	0	0	0	0	0	0.000
156 Si	0.00000	0.68715	0.40958	0	0	0	0	0	0	0	0	0.000
157 O	0.00000	0.61367	0.25337	0	0	0	0	0	0	0	0	0.000
158 O	0.00000	0.64459	0.35409	0	0	0	0	0	0	0	0	0.000
159 O	0.94621	0.55865	0.32848	0	0	0	0	0	0	0	0	0.000
160 Si	0.00000	0.40684	0.31501	0	0	0	0	0	0	0	0	0.000
161 Si	0.00000	0.31285	0.40958	0	0	0	0	0	0	0	0	0.000
162 O	0.00000	0.38633	0.25337	0	0	0	0	0	0	0	0	0.000
163 O	0.00000	0.35541	0.35409	0	0	0	0	0	0	0	0	0.000

164	O	0.05379	0.44135	0.32848	0	0	0	0	0	0	0	0.000
165	Si	0.18499	0.50000	0.59316	0	0	0	0	0	0	0	0.000
166	Si	0.09042	0.50000	0.68715	0	0	0	0	0	0	0	0.000
167	O	0.24663	0.50000	0.61367	0	0	0	0	0	0	0	0.000
168	O	0.14591	0.50000	0.64459	0	0	0	0	0	0	0	0.000
169	O	0.17152	0.55379	0.55865	0	0	0	0	0	0	0	0.000
170	Si	0.18499	0.50000	0.40684	0	0	0	0	0	0	0	0.000
171	Si	0.09042	0.50000	0.31285	0	0	0	0	0	0	0	0.000
172	O	0.24663	0.50000	0.38633	0	0	0	0	0	0	0	0.000
173	O	0.14591	0.50000	0.35541	0	0	0	0	0	0	0	0.000
174	O	0.17152	0.44621	0.44135	0	0	0	0	0	0	0	0.000
175	Si	0.81501	0.50000	0.59316	0	0	0	0	0	0	0	0.000
176	Si	0.90958	0.50000	0.68715	0	0	0	0	0	0	0	0.000
177	O	0.75337	0.50000	0.61367	0	0	0	0	0	0	0	0.000
178	O	0.85409	0.50000	0.64459	0	0	0	0	0	0	0	0.000
179	O	0.82848	0.44621	0.55865	0	0	0	0	0	0	0	0.000
180	Si	0.81501	0.50000	0.40684	0	0	0	0	0	0	0	0.000
181	Si	0.90958	0.50000	0.31285	0	0	0	0	0	0	0	0.000
182	O	0.75337	0.50000	0.38633	0	0	0	0	0	0	0	0.000
183	O	0.85409	0.50000	0.35541	0	0	0	0	0	0	0	0.000
184	O	0.82848	0.55379	0.44135	0	0	0	0	0	0	0	0.000
185	Si	0.09316	0.68499	0.50000	0	0	0	0	0	0	0	0.000
186	Si	0.18715	0.59042	0.50000	0	0	0	0	0	0	0	0.000
187	O	0.11367	0.74663	0.50000	0	0	0	0	0	0	0	0.000
188	O	0.14459	0.64591	0.50000	0	0	0	0	0	0	0	0.000
189	O	0.05865	0.67152	0.55379	0	0	0	0	0	0	0	0.000
190	Si	0.90684	0.68499	0.50000	0	0	0	0	0	0	0	0.000
191	Si	0.81285	0.59042	0.50000	0	0	0	0	0	0	0	0.000
192	O	0.88633	0.74663	0.50000	0	0	0	0	0	0	0	0.000
193	O	0.85541	0.64591	0.50000	0	0	0	0	0	0	0	0.000
194	O	0.94135	0.67152	0.44621	0	0	0	0	0	0	0	0.000
195	Si	0.09316	0.31501	0.50000	0	0	0	0	0	0	0	0.000
196	Si	0.18715	0.40958	0.50000	0	0	0	0	0	0	0	0.000
197	O	0.11367	0.25337	0.50000	0	0	0	0	0	0	0	0.000
198	O	0.14459	0.35409	0.50000	0	0	0	0	0	0	0	0.000
199	O	0.05865	0.32848	0.44621	0	0	0	0	0	0	0	0.000
200	Si	0.90684	0.31501	0.50000	0	0	0	0	0	0	0	0.000
201	Si	0.81285	0.40958	0.50000	0	0	0	0	0	0	0	0.000
202	O	0.88633	0.25337	0.50000	0	0	0	0	0	0	0	0.000
203	O	0.85541	0.35409	0.50000	0	0	0	0	0	0	0	0.000
204	O	0.94135	0.32848	0.55379	0	0	0	0	0	0	0	0.000
205	Si	0.59316	0.00000	0.81501	0	0	0	0	0	0	0	0.000
206	Si	0.68715	0.00000	0.90958	0	0	0	0	0	0	0	0.000
207	O	0.61367	0.00000	0.75337	0	0	0	0	0	0	0	0.000
208	O	0.64459	0.00000	0.85409	0	0	0	0	0	0	0	0.000
209	O	0.55865	0.05379	0.82848	0	0	0	0	0	0	0	0.000
210	Si	0.40684	0.00000	0.81501	0	0	0	0	0	0	0	0.000

211	Si	0.31285	0.00000	0.90958	0	0	0	0	0	0	0	0.000
212	O	0.38633	0.00000	0.75337	0	0	0	0	0	0	0	0.000
213	O	0.35541	0.00000	0.85409	0	0	0	0	0	0	0	0.000
214	O	0.44135	0.94621	0.82848	0	0	0	0	0	0	0	0.000
215	Si	0.59316	0.00000	0.18499	0	0	0	0	0	0	0	0.000
216	Si	0.68715	0.00000	0.09042	0	0	0	0	0	0	0	0.000
217	O	0.61367	0.00000	0.24663	0	0	0	0	0	0	0	0.000
218	O	0.64459	0.00000	0.14591	0	0	0	0	0	0	0	0.000
219	O	0.55865	0.94621	0.17152	0	0	0	0	0	0	0	0.000
220	Si	0.40684	0.00000	0.18499	0	0	0	0	0	0	0	0.000
221	Si	0.31285	0.00000	0.09042	0	0	0	0	0	0	0	0.000
222	O	0.38633	0.00000	0.24663	0	0	0	0	0	0	0	0.000
223	O	0.35541	0.00000	0.14591	0	0	0	0	0	0	0	0.000
224	O	0.44135	0.05379	0.17152	0	0	0	0	0	0	0	0.000
225	Si	0.50000	0.18499	0.90684	0	0	0	0	0	0	0	0.000
226	Si	0.50000	0.09042	0.81285	0	0	0	0	0	0	0	0.000
227	O	0.50000	0.24663	0.88633	0	0	0	0	0	0	0	0.000
228	O	0.50000	0.14591	0.85541	0	0	0	0	0	0	0	0.000
229	O	0.55379	0.17152	0.94135	0	0	0	0	0	0	0	0.000
230	Si	0.50000	0.18499	0.09316	0	0	0	0	0	0	0	0.000
231	Si	0.50000	0.09042	0.18715	0	0	0	0	0	0	0	0.000
232	O	0.50000	0.24663	0.11367	0	0	0	0	0	0	0	0.000
233	O	0.50000	0.14591	0.14459	0	0	0	0	0	0	0	0.000
234	O	0.44621	0.17152	0.05865	0	0	0	0	0	0	0	0.000
235	Si	0.50000	0.81501	0.90684	0	0	0	0	0	0	0	0.000
236	Si	0.50000	0.90958	0.81285	0	0	0	0	0	0	0	0.000
237	O	0.50000	0.75337	0.88633	0	0	0	0	0	0	0	0.000
238	O	0.50000	0.85409	0.85541	0	0	0	0	0	0	0	0.000
239	O	0.44621	0.82848	0.94135	0	0	0	0	0	0	0	0.000
240	Si	0.50000	0.81501	0.09316	0	0	0	0	0	0	0	0.000
241	Si	0.50000	0.90958	0.18715	0	0	0	0	0	0	0	0.000
242	O	0.50000	0.75337	0.11367	0	0	0	0	0	0	0	0.000
243	O	0.50000	0.85409	0.14459	0	0	0	0	0	0	0	0.000
244	O	0.55379	0.82848	0.05865	0	0	0	0	0	0	0	0.000
245	Si	0.68499	0.09316	0.00000	0	0	0	0	0	0	0	0.000
246	Si	0.59042	0.18715	0.00000	0	0	0	0	0	0	0	0.000
247	O	0.74663	0.11367	0.00000	0	0	0	0	0	0	0	0.000
248	O	0.64591	0.14459	0.00000	0	0	0	0	0	0	0	0.000
249	O	0.67152	0.05865	0.94621	0	0	0	0	0	0	0	0.000
250	Si	0.68499	0.90684	0.00000	0	0	0	0	0	0	0	0.000
251	Si	0.59042	0.81285	0.00000	0	0	0	0	0	0	0	0.000
252	O	0.74663	0.88633	0.00000	0	0	0	0	0	0	0	0.000
253	O	0.64591	0.85541	0.00000	0	0	0	0	0	0	0	0.000
254	O	0.67152	0.94135	0.05379	0	0	0	0	0	0	0	0.000
255	Si	0.31501	0.09316	0.00000	0	0	0	0	0	0	0	0.000
256	Si	0.40958	0.18715	0.00000	0	0	0	0	0	0	0	0.000
257	O	0.25337	0.11367	0.00000	0	0	0	0	0	0	0	0.000

258	O	0.35409	0.14459	0.00000	0	0	0	0	0	0	0	0.000
259	O	0.32848	0.05865	0.05379	0	0	0	0	0	0	0	0.000
260	Si	0.31501	0.90684	0.00000	0	0	0	0	0	0	0	0.000
261	Si	0.40958	0.81285	0.00000	0	0	0	0	0	0	0	0.000
262	O	0.25337	0.88633	0.00000	0	0	0	0	0	0	0	0.000
263	O	0.35409	0.85541	0.00000	0	0	0	0	0	0	0	0.000
264	O	0.32848	0.94135	0.94621	0	0	0	0	0	0	0	0.000
265	O	0.94621	0.44135	0.32848	0	0	0	0	0	0	0	0.000
266	O	0.05379	0.55865	0.32848	0	0	0	0	0	0	0	0.000
267	O	0.05379	0.44135	0.67152	0	0	0	0	0	0	0	0.000
268	O	0.94621	0.55865	0.67152	0	0	0	0	0	0	0	0.000
269	O	0.82848	0.44621	0.44135	0	0	0	0	0	0	0	0.000
270	O	0.82848	0.55379	0.55865	0	0	0	0	0	0	0	0.000
271	O	0.17152	0.55379	0.44135	0	0	0	0	0	0	0	0.000
272	O	0.17152	0.44621	0.55865	0	0	0	0	0	0	0	0.000
273	O	0.94135	0.32848	0.44621	0	0	0	0	0	0	0	0.000
274	O	0.05865	0.32848	0.55379	0	0	0	0	0	0	0	0.000
275	O	0.94135	0.67152	0.55379	0	0	0	0	0	0	0	0.000
276	O	0.05865	0.67152	0.44621	0	0	0	0	0	0	0	0.000
277	O	0.44135	0.94621	0.17152	0	0	0	0	0	0	0	0.000
278	O	0.55865	0.05379	0.17152	0	0	0	0	0	0	0	0.000
279	O	0.44135	0.05379	0.82848	0	0	0	0	0	0	0	0.000
280	O	0.55865	0.94621	0.82848	0	0	0	0	0	0	0	0.000
281	O	0.44621	0.82848	0.05865	0	0	0	0	0	0	0	0.000
282	O	0.55379	0.82848	0.94135	0	0	0	0	0	0	0	0.000
283	O	0.55379	0.17152	0.05865	0	0	0	0	0	0	0	0.000
284	O	0.44621	0.17152	0.94135	0	0	0	0	0	0	0	0.000
285	O	0.32848	0.94135	0.05379	0	0	0	0	0	0	0	0.000
286	O	0.32848	0.05865	0.94621	0	0	0	0	0	0	0	0.000
287	O	0.67152	0.94135	0.94621	0	0	0	0	0	0	0	0.000
288	O	0.67152	0.05865	0.05379	0	0	0	0	0	0	0	0.000
289	Si	0.50000	0.09316	0.68499	0	0	0	0	0	0	0	0.000
290	Si	0.50000	0.18715	0.59042	0	0	0	0	0	0	0	0.000
291	O	0.50000	0.11367	0.74663	0	0	0	0	0	0	0	0.000
292	O	0.50000	0.14459	0.64591	0	0	0	0	0	0	0	0.000
293	O	0.55379	0.05865	0.67152	0	0	0	0	0	0	0	0.000
294	Si	0.50000	0.90684	0.68499	0	0	0	0	0	0	0	0.000
295	Si	0.50000	0.81285	0.59042	0	0	0	0	0	0	0	0.000
296	O	0.50000	0.88633	0.74663	0	0	0	0	0	0	0	0.000
297	O	0.50000	0.85541	0.64591	0	0	0	0	0	0	0	0.000
298	O	0.44621	0.94135	0.67152	0	0	0	0	0	0	0	0.000
299	Si	0.50000	0.09316	0.31501	0	0	0	0	0	0	0	0.000
300	Si	0.50000	0.18715	0.40958	0	0	0	0	0	0	0	0.000
301	O	0.50000	0.11367	0.25337	0	0	0	0	0	0	0	0.000
302	O	0.50000	0.14459	0.35409	0	0	0	0	0	0	0	0.000
303	O	0.44621	0.05865	0.32848	0	0	0	0	0	0	0	0.000
304	Si	0.50000	0.90684	0.31501	0	0	0	0	0	0	0	0.000

305	Si	0.50000	0.81285	0.40958	0	0	0	0	0	0	0	0.000
306	O	0.50000	0.88633	0.25337	0	0	0	0	0	0	0	0.000
307	O	0.50000	0.85541	0.35409	0	0	0	0	0	0	0	0.000
308	O	0.55379	0.94135	0.32848	0	0	0	0	0	0	0	0.000
309	Si	0.68499	0.00000	0.59316	0	0	0	0	0	0	0	0.000
310	Si	0.59042	0.00000	0.68715	0	0	0	0	0	0	0	0.000
311	O	0.74663	0.00000	0.61367	0	0	0	0	0	0	0	0.000
312	O	0.64591	0.00000	0.64459	0	0	0	0	0	0	0	0.000
313	O	0.67152	0.05379	0.55865	0	0	0	0	0	0	0	0.000
314	Si	0.68499	0.00000	0.40684	0	0	0	0	0	0	0	0.000
315	Si	0.59042	0.00000	0.31285	0	0	0	0	0	0	0	0.000
316	O	0.74663	0.00000	0.38633	0	0	0	0	0	0	0	0.000
317	O	0.64591	0.00000	0.35541	0	0	0	0	0	0	0	0.000
318	O	0.67152	0.94621	0.44135	0	0	0	0	0	0	0	0.000
319	Si	0.31501	0.00000	0.59316	0	0	0	0	0	0	0	0.000
320	Si	0.40958	0.00000	0.68715	0	0	0	0	0	0	0	0.000
321	O	0.25337	0.00000	0.61367	0	0	0	0	0	0	0	0.000
322	O	0.35409	0.00000	0.64459	0	0	0	0	0	0	0	0.000
323	O	0.32848	0.94621	0.55865	0	0	0	0	0	0	0	0.000
324	Si	0.31501	0.00000	0.40684	0	0	0	0	0	0	0	0.000
325	Si	0.40958	0.00000	0.31285	0	0	0	0	0	0	0	0.000
326	O	0.25337	0.00000	0.38633	0	0	0	0	0	0	0	0.000
327	O	0.35409	0.00000	0.35541	0	0	0	0	0	0	0	0.000
328	O	0.32848	0.05379	0.44135	0	0	0	0	0	0	0	0.000
329	Si	0.59316	0.18499	0.50000	0	0	0	0	0	0	0	0.000
330	Si	0.68715	0.09042	0.50000	0	0	0	0	0	0	0	0.000
331	O	0.61367	0.24663	0.50000	0	0	0	0	0	0	0	0.000
332	O	0.64459	0.14591	0.50000	0	0	0	0	0	0	0	0.000
333	O	0.55865	0.17152	0.55379	0	0	0	0	0	0	0	0.000
334	Si	0.40684	0.18499	0.50000	0	0	0	0	0	0	0	0.000
335	Si	0.31285	0.09042	0.50000	0	0	0	0	0	0	0	0.000
336	O	0.38633	0.24663	0.50000	0	0	0	0	0	0	0	0.000
337	O	0.35541	0.14591	0.50000	0	0	0	0	0	0	0	0.000
338	O	0.44135	0.17152	0.44621	0	0	0	0	0	0	0	0.000
339	Si	0.59316	0.81501	0.50000	0	0	0	0	0	0	0	0.000
340	Si	0.68715	0.90958	0.50000	0	0	0	0	0	0	0	0.000
341	O	0.61367	0.75337	0.50000	0	0	0	0	0	0	0	0.000
342	O	0.64459	0.85409	0.50000	0	0	0	0	0	0	0	0.000
343	O	0.55865	0.82848	0.44621	0	0	0	0	0	0	0	0.000
344	Si	0.40684	0.81501	0.50000	0	0	0	0	0	0	0	0.000
345	Si	0.31285	0.90958	0.50000	0	0	0	0	0	0	0	0.000
346	O	0.38633	0.75337	0.50000	0	0	0	0	0	0	0	0.000
347	O	0.35541	0.85409	0.50000	0	0	0	0	0	0	0	0.000
348	O	0.44135	0.82848	0.55379	0	0	0	0	0	0	0	0.000
349	Si	0.09316	0.50000	0.81501	0	0	0	0	0	0	0	0.000
350	Si	0.18715	0.50000	0.90958	0	0	0	0	0	0	0	0.000
351	O	0.11367	0.50000	0.75337	0	0	0	0	0	0	0	0.000

352	O	0.14459	0.50000	0.85409	0	0	0	0	0	0	0	0.000
353	O	0.05865	0.55379	0.82848	0	0	0	0	0	0	0	0.000
354	Si	0.90684	0.50000	0.81501	0	0	0	0	0	0	0	0.000
355	Si	0.81285	0.50000	0.90958	0	0	0	0	0	0	0	0.000
356	O	0.88633	0.50000	0.75337	0	0	0	0	0	0	0	0.000
357	O	0.85541	0.50000	0.85409	0	0	0	0	0	0	0	0.000
358	O	0.94135	0.44621	0.82848	0	0	0	0	0	0	0	0.000
359	Si	0.09316	0.50000	0.18499	0	0	0	0	0	0	0	0.000
360	Si	0.18715	0.50000	0.09042	0	0	0	0	0	0	0	0.000
361	O	0.11367	0.50000	0.24663	0	0	0	0	0	0	0	0.000
362	O	0.14459	0.50000	0.14591	0	0	0	0	0	0	0	0.000
363	O	0.05865	0.44621	0.17152	0	0	0	0	0	0	0	0.000
364	Si	0.90684	0.50000	0.18499	0	0	0	0	0	0	0	0.000
365	Si	0.81285	0.50000	0.09042	0	0	0	0	0	0	0	0.000
366	O	0.88633	0.50000	0.24663	0	0	0	0	0	0	0	0.000
367	O	0.85541	0.50000	0.14591	0	0	0	0	0	0	0	0.000
368	O	0.94135	0.55379	0.17152	0	0	0	0	0	0	0	0.000
369	Si	0.00000	0.68499	0.90684	0	0	0	0	0	0	0	0.000
370	Si	0.00000	0.59042	0.81285	0	0	0	0	0	0	0	0.000
371	O	0.00000	0.74663	0.88633	0	0	0	0	0	0	0	0.000
372	O	0.00000	0.64591	0.85541	0	0	0	0	0	0	0	0.000
373	O	0.05379	0.67152	0.94135	0	0	0	0	0	0	0	0.000
374	Si	0.00000	0.68499	0.09316	0	0	0	0	0	0	0	0.000
375	Si	0.00000	0.59042	0.18715	0	0	0	0	0	0	0	0.000
376	O	0.00000	0.74663	0.11367	0	0	0	0	0	0	0	0.000
377	O	0.00000	0.64591	0.14459	0	0	0	0	0	0	0	0.000
378	O	0.94621	0.67152	0.05865	0	0	0	0	0	0	0	0.000
379	Si	0.00000	0.31501	0.90684	0	0	0	0	0	0	0	0.000
380	Si	0.00000	0.40958	0.81285	0	0	0	0	0	0	0	0.000
381	O	0.00000	0.25337	0.88633	0	0	0	0	0	0	0	0.000
382	O	0.00000	0.35409	0.85541	0	0	0	0	0	0	0	0.000
383	O	0.94621	0.32848	0.94135	0	0	0	0	0	0	0	0.000
384	Si	0.00000	0.31501	0.09316	0	0	0	0	0	0	0	0.000
385	Si	0.00000	0.40958	0.18715	0	0	0	0	0	0	0	0.000
386	O	0.00000	0.25337	0.11367	0	0	0	0	0	0	0	0.000
387	O	0.00000	0.35409	0.14459	0	0	0	0	0	0	0	0.000
388	O	0.05379	0.32848	0.05865	0	0	0	0	0	0	0	0.000
389	Si	0.18499	0.59316	0.00000	0	0	0	0	0	0	0	0.000
390	Si	0.09042	0.68715	0.00000	0	0	0	0	0	0	0	0.000
391	O	0.24663	0.61367	0.00000	0	0	0	0	0	0	0	0.000
392	O	0.14591	0.64459	0.00000	0	0	0	0	0	0	0	0.000
393	O	0.17152	0.55865	0.94621	0	0	0	0	0	0	0	0.000
394	Si	0.18499	0.40684	0.00000	0	0	0	0	0	0	0	0.000
395	Si	0.09042	0.31285	0.00000	0	0	0	0	0	0	0	0.000
396	O	0.24663	0.38633	0.00000	0	0	0	0	0	0	0	0.000
397	O	0.14591	0.35541	0.00000	0	0	0	0	0	0	0	0.000
398	O	0.17152	0.44135	0.05379	0	0	0	0	0	0	0	0.000

399	Si	0.81501	0.59316	0.00000	0	0	0	0	0	0	0	0.000
400	Si	0.90958	0.68715	0.00000	0	0	0	0	0	0	0	0.000
401	O	0.75337	0.61367	0.00000	0	0	0	0	0	0	0	0.000
402	O	0.85409	0.64459	0.00000	0	0	0	0	0	0	0	0.000
403	O	0.82848	0.55865	0.05379	0	0	0	0	0	0	0	0.000
404	Si	0.81501	0.40684	0.00000	0	0	0	0	0	0	0	0.000
405	Si	0.90958	0.31285	0.00000	0	0	0	0	0	0	0	0.000
406	O	0.75337	0.38633	0.00000	0	0	0	0	0	0	0	0.000
407	O	0.85409	0.35541	0.00000	0	0	0	0	0	0	0	0.000
408	O	0.82848	0.44135	0.94621	0	0	0	0	0	0	0	0.000
409	O	0.44621	0.94135	0.32848	0	0	0	0	0	0	0	0.000
410	O	0.55379	0.05865	0.32848	0	0	0	0	0	0	0	0.000
411	O	0.55379	0.94135	0.67152	0	0	0	0	0	0	0	0.000
412	O	0.44621	0.05865	0.67152	0	0	0	0	0	0	0	0.000
413	O	0.32848	0.94621	0.44135	0	0	0	0	0	0	0	0.000
414	O	0.32848	0.05379	0.55865	0	0	0	0	0	0	0	0.000
415	O	0.67152	0.05379	0.44135	0	0	0	0	0	0	0	0.000
416	O	0.67152	0.94621	0.55865	0	0	0	0	0	0	0	0.000
417	O	0.44135	0.82848	0.44621	0	0	0	0	0	0	0	0.000
418	O	0.55865	0.82848	0.55379	0	0	0	0	0	0	0	0.000
419	O	0.44135	0.17152	0.55379	0	0	0	0	0	0	0	0.000
420	O	0.55865	0.17152	0.44621	0	0	0	0	0	0	0	0.000
421	O	0.94135	0.44621	0.17152	0	0	0	0	0	0	0	0.000
422	O	0.05865	0.55379	0.17152	0	0	0	0	0	0	0	0.000
423	O	0.94135	0.55379	0.82848	0	0	0	0	0	0	0	0.000
424	O	0.05865	0.44621	0.82848	0	0	0	0	0	0	0	0.000
425	O	0.94621	0.32848	0.05865	0	0	0	0	0	0	0	0.000
426	O	0.05379	0.32848	0.94135	0	0	0	0	0	0	0	0.000
427	O	0.05379	0.67152	0.05865	0	0	0	0	0	0	0	0.000
428	O	0.94621	0.67152	0.94135	0	0	0	0	0	0	0	0.000
429	O	0.82848	0.44135	0.05379	0	0	0	0	0	0	0	0.000
430	O	0.82848	0.55865	0.94621	0	0	0	0	0	0	0	0.000
431	O	0.17152	0.44135	0.94621	0	0	0	0	0	0	0	0.000
432	O	0.17152	0.55865	0.05379	0	0	0	0	0	0	0	0.000
433	Si	0.50000	0.59316	0.18499	0	0	0	0	0	0	0	0.000
434	Si	0.50000	0.68715	0.09042	0	0	0	0	0	0	0	0.000
435	O	0.50000	0.61367	0.24663	0	0	0	0	0	0	0	0.000
436	O	0.50000	0.64459	0.14591	0	0	0	0	0	0	0	0.000
437	O	0.55379	0.55865	0.17152	0	0	0	0	0	0	0	0.000
438	Si	0.50000	0.40684	0.18499	0	0	0	0	0	0	0	0.000
439	Si	0.50000	0.31285	0.09042	0	0	0	0	0	0	0	0.000
440	O	0.50000	0.38633	0.24663	0	0	0	0	0	0	0	0.000
441	O	0.50000	0.35541	0.14591	0	0	0	0	0	0	0	0.000
442	O	0.44621	0.44135	0.17152	0	0	0	0	0	0	0	0.000
443	Si	0.50000	0.59316	0.81501	0	0	0	0	0	0	0	0.000
444	Si	0.50000	0.68715	0.90958	0	0	0	0	0	0	0	0.000
445	O	0.50000	0.61367	0.75337	0	0	0	0	0	0	0	0.000

446	O	0.50000	0.64459	0.85409	0	0	0	0	0	0	0	0.000
447	O	0.44621	0.55865	0.82848	0	0	0	0	0	0	0	0.000
448	Si	0.50000	0.40684	0.81501	0	0	0	0	0	0	0	0.000
449	Si	0.50000	0.31285	0.90958	0	0	0	0	0	0	0	0.000
450	O	0.50000	0.38633	0.75337	0	0	0	0	0	0	0	0.000
451	O	0.50000	0.35541	0.85409	0	0	0	0	0	0	0	0.000
452	O	0.55379	0.44135	0.82848	0	0	0	0	0	0	0	0.000
453	Si	0.68499	0.50000	0.09316	0	0	0	0	0	0	0	0.000
454	Si	0.59042	0.50000	0.18715	0	0	0	0	0	0	0	0.000
455	O	0.74663	0.50000	0.11367	0	0	0	0	0	0	0	0.000
456	O	0.64591	0.50000	0.14459	0	0	0	0	0	0	0	0.000
457	O	0.67152	0.55379	0.05865	0	0	0	0	0	0	0	0.000
458	Si	0.68499	0.50000	0.90684	0	0	0	0	0	0	0	0.000
459	Si	0.59042	0.50000	0.81285	0	0	0	0	0	0	0	0.000
460	O	0.74663	0.50000	0.88633	0	0	0	0	0	0	0	0.000
461	O	0.64591	0.50000	0.85541	0	0	0	0	0	0	0	0.000
462	O	0.67152	0.44621	0.94135	0	0	0	0	0	0	0	0.000
463	Si	0.31501	0.50000	0.09316	0	0	0	0	0	0	0	0.000
464	Si	0.40958	0.50000	0.18715	0	0	0	0	0	0	0	0.000
465	O	0.25337	0.50000	0.11367	0	0	0	0	0	0	0	0.000
466	O	0.35409	0.50000	0.14459	0	0	0	0	0	0	0	0.000
467	O	0.32848	0.44621	0.05865	0	0	0	0	0	0	0	0.000
468	Si	0.31501	0.50000	0.90684	0	0	0	0	0	0	0	0.000
469	Si	0.40958	0.50000	0.81285	0	0	0	0	0	0	0	0.000
470	O	0.25337	0.50000	0.88633	0	0	0	0	0	0	0	0.000
471	O	0.35409	0.50000	0.85541	0	0	0	0	0	0	0	0.000
472	O	0.32848	0.55379	0.94135	0	0	0	0	0	0	0	0.000
473	Si	0.59316	0.68499	0.00000	0	0	0	0	0	0	0	0.000
474	Si	0.68715	0.59042	0.00000	0	0	0	0	0	0	0	0.000
475	O	0.61367	0.74663	0.00000	0	0	0	0	0	0	0	0.000
476	O	0.64459	0.64591	0.00000	0	0	0	0	0	0	0	0.000
477	O	0.55865	0.67152	0.05379	0	0	0	0	0	0	0	0.000
478	Si	0.40684	0.68499	0.00000	0	0	0	0	0	0	0	0.000
479	Si	0.31285	0.59042	0.00000	0	0	0	0	0	0	0	0.000
480	O	0.38633	0.74663	0.00000	0	0	0	0	0	0	0	0.000
481	O	0.35541	0.64591	0.00000	0	0	0	0	0	0	0	0.000
482	O	0.44135	0.67152	0.94621	0	0	0	0	0	0	0	0.000
483	Si	0.59316	0.31501	0.00000	0	0	0	0	0	0	0	0.000
484	Si	0.68715	0.40958	0.00000	0	0	0	0	0	0	0	0.000
485	O	0.61367	0.25337	0.00000	0	0	0	0	0	0	0	0.000
486	O	0.64459	0.35409	0.00000	0	0	0	0	0	0	0	0.000
487	O	0.55865	0.32848	0.94621	0	0	0	0	0	0	0	0.000
488	Si	0.40684	0.31501	0.00000	0	0	0	0	0	0	0	0.000
489	Si	0.31285	0.40958	0.00000	0	0	0	0	0	0	0	0.000
490	O	0.38633	0.25337	0.00000	0	0	0	0	0	0	0	0.000
491	O	0.35541	0.35409	0.00000	0	0	0	0	0	0	0	0.000
492	O	0.44135	0.32848	0.05379	0	0	0	0	0	0	0	0.000

493	Si	0.09316	0.00000	0.31501	0	0	0	0	0	0	0	0.000
494	Si	0.18715	0.00000	0.40958	0	0	0	0	0	0	0	0.000
495	O	0.11367	0.00000	0.25337	0	0	0	0	0	0	0	0.000
496	O	0.14459	0.00000	0.35409	0	0	0	0	0	0	0	0.000
497	O	0.05865	0.05379	0.32848	0	0	0	0	0	0	0	0.000
498	Si	0.90684	0.00000	0.31501	0	0	0	0	0	0	0	0.000
499	Si	0.81285	0.00000	0.40958	0	0	0	0	0	0	0	0.000
500	O	0.88633	0.00000	0.25337	0	0	0	0	0	0	0	0.000
501	O	0.85541	0.00000	0.35409	0	0	0	0	0	0	0	0.000
502	O	0.94135	0.94621	0.32848	0	0	0	0	0	0	0	0.000
503	Si	0.09316	0.00000	0.68499	0	0	0	0	0	0	0	0.000
504	Si	0.18715	0.00000	0.59042	0	0	0	0	0	0	0	0.000
505	O	0.11367	0.00000	0.74663	0	0	0	0	0	0	0	0.000
506	O	0.14459	0.00000	0.64591	0	0	0	0	0	0	0	0.000
507	O	0.05865	0.94621	0.67152	0	0	0	0	0	0	0	0.000
508	Si	0.90684	0.00000	0.68499	0	0	0	0	0	0	0	0.000
509	Si	0.81285	0.00000	0.59042	0	0	0	0	0	0	0	0.000
510	O	0.88633	0.00000	0.74663	0	0	0	0	0	0	0	0.000
511	O	0.85541	0.00000	0.64591	0	0	0	0	0	0	0	0.000
512	O	0.94135	0.05379	0.67152	0	0	0	0	0	0	0	0.000
513	Si	0.00000	0.18499	0.40684	0	0	0	0	0	0	0	0.000
514	Si	0.00000	0.09042	0.31285	0	0	0	0	0	0	0	0.000
515	O	0.00000	0.24663	0.38633	0	0	0	0	0	0	0	0.000
516	O	0.00000	0.14591	0.35541	0	0	0	0	0	0	0	0.000
517	O	0.05379	0.17152	0.44135	0	0	0	0	0	0	0	0.000
518	Si	0.00000	0.18499	0.59316	0	0	0	0	0	0	0	0.000
519	Si	0.00000	0.09042	0.68715	0	0	0	0	0	0	0	0.000
520	O	0.00000	0.24663	0.61367	0	0	0	0	0	0	0	0.000
521	O	0.00000	0.14591	0.64459	0	0	0	0	0	0	0	0.000
522	O	0.94621	0.17152	0.55865	0	0	0	0	0	0	0	0.000
523	Si	0.00000	0.81501	0.40684	0	0	0	0	0	0	0	0.000
524	Si	0.00000	0.90958	0.31285	0	0	0	0	0	0	0	0.000
525	O	0.00000	0.75337	0.38633	0	0	0	0	0	0	0	0.000
526	O	0.00000	0.85409	0.35541	0	0	0	0	0	0	0	0.000
527	O	0.94621	0.82848	0.44135	0	0	0	0	0	0	0	0.000
528	Si	0.00000	0.81501	0.59316	0	0	0	0	0	0	0	0.000
529	Si	0.00000	0.90958	0.68715	0	0	0	0	0	0	0	0.000
530	O	0.00000	0.75337	0.61367	0	0	0	0	0	0	0	0.000
531	O	0.00000	0.85409	0.64459	0	0	0	0	0	0	0	0.000
532	O	0.05379	0.82848	0.55865	0	0	0	0	0	0	0	0.000
533	Si	0.18499	0.09316	0.50000	0	0	0	0	0	0	0	0.000
534	Si	0.09042	0.18715	0.50000	0	0	0	0	0	0	0	0.000
535	O	0.24663	0.11367	0.50000	0	0	0	0	0	0	0	0.000
536	O	0.14591	0.14459	0.50000	0	0	0	0	0	0	0	0.000
537	O	0.17152	0.05865	0.44621	0	0	0	0	0	0	0	0.000
538	Si	0.18499	0.90684	0.50000	0	0	0	0	0	0	0	0.000
539	Si	0.09042	0.81285	0.50000	0	0	0	0	0	0	0	0.000

540	O	0.24663	0.88633	0.50000	0	0	0	0	0	0	0	0.000
541	O	0.14591	0.85541	0.50000	0	0	0	0	0	0	0	0.000
542	O	0.17152	0.94135	0.55379	0	0	0	0	0	0	0	0.000
543	Si	0.81501	0.09316	0.50000	0	0	0	0	0	0	0	0.000
544	Si	0.90958	0.18715	0.50000	0	0	0	0	0	0	0	0.000
545	O	0.75337	0.11367	0.50000	0	0	0	0	0	0	0	0.000
546	O	0.85409	0.14459	0.50000	0	0	0	0	0	0	0	0.000
547	O	0.82848	0.05865	0.55379	0	0	0	0	0	0	0	0.000
548	Si	0.81501	0.90684	0.50000	0	0	0	0	0	0	0	0.000
549	Si	0.90958	0.81285	0.50000	0	0	0	0	0	0	0	0.000
550	O	0.75337	0.88633	0.50000	0	0	0	0	0	0	0	0.000
551	O	0.85409	0.85541	0.50000	0	0	0	0	0	0	0	0.000
552	O	0.82848	0.94135	0.44621	0	0	0	0	0	0	0	0.000
553	O	0.44621	0.44135	0.82848	0	0	0	0	0	0	0	0.000
554	O	0.55379	0.55865	0.82848	0	0	0	0	0	0	0	0.000
555	O	0.55379	0.44135	0.17152	0	0	0	0	0	0	0	0.000
556	O	0.44621	0.55865	0.17152	0	0	0	0	0	0	0	0.000
557	O	0.32848	0.44621	0.94135	0	0	0	0	0	0	0	0.000
558	O	0.32848	0.55379	0.05865	0	0	0	0	0	0	0	0.000
559	O	0.67152	0.55379	0.94135	0	0	0	0	0	0	0	0.000
560	O	0.67152	0.44621	0.05865	0	0	0	0	0	0	0	0.000
561	O	0.44135	0.32848	0.94621	0	0	0	0	0	0	0	0.000
562	O	0.55865	0.32848	0.05379	0	0	0	0	0	0	0	0.000
563	O	0.44135	0.67152	0.05379	0	0	0	0	0	0	0	0.000
564	O	0.55865	0.67152	0.94621	0	0	0	0	0	0	0	0.000
565	O	0.94135	0.94621	0.67152	0	0	0	0	0	0	0	0.000
566	O	0.05865	0.05379	0.67152	0	0	0	0	0	0	0	0.000
567	O	0.94135	0.05379	0.32848	0	0	0	0	0	0	0	0.000
568	O	0.05865	0.94621	0.32848	0	0	0	0	0	0	0	0.000
569	O	0.94621	0.82848	0.55865	0	0	0	0	0	0	0	0.000
570	O	0.05379	0.82848	0.44135	0	0	0	0	0	0	0	0.000
571	O	0.05379	0.17152	0.55865	0	0	0	0	0	0	0	0.000
572	O	0.94621	0.17152	0.44135	0	0	0	0	0	0	0	0.000
573	O	0.82848	0.94135	0.55379	0	0	0	0	0	0	0	0.000
574	O	0.82848	0.05865	0.44621	0	0	0	0	0	0	0	0.000
575	O	0.17152	0.94135	0.44621	0	0	0	0	0	0	0	0.000
576	O	0.17152	0.05865	0.55379	0	0	0	0	0	0	0	0.000

3.4. SAS – IZA [10]

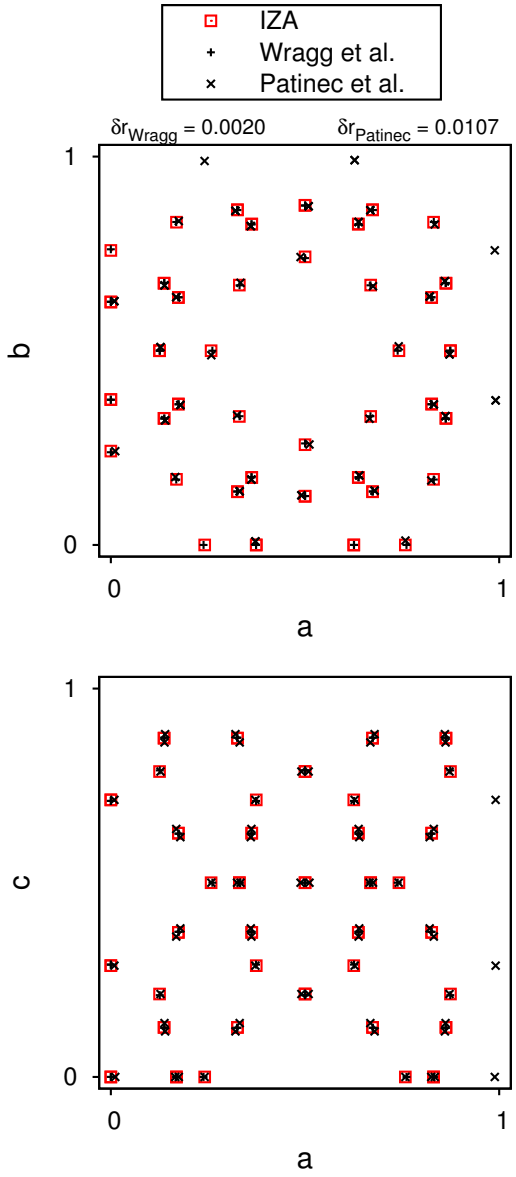

Figure 5. Plot of the fractional coordinates of the oxygen atoms of the three different SAS materials studied; top: a vs. b; bottom: a vs. c.

```
                                        14.349   14.349   10.398
                          90.000  90.000  90.000    SPGR =  1 P 1         OPT = 1
 96   0
    0 SAS          : SAS
 1  0      0.24180  0.00000  0.00000       0 0 0 0 0 0 0 0 0.00
 2  0      0.00000  0.24180  0.00000       0 0 0 0 0 0 0 0 0.00
 3  0      0.00000  0.75820  0.00000       0 0 0 0 0 0 0 0 0.00
 4  0      0.75820  0.00000  0.00000       0 0 0 0 0 0 0 0 0.00
 5  0      0.74180  0.50000  0.50000       0 0 0 0 0 0 0 0 0.00
 6  0      0.50000  0.74180  0.50000       0 0 0 0 0 0 0 0 0.00
 7  0      0.50000  0.25820  0.50000       0 0 0 0 0 0 0 0 0.00
 8  0      0.25820  0.50000  0.50000       0 0 0 0 0 0 0 0 0.00
 9  0      0.16900  0.16900  0.00000       0 0 0 0 0 0 0 0 0.00
10  0      0.83100  0.16900  0.00000       0 0 0 0 0 0 0 0 0.00
11  0      0.16900  0.83100  0.00000       0 0 0 0 0 0 0 0 0.00
12  0      0.83100  0.83100  0.00000       0 0 0 0 0 0 0 0 0.00
13  0      0.66900  0.66900  0.50000       0 0 0 0 0 0 0 0 0.00
14  0      0.33100  0.66900  0.50000       0 0 0 0 0 0 0 0 0.00
15  0      0.66900  0.33100  0.50000       0 0 0 0 0 0 0 0 0.00
16  0      0.33100  0.33100  0.50000       0 0 0 0 0 0 0 0 0.00
17  0      0.50000  0.87450  0.78650       0 0 0 0 0 0 0 0 0.00
18  0      0.12550  0.50000  0.78650       0 0 0 0 0 0 0 0 0.00
19  0      0.87450  0.50000  0.78650       0 0 0 0 0 0 0 0 0.00
20  0      0.50000  0.12550  0.21350       0 0 0 0 0 0 0 0 0.00
21  0      0.50000  0.87450  0.21350       0 0 0 0 0 0 0 0 0.00
22  0      0.50000  0.12550  0.78650       0 0 0 0 0 0 0 0 0.00
23  0      0.87450  0.50000  0.21350       0 0 0 0 0 0 0 0 0.00
24  0      0.12550  0.50000  0.21350       0 0 0 0 0 0 0 0 0.00
25  0      0.00000  0.37450  0.28650       0 0 0 0 0 0 0 0 0.00
26  0      0.62550  0.00000  0.28650       0 0 0 0 0 0 0 0 0.00
27  0      0.37450  0.00000  0.28650       0 0 0 0 0 0 0 0 0.00
28  0      0.00000  0.62550  0.71350       0 0 0 0 0 0 0 0 0.00
29  0      0.00000  0.37450  0.71350       0 0 0 0 0 0 0 0 0.00
30  0      0.00000  0.62550  0.28650       0 0 0 0 0 0 0 0 0.00
31  0      0.37450  0.00000  0.71350       0 0 0 0 0 0 0 0 0.00
32  0      0.62550  0.00000  0.71350       0 0 0 0 0 0 0 0 0.00
33  0      0.32610  0.86290  0.87230       0 0 0 0 0 0 0 0 0.00
34  0      0.13710  0.32610  0.87230       0 0 0 0 0 0 0 0 0.00
35  0      0.86290  0.67390  0.87230       0 0 0 0 0 0 0 0 0.00
36  0      0.32610  0.13710  0.12770       0 0 0 0 0 0 0 0 0.00
37  0      0.67390  0.86290  0.12770       0 0 0 0 0 0 0 0 0.00
38  0      0.67390  0.13710  0.87230       0 0 0 0 0 0 0 0 0.00
39  0      0.86290  0.32610  0.12770       0 0 0 0 0 0 0 0 0.00
40  0      0.13710  0.67390  0.12770       0 0 0 0 0 0 0 0 0.00
41  0      0.67390  0.13710  0.12770       0 0 0 0 0 0 0 0 0.00
42  0      0.86290  0.67390  0.12770       0 0 0 0 0 0 0 0 0.00
43  0      0.13710  0.32610  0.12770       0 0 0 0 0 0 0 0 0.00
```

```
44  O     0.67390  0.86290  0.87230      0 0 0 0 0 0 0 0 0.00
45  O     0.32610  0.13710  0.87230      0 0 0 0 0 0 0 0 0.00
46  O     0.32610  0.86290  0.12770      0 0 0 0 0 0 0 0 0.00
47  O     0.13710  0.67390  0.87230      0 0 0 0 0 0 0 0 0.00
48  O     0.86290  0.32610  0.87230      0 0 0 0 0 0 0 0 0.00
49  O     0.82610  0.36290  0.37230      0 0 0 0 0 0 0 0 0.00
50  O     0.63710  0.82610  0.37230      0 0 0 0 0 0 0 0 0.00
51  O     0.36290  0.17390  0.37230      0 0 0 0 0 0 0 0 0.00
52  O     0.82610  0.63710  0.62770      0 0 0 0 0 0 0 0 0.00
53  O     0.17390  0.36290  0.62770      0 0 0 0 0 0 0 0 0.00
54  O     0.17390  0.63710  0.37230      0 0 0 0 0 0 0 0 0.00
55  O     0.36290  0.82610  0.62770      0 0 0 0 0 0 0 0 0.00
56  O     0.63710  0.17390  0.62770      0 0 0 0 0 0 0 0 0.00
57  O     0.17390  0.63710  0.62770      0 0 0 0 0 0 0 0 0.00
58  O     0.36290  0.17390  0.62770      0 0 0 0 0 0 0 0 0.00
59  O     0.63710  0.82610  0.62770      0 0 0 0 0 0 0 0 0.00
60  O     0.17390  0.36290  0.37230      0 0 0 0 0 0 0 0 0.00
61  O     0.82610  0.63710  0.37230      0 0 0 0 0 0 0 0 0.00
62  O     0.82610  0.36290  0.62770      0 0 0 0 0 0 0 0 0.00
63  O     0.63710  0.17390  0.37230      0 0 0 0 0 0 0 0 0.00
64  O     0.36290  0.82610  0.37230      0 0 0 0 0 0 0 0 0.00
65  Si    0.26620  0.88930  0.00000      0 0 0 0 0 0 0 0 0.00
66  Si    0.11070  0.26620  0.00000      0 0 0 0 0 0 0 0 0.00
67  Si    0.88930  0.73380  0.00000      0 0 0 0 0 0 0 0 0.00
68  Si    0.26620  0.11070  0.00000      0 0 0 0 0 0 0 0 0.00
69  Si    0.73380  0.88930  0.00000      0 0 0 0 0 0 0 0 0.00
70  Si    0.73380  0.11070  0.00000      0 0 0 0 0 0 0 0 0.00
71  Si    0.88930  0.26620  0.00000      0 0 0 0 0 0 0 0 0.00
72  Si    0.11070  0.73380  0.00000      0 0 0 0 0 0 0 0 0.00
73  Si    0.76620  0.38930  0.50000      0 0 0 0 0 0 0 0 0.00
74  Si    0.61070  0.76620  0.50000      0 0 0 0 0 0 0 0 0.00
75  Si    0.38930  0.23380  0.50000      0 0 0 0 0 0 0 0 0.00
76  Si    0.76620  0.61070  0.50000      0 0 0 0 0 0 0 0 0.00
77  Si    0.23380  0.38930  0.50000      0 0 0 0 0 0 0 0 0.00
78  Si    0.23380  0.61070  0.50000      0 0 0 0 0 0 0 0 0.00
79  Si    0.38930  0.76620  0.50000      0 0 0 0 0 0 0 0 0.00
80  Si    0.61070  0.23380  0.50000      0 0 0 0 0 0 0 0 0.00
81  Si    0.60900  0.89100  0.75000      0 0 0 0 0 0 0 0 0.00
82  Si    0.10900  0.60900  0.75000      0 0 0 0 0 0 0 0 0.00
83  Si    0.89100  0.39100  0.75000      0 0 0 0 0 0 0 0 0.00
84  Si    0.60900  0.10900  0.25000      0 0 0 0 0 0 0 0 0.00
85  Si    0.39100  0.89100  0.25000      0 0 0 0 0 0 0 0 0.00
86  Si    0.39100  0.10900  0.75000      0 0 0 0 0 0 0 0 0.00
87  Si    0.89100  0.60900  0.25000      0 0 0 0 0 0 0 0 0.00
88  Si    0.10900  0.39100  0.25000      0 0 0 0 0 0 0 0 0.00
89  Si    0.39100  0.10900  0.25000      0 0 0 0 0 0 0 0 0.00
90  Si    0.89100  0.39100  0.25000      0 0 0 0 0 0 0 0 0.00
```

```
91  Si    0.10900  0.60900  0.25000      0 0 0 0 0 0 0 0 0.00
92  Si    0.39100  0.89100  0.75000      0 0 0 0 0 0 0 0 0.00
93  Si    0.60900  0.10900  0.75000      0 0 0 0 0 0 0 0 0.00
94  Si    0.60900  0.89100  0.25000      0 0 0 0 0 0 0 0 0.00
95  Si    0.10900  0.39100  0.75000      0 0 0 0 0 0 0 0 0.00
96  Si    0.89100  0.60900  0.75000      0 0 0 0 0 0 0 0 0.00
```

3.5. SAS – Wragg *et al.* [7]

```
                                      14.1039   14.1039   10.1875
                     90.000  90.000  90.000    SPGR =  1 P 1         OPT = 1
 96   0
    0 SAS         : SAS
 1  O     0.23860  0.00000  0.00000      0 0 0 0 0 0 0 0 0.00
 2  O     0.00000  0.23860  0.00000      0 0 0 0 0 0 0 0 0.00
 3  O     0.00000  0.76140  0.00000      0 0 0 0 0 0 0 0 0.00
 4  O     0.76140  0.00000  0.00000      0 0 0 0 0 0 0 0 0.00
 5  O     0.73860  0.50000  0.50000      0 0 0 0 0 0 0 0 0.00
 6  O     0.50000  0.73860  0.50000      0 0 0 0 0 0 0 0 0.00
 7  O     0.50000  0.26140  0.50000      0 0 0 0 0 0 0 0 0.00
 8  O     0.26140  0.50000  0.50000      0 0 0 0 0 0 0 0 0.00
 9  O     0.32550  0.86230  0.87350      0 0 0 0 0 0 0 0 0.00
10  O     0.13770  0.32550  0.87350      0 0 0 0 0 0 0 0 0.00
11  O     0.86230  0.67450  0.87350      0 0 0 0 0 0 0 0 0.00
12  O     0.32550  0.13770  0.12650      0 0 0 0 0 0 0 0 0.00
13  O     0.67450  0.86230  0.12650      0 0 0 0 0 0 0 0 0.00
14  O     0.67450  0.13770  0.87350      0 0 0 0 0 0 0 0 0.00
15  O     0.86230  0.32550  0.12650      0 0 0 0 0 0 0 0 0.00
16  O     0.13770  0.67450  0.12650      0 0 0 0 0 0 0 0 0.00
17  O     0.67450  0.13770  0.12650      0 0 0 0 0 0 0 0 0.00
18  O     0.86230  0.67450  0.12650      0 0 0 0 0 0 0 0 0.00
19  O     0.13770  0.32550  0.12650      0 0 0 0 0 0 0 0 0.00
20  O     0.67450  0.86230  0.87350      0 0 0 0 0 0 0 0 0.00
21  O     0.32550  0.13770  0.87350      0 0 0 0 0 0 0 0 0.00
22  O     0.32550  0.86230  0.12650      0 0 0 0 0 0 0 0 0.00
23  O     0.13770  0.67450  0.87350      0 0 0 0 0 0 0 0 0.00
24  O     0.86230  0.32550  0.87350      0 0 0 0 0 0 0 0 0.00
25  O     0.82550  0.36230  0.37350      0 0 0 0 0 0 0 0 0.00
26  O     0.63770  0.82550  0.37350      0 0 0 0 0 0 0 0 0.00
27  O     0.36230  0.17450  0.37350      0 0 0 0 0 0 0 0 0.00
28  O     0.82550  0.63770  0.62650      0 0 0 0 0 0 0 0 0.00
29  O     0.17450  0.36230  0.62650      0 0 0 0 0 0 0 0 0.00
30  O     0.17450  0.63770  0.37350      0 0 0 0 0 0 0 0 0.00
31  O     0.36230  0.82550  0.62650      0 0 0 0 0 0 0 0 0.00
32  O     0.63770  0.17450  0.62650      0 0 0 0 0 0 0 0 0.00
```

```
33  O     0.17450  0.63770  0.62650     0 0 0 0 0 0 0 0 0.00
34  O     0.36230  0.17450  0.62650     0 0 0 0 0 0 0 0 0.00
35  O     0.63770  0.82550  0.62650     0 0 0 0 0 0 0 0 0.00
36  O     0.17450  0.36230  0.37350     0 0 0 0 0 0 0 0 0.00
37  O     0.82550  0.63770  0.37350     0 0 0 0 0 0 0 0 0.00
38  O     0.82550  0.36230  0.62650     0 0 0 0 0 0 0 0 0.00
39  O     0.63770  0.17450  0.37350     0 0 0 0 0 0 0 0 0.00
40  O     0.36230  0.82550  0.37350     0 0 0 0 0 0 0 0 0.00
41  O     0.50000  0.87390  0.78930     0 0 0 0 0 0 0 0 0.00
42  O     0.12610  0.50000  0.78930     0 0 0 0 0 0 0 0 0.00
43  O     0.87390  0.50000  0.78930     0 0 0 0 0 0 0 0 0.00
44  O     0.50000  0.12610  0.21070     0 0 0 0 0 0 0 0 0.00
45  O     0.50000  0.87390  0.21070     0 0 0 0 0 0 0 0 0.00
46  O     0.50000  0.12610  0.78930     0 0 0 0 0 0 0 0 0.00
47  O     0.87390  0.50000  0.21070     0 0 0 0 0 0 0 0 0.00
48  O     0.12610  0.50000  0.21070     0 0 0 0 0 0 0 0 0.00
49  O     0.00000  0.37390  0.28930     0 0 0 0 0 0 0 0 0.00
50  O     0.62610  0.00000  0.28930     0 0 0 0 0 0 0 0 0.00
51  O     0.37390  0.00000  0.28930     0 0 0 0 0 0 0 0 0.00
52  O     0.00000  0.62610  0.71070     0 0 0 0 0 0 0 0 0.00
53  O     0.00000  0.37390  0.71070     0 0 0 0 0 0 0 0 0.00
54  O     0.00000  0.62610  0.28930     0 0 0 0 0 0 0 0 0.00
55  O     0.37390  0.00000  0.71070     0 0 0 0 0 0 0 0 0.00
56  O     0.62610  0.00000  0.71070     0 0 0 0 0 0 0 0 0.00
57  O     0.16845  0.83155  0.00000     0 0 0 0 0 0 0 0 0.00
58  O     0.16845  0.16845  0.00000     0 0 0 0 0 0 0 0 0.00
59  O     0.83155  0.83155  0.00000     0 0 0 0 0 0 0 0 0.00
60  O     0.83155  0.16845  0.00000     0 0 0 0 0 0 0 0 0.00
61  O     0.66845  0.33155  0.50000     0 0 0 0 0 0 0 0 0.00
62  O     0.66845  0.66845  0.50000     0 0 0 0 0 0 0 0 0.00
63  O     0.33155  0.33155  0.50000     0 0 0 0 0 0 0 0 0.00
64  O     0.33155  0.66845  0.50000     0 0 0 0 0 0 0 0 0.00
65  Si    0.26580  0.10980  0.00000     0 0 0 0 0 0 0 0 0.00
66  Si    0.89020  0.26580  0.00000     0 0 0 0 0 0 0 0 0.00
67  Si    0.10980  0.73420  0.00000     0 0 0 0 0 0 0 0 0.00
68  Si    0.26580  0.89020  0.00000     0 0 0 0 0 0 0 0 0.00
69  Si    0.73420  0.10980  0.00000     0 0 0 0 0 0 0 0 0.00
70  Si    0.73420  0.89020  0.00000     0 0 0 0 0 0 0 0 0.00
71  Si    0.10980  0.26580  0.00000     0 0 0 0 0 0 0 0 0.00
72  Si    0.89020  0.73420  0.00000     0 0 0 0 0 0 0 0 0.00
73  Si    0.76580  0.60980  0.50000     0 0 0 0 0 0 0 0 0.00
74  Si    0.39020  0.76580  0.50000     0 0 0 0 0 0 0 0 0.00
75  Si    0.60980  0.23420  0.50000     0 0 0 0 0 0 0 0 0.00
76  Si    0.76580  0.39020  0.50000     0 0 0 0 0 0 0 0 0.00
77  Si    0.23420  0.60980  0.50000     0 0 0 0 0 0 0 0 0.00
78  Si    0.23420  0.39020  0.50000     0 0 0 0 0 0 0 0 0.00
79  Si    0.60980  0.76580  0.50000     0 0 0 0 0 0 0 0 0.00
```

```
80  Si    0.39020  0.23420  0.50000      0 0 0 0 0 0 0 0 0.00
81  Si    0.60900  0.89100  0.75000      0 0 0 0 0 0 0 0 0.00
82  Si    0.10900  0.60900  0.75000      0 0 0 0 0 0 0 0 0.00
83  Si    0.89100  0.39100  0.75000      0 0 0 0 0 0 0 0 0.00
84  Si    0.60900  0.10900  0.25000      0 0 0 0 0 0 0 0 0.00
85  Si    0.39100  0.89100  0.25000      0 0 0 0 0 0 0 0 0.00
86  Si    0.39100  0.10900  0.75000      0 0 0 0 0 0 0 0 0.00
87  Si    0.89100  0.60900  0.25000      0 0 0 0 0 0 0 0 0.00
88  Si    0.10900  0.39100  0.25000      0 0 0 0 0 0 0 0 0.00
89  Si    0.39100  0.10900  0.25000      0 0 0 0 0 0 0 0 0.00
90  Si    0.89100  0.39100  0.25000      0 0 0 0 0 0 0 0 0.00
91  Si    0.10900  0.60900  0.25000      0 0 0 0 0 0 0 0 0.00
92  Si    0.39100  0.89100  0.75000      0 0 0 0 0 0 0 0 0.00
93  Si    0.60900  0.10900  0.75000      0 0 0 0 0 0 0 0 0.00
94  Si    0.60900  0.89100  0.25000      0 0 0 0 0 0 0 0 0.00
95  Si    0.10900  0.39100  0.75000      0 0 0 0 0 0 0 0 0.00
96  Si    0.89100  0.60900  0.75000      0 0 0 0 0 0 0 0 0.00
```

3.6. SAS – Patinec *et al.* [9]

```
                                    14.322   14.322   10.424
                    90.000  90.000  90.000    SPGR =  1 P 1         OPT = 1
 96   0
    0 SAS          : SAS
 1  Si    0.26890  0.10910  0.00000      0 0 0 0 0 0 0 0 0.00
 2  Si    0.89090  0.26890  0.00000      0 0 0 0 0 0 0 0 0.00
 3  Si    0.10910  0.73110  0.00000      0 0 0 0 0 0 0 0 0.00
 4  Si    0.76890  0.39090  0.50000      0 0 0 0 0 0 0 0 0.00
 5  Si    0.23110  0.60910  0.50000      0 0 0 0 0 0 0 0 0.00
 6  Si    0.73110  0.89090  0.00000      0 0 0 0 0 0 0 0 0.00
 7  Si    0.60910  0.76890  0.50000      0 0 0 0 0 0 0 0 0.00
 8  Si    0.39090  0.23110  0.50000      0 0 0 0 0 0 0 0 0.00
 9  Si    0.39070  0.89070  0.75000      0 0 0 0 0 0 0 0 0.00
10  Si    0.10930  0.39070  0.75000      0 0 0 0 0 0 0 0 0.00
11  Si    0.89070  0.60930  0.75000      0 0 0 0 0 0 0 0 0.00
12  Si    0.60930  0.10930  0.75000      0 0 0 0 0 0 0 0 0.00
13  Si    0.60930  0.10930  0.25000      0 0 0 0 0 0 0 0 0.00
14  Si    0.89070  0.60930  0.25000      0 0 0 0 0 0 0 0 0.00
15  Si    0.10930  0.39070  0.25000      0 0 0 0 0 0 0 0 0.00
16  Si    0.39070  0.89070  0.25000      0 0 0 0 0 0 0 0 0.00
17  Si    0.61010  0.88990  0.75000      0 0 0 0 0 0 0 0 0.00
18  Si    0.11010  0.61010  0.75000      0 0 0 0 0 0 0 0 0.00
19  Si    0.88990  0.38990  0.75000      0 0 0 0 0 0 0 0 0.00
20  Si    0.38990  0.11010  0.75000      0 0 0 0 0 0 0 0 0.00
21  Si    0.38990  0.11010  0.25000      0 0 0 0 0 0 0 0 0.00
```

```
22  Si    0.88990  0.38990  0.25000      0 0 0 0 0 0 0 0 0.00
23  Si    0.11010  0.61010  0.25000      0 0 0 0 0 0 0 0 0.00
24  Si    0.61010  0.88990  0.25000      0 0 0 0 0 0 0 0 0.00
25  Si    0.26660  0.88630  0.00000      0 0 0 0 0 0 0 0 0.00
26  Si    0.11370  0.26660  0.00000      0 0 0 0 0 0 0 0 0.00
27  Si    0.88630  0.73340  0.00000      0 0 0 0 0 0 0 0 0.00
28  Si    0.76660  0.61370  0.50000      0 0 0 0 0 0 0 0 0.00
29  Si    0.23340  0.38630  0.50000      0 0 0 0 0 0 0 0 0.00
30  Si    0.73340  0.11370  0.00000      0 0 0 0 0 0 0 0 0.00
31  Si    0.38630  0.76660  0.50000      0 0 0 0 0 0 0 0 0.00
32  Si    0.61370  0.23340  0.50000      0 0 0 0 0 0 0 0 0.00
33  O     0.24140  0.98860  0.00000      0 0 0 0 0 0 0 0 0.00
34  O     0.01140  0.24140  0.00000      0 0 0 0 0 0 0 0 0.00
35  O     0.98860  0.75860  0.00000      0 0 0 0 0 0 0 0 0.00
36  O     0.74140  0.51140  0.50000      0 0 0 0 0 0 0 0 0.00
37  O     0.25860  0.48860  0.50000      0 0 0 0 0 0 0 0 0.00
38  O     0.75860  0.01140  0.00000      0 0 0 0 0 0 0 0 0.00
39  O     0.48860  0.74140  0.50000      0 0 0 0 0 0 0 0 0.00
40  O     0.51140  0.25860  0.50000      0 0 0 0 0 0 0 0 0.00
41  O     0.32090  0.86030  0.88260      0 0 0 0 0 0 0 0 0.00
42  O     0.13970  0.32090  0.88260      0 0 0 0 0 0 0 0 0.00
43  O     0.86030  0.67910  0.88260      0 0 0 0 0 0 0 0 0.00
44  O     0.82090  0.63970  0.61740      0 0 0 0 0 0 0 0 0.00
45  O     0.17910  0.36030  0.61740      0 0 0 0 0 0 0 0 0.00
46  O     0.67910  0.13970  0.88260      0 0 0 0 0 0 0 0 0.00
47  O     0.36030  0.82090  0.61740      0 0 0 0 0 0 0 0 0.00
48  O     0.63970  0.17910  0.61740      0 0 0 0 0 0 0 0 0.00
49  O     0.67910  0.13970  0.11740      0 0 0 0 0 0 0 0 0.00
50  O     0.86030  0.67910  0.11740      0 0 0 0 0 0 0 0 0.00
51  O     0.13970  0.32090  0.11740      0 0 0 0 0 0 0 0 0.00
52  O     0.17910  0.36030  0.38260      0 0 0 0 0 0 0 0 0.00
53  O     0.82090  0.63970  0.38260      0 0 0 0 0 0 0 0 0.00
54  O     0.32090  0.86030  0.11740      0 0 0 0 0 0 0 0 0.00
55  O     0.63970  0.17910  0.38260      0 0 0 0 0 0 0 0 0.00
56  O     0.36030  0.82090  0.38260      0 0 0 0 0 0 0 0 0.00
57  O     0.50930  0.87220  0.78650      0 0 0 0 0 0 0 0 0.00
58  O     0.12780  0.50930  0.78650      0 0 0 0 0 0 0 0 0.00
59  O     0.87220  0.49070  0.78650      0 0 0 0 0 0 0 0 0.00
60  O     0.00930  0.62780  0.71350      0 0 0 0 0 0 0 0 0.00
61  O     0.99070  0.37220  0.71350      0 0 0 0 0 0 0 0 0.00
62  O     0.49070  0.12780  0.78650      0 0 0 0 0 0 0 0 0.00
63  O     0.37220  0.00930  0.71350      0 0 0 0 0 0 0 0 0.00
64  O     0.62780  0.99070  0.71350      0 0 0 0 0 0 0 0 0.00
65  O     0.49070  0.12780  0.21350      0 0 0 0 0 0 0 0 0.00
66  O     0.87220  0.49070  0.21350      0 0 0 0 0 0 0 0 0.00
67  O     0.12780  0.50930  0.21350      0 0 0 0 0 0 0 0 0.00
68  O     0.99070  0.37220  0.28650      0 0 0 0 0 0 0 0 0.00
```

```
69  0     0.00930  0.62780  0.28650     0 0 0 0 0 0 0 0 0.00
70  0     0.50930  0.87220  0.21350     0 0 0 0 0 0 0 0 0.00
71  0     0.62780  0.99070  0.28650     0 0 0 0 0 0 0 0 0.00
72  0     0.37220  0.00930  0.28650     0 0 0 0 0 0 0 0 0.00
73  0     0.17500  0.83390  0.00000     0 0 0 0 0 0 0 0 0.00
74  0     0.16610  0.17500  0.00000     0 0 0 0 0 0 0 0 0.00
75  0     0.83390  0.82500  0.00000     0 0 0 0 0 0 0 0 0.00
76  0     0.67500  0.66610  0.50000     0 0 0 0 0 0 0 0 0.00
77  0     0.32500  0.33390  0.50000     0 0 0 0 0 0 0 0 0.00
78  0     0.82500  0.16610  0.00000     0 0 0 0 0 0 0 0 0.00
79  0     0.33390  0.67500  0.50000     0 0 0 0 0 0 0 0 0.00
80  0     0.66610  0.32500  0.50000     0 0 0 0 0 0 0 0 0.00
81  0     0.66830  0.86190  0.86140     0 0 0 0 0 0 0 0 0.00
82  0     0.13810  0.66830  0.86140     0 0 0 0 0 0 0 0 0.00
83  0     0.86190  0.33170  0.86140     0 0 0 0 0 0 0 0 0.00
84  0     0.16830  0.63810  0.63860     0 0 0 0 0 0 0 0 0.00
85  0     0.83170  0.36190  0.63860     0 0 0 0 0 0 0 0 0.00
86  0     0.33170  0.13810  0.86140     0 0 0 0 0 0 0 0 0.00
87  0     0.36190  0.16830  0.63860     0 0 0 0 0 0 0 0 0.00
88  0     0.63810  0.83170  0.63860     0 0 0 0 0 0 0 0 0.00
89  0     0.33170  0.13810  0.13860     0 0 0 0 0 0 0 0 0.00
90  0     0.86190  0.33170  0.13860     0 0 0 0 0 0 0 0 0.00
91  0     0.13810  0.66830  0.13860     0 0 0 0 0 0 0 0 0.00
92  0     0.83170  0.36190  0.36140     0 0 0 0 0 0 0 0 0.00
93  0     0.16830  0.63810  0.36140     0 0 0 0 0 0 0 0 0.00
94  0     0.66830  0.86190  0.13860     0 0 0 0 0 0 0 0 0.00
95  0     0.63810  0.83170  0.36140     0 0 0 0 0 0 0 0 0.00
96  0     0.36190  0.16830  0.36140     0 0 0 0 0 0 0 0 0.00
```

3.7. ITE – IZA [10]

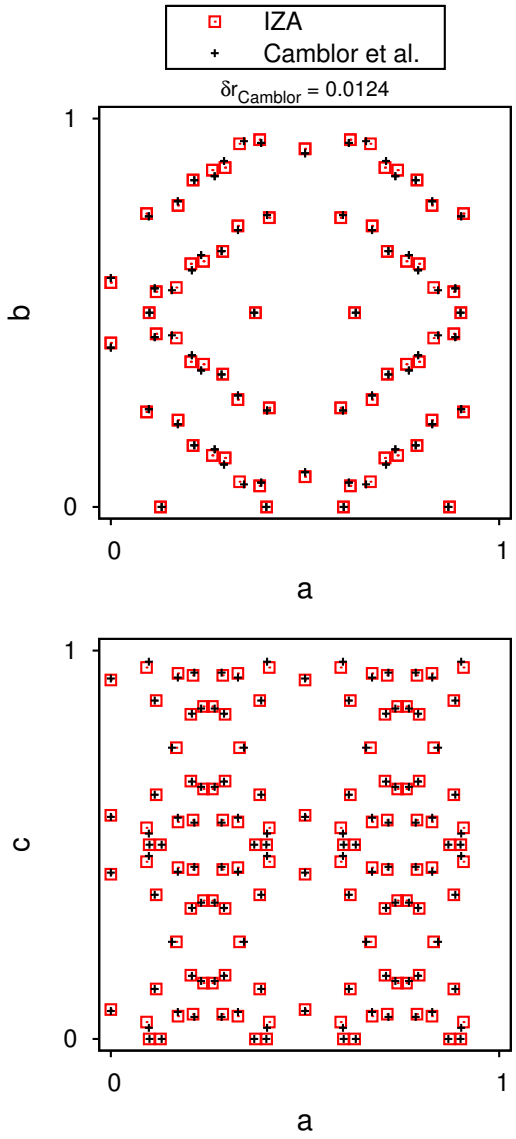

Figure 6. Plot of the fractional coordinates of the oxygen atoms of the three different ITE materials studied; top: a vs. b; bottom: a vs. c.

```
                                        20.753   9.804   20.009
                      90.000  90.000  90.000    SPGR =  1 P 1         OPT = 1
 192   0
    0 ITE          : ITE
 1  0     0.26140  0.86730  0.14380      0 0 0 0 0 0 0 0 0.00
 2  0     0.26140  0.13270  0.85620      0 0 0 0 0 0 0 0 0.00
 3  0     0.73860  0.86730  0.35620      0 0 0 0 0 0 0 0 0.00
 4  0     0.73860  0.13270  0.64380      0 0 0 0 0 0 0 0 0.00
 5  0     0.73860  0.13270  0.85620      0 0 0 0 0 0 0 0 0.00
 6  0     0.73860  0.86730  0.14380      0 0 0 0 0 0 0 0 0.00
 7  0     0.26140  0.13270  0.64380      0 0 0 0 0 0 0 0 0.00
 8  0     0.26140  0.86730  0.35620      0 0 0 0 0 0 0 0 0.00
 9  0     0.76140  0.36730  0.14380      0 0 0 0 0 0 0 0 0.00
10  0     0.76140  0.63270  0.85620      0 0 0 0 0 0 0 0 0.00
11  0     0.23860  0.36730  0.35620      0 0 0 0 0 0 0 0 0.00
12  0     0.23860  0.63270  0.64380      0 0 0 0 0 0 0 0 0.00
13  0     0.23860  0.63270  0.85620      0 0 0 0 0 0 0 0 0.00
14  0     0.23860  0.36730  0.14380      0 0 0 0 0 0 0 0 0.00
15  0     0.76140  0.63270  0.64380      0 0 0 0 0 0 0 0 0.00
16  0     0.76140  0.36730  0.35620      0 0 0 0 0 0 0 0 0.00
17  0     0.33140  0.93500  0.25000      0 0 0 0 0 0 0 0 0.00
18  0     0.33140  0.06500  0.75000      0 0 0 0 0 0 0 0 0.00
19  0     0.66860  0.93500  0.25000      0 0 0 0 0 0 0 0 0.00
20  0     0.66860  0.06500  0.75000      0 0 0 0 0 0 0 0 0.00
21  0     0.83140  0.43500  0.25000      0 0 0 0 0 0 0 0 0.00
22  0     0.83140  0.56500  0.75000      0 0 0 0 0 0 0 0 0.00
23  0     0.16860  0.43500  0.25000      0 0 0 0 0 0 0 0 0.00
24  0     0.16860  0.56500  0.75000      0 0 0 0 0 0 0 0 0.00
25  0     0.29410  0.12620  0.16400      0 0 0 0 0 0 0 0 0.00
26  0     0.29410  0.87380  0.83600      0 0 0 0 0 0 0 0 0.00
27  0     0.70590  0.12620  0.33600      0 0 0 0 0 0 0 0 0.00
28  0     0.70590  0.87380  0.66400      0 0 0 0 0 0 0 0 0.00
29  0     0.70590  0.87380  0.83600      0 0 0 0 0 0 0 0 0.00
30  0     0.70590  0.12620  0.16400      0 0 0 0 0 0 0 0 0.00
31  0     0.29410  0.87380  0.66400      0 0 0 0 0 0 0 0 0.00
32  0     0.29410  0.12620  0.33600      0 0 0 0 0 0 0 0 0.00
33  0     0.79410  0.62620  0.16400      0 0 0 0 0 0 0 0 0.00
34  0     0.79410  0.37380  0.83600      0 0 0 0 0 0 0 0 0.00
35  0     0.20590  0.62620  0.33600      0 0 0 0 0 0 0 0 0.00
36  0     0.20590  0.37380  0.66400      0 0 0 0 0 0 0 0 0.00
37  0     0.20590  0.37380  0.83600      0 0 0 0 0 0 0 0 0.00
38  0     0.20590  0.62620  0.16400      0 0 0 0 0 0 0 0 0.00
39  0     0.79410  0.37380  0.66400      0 0 0 0 0 0 0 0 0.00
40  0     0.79410  0.62620  0.33600      0 0 0 0 0 0 0 0 0.00
41  0     0.38330  0.94570  0.12880      0 0 0 0 0 0 0 0 0.00
42  0     0.38330  0.05430  0.87120      0 0 0 0 0 0 0 0 0.00
43  0     0.61670  0.94570  0.37120      0 0 0 0 0 0 0 0 0.00
```

```
44  0     0.61670  0.05430  0.62880     0 0 0 0 0 0 0 0 0.00
45  0     0.61670  0.05430  0.87120     0 0 0 0 0 0 0 0 0.00
46  0     0.61670  0.94570  0.12880     0 0 0 0 0 0 0 0 0.00
47  0     0.38330  0.05430  0.62880     0 0 0 0 0 0 0 0 0.00
48  0     0.38330  0.94570  0.37120     0 0 0 0 0 0 0 0 0.00
49  0     0.88330  0.44570  0.12880     0 0 0 0 0 0 0 0 0.00
50  0     0.88330  0.55430  0.87120     0 0 0 0 0 0 0 0 0.00
51  0     0.11670  0.44570  0.37120     0 0 0 0 0 0 0 0 0.00
52  0     0.11670  0.55430  0.62880     0 0 0 0 0 0 0 0 0.00
53  0     0.11670  0.55430  0.87120     0 0 0 0 0 0 0 0 0.00
54  0     0.11670  0.44570  0.12880     0 0 0 0 0 0 0 0 0.00
55  0     0.88330  0.55430  0.62880     0 0 0 0 0 0 0 0 0.00
56  0     0.88330  0.44570  0.37120     0 0 0 0 0 0 0 0 0.00
57  0     0.09870  0.50000  0.00000     0 0 0 0 0 0 0 0 0.00
58  0     0.90130  0.50000  0.50000     0 0 0 0 0 0 0 0 0.00
59  0     0.90130  0.50000  0.00000     0 0 0 0 0 0 0 0 0.00
60  0     0.09870  0.50000  0.50000     0 0 0 0 0 0 0 0 0.00
61  0     0.59870  0.00000  0.00000     0 0 0 0 0 0 0 0 0.00
62  0     0.40130  0.00000  0.50000     0 0 0 0 0 0 0 0 0.00
63  0     0.40130  0.00000  0.00000     0 0 0 0 0 0 0 0 0.00
64  0     0.59870  0.00000  0.50000     0 0 0 0 0 0 0 0 0.00
65  0     0.00000  0.42220  0.07580     0 0 0 0 0 0 0 0 0.00
66  0     0.00000  0.57780  0.92420     0 0 0 0 0 0 0 0 0.00
67  0     0.00000  0.42220  0.42420     0 0 0 0 0 0 0 0 0.00
68  0     0.00000  0.57780  0.57580     0 0 0 0 0 0 0 0 0.00
69  0     0.50000  0.92220  0.07580     0 0 0 0 0 0 0 0 0.00
70  0     0.50000  0.07780  0.92420     0 0 0 0 0 0 0 0 0.00
71  0     0.50000  0.92220  0.42420     0 0 0 0 0 0 0 0 0.00
72  0     0.50000  0.07780  0.57580     0 0 0 0 0 0 0 0 0.00
73  0     0.09200  0.24470  0.04360     0 0 0 0 0 0 0 0 0.00
74  0     0.09200  0.75530  0.95640     0 0 0 0 0 0 0 0 0.00
75  0     0.90800  0.24470  0.45640     0 0 0 0 0 0 0 0 0.00
76  0     0.90800  0.75530  0.54360     0 0 0 0 0 0 0 0 0.00
77  0     0.90800  0.75530  0.95640     0 0 0 0 0 0 0 0 0.00
78  0     0.90800  0.24470  0.04360     0 0 0 0 0 0 0 0 0.00
79  0     0.09200  0.75530  0.54360     0 0 0 0 0 0 0 0 0.00
80  0     0.09200  0.24470  0.45640     0 0 0 0 0 0 0 0 0.00
81  0     0.59200  0.74470  0.04360     0 0 0 0 0 0 0 0 0.00
82  0     0.59200  0.25530  0.95640     0 0 0 0 0 0 0 0 0.00
83  0     0.40800  0.74470  0.45640     0 0 0 0 0 0 0 0 0.00
84  0     0.40800  0.25530  0.54360     0 0 0 0 0 0 0 0 0.00
85  0     0.40800  0.25530  0.95640     0 0 0 0 0 0 0 0 0.00
86  0     0.40800  0.74470  0.04360     0 0 0 0 0 0 0 0 0.00
87  0     0.59200  0.25530  0.54360     0 0 0 0 0 0 0 0 0.00
88  0     0.59200  0.74470  0.45640     0 0 0 0 0 0 0 0 0.00
89  0     0.32700  0.27630  0.05880     0 0 0 0 0 0 0 0 0.00
90  0     0.32700  0.72370  0.94120     0 0 0 0 0 0 0 0 0.00
```

91	O	0.67300	0.27630	0.44120	0	0	0	0	0	0	0	0	0.00
92	O	0.67300	0.72370	0.55880	0	0	0	0	0	0	0	0	0.00
93	O	0.67300	0.72370	0.94120	0	0	0	0	0	0	0	0	0.00
94	O	0.67300	0.27630	0.05880	0	0	0	0	0	0	0	0	0.00
95	O	0.32700	0.72370	0.55880	0	0	0	0	0	0	0	0	0.00
96	O	0.32700	0.27630	0.44120	0	0	0	0	0	0	0	0	0.00
97	O	0.82700	0.77630	0.05880	0	0	0	0	0	0	0	0	0.00
98	O	0.82700	0.22370	0.94120	0	0	0	0	0	0	0	0	0.00
99	O	0.17300	0.77630	0.44120	0	0	0	0	0	0	0	0	0.00
100	O	0.17300	0.22370	0.55880	0	0	0	0	0	0	0	0	0.00
101	O	0.17300	0.22370	0.94120	0	0	0	0	0	0	0	0	0.00
102	O	0.17300	0.77630	0.05880	0	0	0	0	0	0	0	0	0.00
103	O	0.82700	0.22370	0.55880	0	0	0	0	0	0	0	0	0.00
104	O	0.82700	0.77630	0.44120	0	0	0	0	0	0	0	0	0.00
105	O	0.21180	0.15810	0.06370	0	0	0	0	0	0	0	0	0.00
106	O	0.21180	0.84190	0.93630	0	0	0	0	0	0	0	0	0.00
107	O	0.78820	0.15810	0.43630	0	0	0	0	0	0	0	0	0.00
108	O	0.78820	0.84190	0.56370	0	0	0	0	0	0	0	0	0.00
109	O	0.78820	0.84190	0.93630	0	0	0	0	0	0	0	0	0.00
110	O	0.78820	0.15810	0.06370	0	0	0	0	0	0	0	0	0.00
111	O	0.21180	0.84190	0.56370	0	0	0	0	0	0	0	0	0.00
112	O	0.21180	0.15810	0.43630	0	0	0	0	0	0	0	0	0.00
113	O	0.71180	0.65810	0.06370	0	0	0	0	0	0	0	0	0.00
114	O	0.71180	0.34190	0.93630	0	0	0	0	0	0	0	0	0.00
115	O	0.28820	0.65810	0.43630	0	0	0	0	0	0	0	0	0.00
116	O	0.28820	0.34190	0.56370	0	0	0	0	0	0	0	0	0.00
117	O	0.28820	0.34190	0.93630	0	0	0	0	0	0	0	0	0.00
118	O	0.28820	0.65810	0.06370	0	0	0	0	0	0	0	0	0.00
119	O	0.71180	0.34190	0.56370	0	0	0	0	0	0	0	0	0.00
120	O	0.71180	0.65810	0.43630	0	0	0	0	0	0	0	0	0.00
121	O	0.12780	0.00000	0.00000	0	0	0	0	0	0	0	0	0.00
122	O	0.87220	0.00000	0.50000	0	0	0	0	0	0	0	0	0.00
123	O	0.87220	0.00000	0.00000	0	0	0	0	0	0	0	0	0.00
124	O	0.12780	0.00000	0.50000	0	0	0	0	0	0	0	0	0.00
125	O	0.62780	0.50000	0.00000	0	0	0	0	0	0	0	0	0.00
126	O	0.37220	0.50000	0.50000	0	0	0	0	0	0	0	0	0.00
127	O	0.37220	0.50000	0.00000	0	0	0	0	0	0	0	0	0.00
128	O	0.62780	0.50000	0.50000	0	0	0	0	0	0	0	0	0.00
129	Si	0.31750	0.96850	0.17170	0	0	0	0	0	0	0	0	0.00
130	Si	0.31750	0.03150	0.82830	0	0	0	0	0	0	0	0	0.00
131	Si	0.68250	0.96850	0.32830	0	0	0	0	0	0	0	0	0.00
132	Si	0.68250	0.03150	0.67170	0	0	0	0	0	0	0	0	0.00
133	Si	0.68250	0.03150	0.82830	0	0	0	0	0	0	0	0	0.00
134	Si	0.68250	0.96850	0.17170	0	0	0	0	0	0	0	0	0.00
135	Si	0.31750	0.03150	0.67170	0	0	0	0	0	0	0	0	0.00
136	Si	0.31750	0.96850	0.32830	0	0	0	0	0	0	0	0	0.00
137	Si	0.81750	0.46850	0.17170	0	0	0	0	0	0	0	0	0.00

```
138  Si    0.81750  0.53150  0.82830      0 0 0 0 0 0 0 0 0.00
139  Si    0.18250  0.46850  0.32830      0 0 0 0 0 0 0 0 0.00
140  Si    0.18250  0.53150  0.67170      0 0 0 0 0 0 0 0 0.00
141  Si    0.18250  0.53150  0.82830      0 0 0 0 0 0 0 0 0.00
142  Si    0.18250  0.46850  0.17170      0 0 0 0 0 0 0 0 0.00
143  Si    0.81750  0.53150  0.67170      0 0 0 0 0 0 0 0 0.00
144  Si    0.81750  0.46850  0.32830      0 0 0 0 0 0 0 0 0.00
145  Si    0.07670  0.40320  0.06200      0 0 0 0 0 0 0 0 0.00
146  Si    0.07670  0.59680  0.93800      0 0 0 0 0 0 0 0 0.00
147  Si    0.92330  0.40320  0.43800      0 0 0 0 0 0 0 0 0.00
148  Si    0.92330  0.59680  0.56200      0 0 0 0 0 0 0 0 0.00
149  Si    0.92330  0.59680  0.93800      0 0 0 0 0 0 0 0 0.00
150  Si    0.92330  0.40320  0.06200      0 0 0 0 0 0 0 0 0.00
151  Si    0.07670  0.59680  0.56200      0 0 0 0 0 0 0 0 0.00
152  Si    0.07670  0.40320  0.43800      0 0 0 0 0 0 0 0 0.00
153  Si    0.57670  0.90320  0.06200      0 0 0 0 0 0 0 0 0.00
154  Si    0.57670  0.09680  0.93800      0 0 0 0 0 0 0 0 0.00
155  Si    0.42330  0.90320  0.43800      0 0 0 0 0 0 0 0 0.00
156  Si    0.42330  0.09680  0.56200      0 0 0 0 0 0 0 0 0.00
157  Si    0.42330  0.09680  0.93800      0 0 0 0 0 0 0 0 0.00
158  Si    0.42330  0.90320  0.06200      0 0 0 0 0 0 0 0 0.00
159  Si    0.57670  0.09680  0.56200      0 0 0 0 0 0 0 0 0.00
160  Si    0.57670  0.90320  0.43800      0 0 0 0 0 0 0 0 0.00
161  Si    0.26770  0.23220  0.10760      0 0 0 0 0 0 0 0 0.00
162  Si    0.26770  0.76780  0.89240      0 0 0 0 0 0 0 0 0.00
163  Si    0.73230  0.23220  0.39240      0 0 0 0 0 0 0 0 0.00
164  Si    0.73230  0.76780  0.60760      0 0 0 0 0 0 0 0 0.00
165  Si    0.73230  0.76780  0.89240      0 0 0 0 0 0 0 0 0.00
166  Si    0.73230  0.23220  0.10760      0 0 0 0 0 0 0 0 0.00
167  Si    0.26770  0.76780  0.60760      0 0 0 0 0 0 0 0 0.00
168  Si    0.26770  0.23220  0.39240      0 0 0 0 0 0 0 0 0.00
169  Si    0.76770  0.73220  0.10760      0 0 0 0 0 0 0 0 0.00
170  Si    0.76770  0.26780  0.89240      0 0 0 0 0 0 0 0 0.00
171  Si    0.23230  0.73220  0.39240      0 0 0 0 0 0 0 0 0.00
172  Si    0.23230  0.26780  0.60760      0 0 0 0 0 0 0 0 0.00
173  Si    0.23230  0.26780  0.89240      0 0 0 0 0 0 0 0 0.00
174  Si    0.23230  0.73220  0.10760      0 0 0 0 0 0 0 0 0.00
175  Si    0.76770  0.26780  0.60760      0 0 0 0 0 0 0 0 0.00
176  Si    0.76770  0.73220  0.39240      0 0 0 0 0 0 0 0 0.00
177  Si    0.15120  0.15650  0.01210      0 0 0 0 0 0 0 0 0.00
178  Si    0.15120  0.84350  0.98790      0 0 0 0 0 0 0 0 0.00
179  Si    0.84880  0.15650  0.48790      0 0 0 0 0 0 0 0 0.00
180  Si    0.84880  0.84350  0.51210      0 0 0 0 0 0 0 0 0.00
181  Si    0.84880  0.84350  0.98790      0 0 0 0 0 0 0 0 0.00
182  Si    0.84880  0.15650  0.01210      0 0 0 0 0 0 0 0 0.00
183  Si    0.15120  0.84350  0.51210      0 0 0 0 0 0 0 0 0.00
184  Si    0.15120  0.15650  0.48790      0 0 0 0 0 0 0 0 0.00
```

```
185  Si    0.65120  0.65650  0.01210      0 0 0 0 0 0 0 0 0.00
186  Si    0.65120  0.34350  0.98790      0 0 0 0 0 0 0 0 0.00
187  Si    0.34880  0.65650  0.48790      0 0 0 0 0 0 0 0 0.00
188  Si    0.34880  0.34350  0.51210      0 0 0 0 0 0 0 0 0.00
189  Si    0.34880  0.34350  0.98790      0 0 0 0 0 0 0 0 0.00
190  Si    0.34880  0.65650  0.01210      0 0 0 0 0 0 0 0 0.00
191  Si    0.65120  0.34350  0.51210      0 0 0 0 0 0 0 0 0.00
192  Si    0.65120  0.65650  0.48790      0 0 0 0 0 0 0 0 0.00
```

3.8. ITE – Camblor *et al.* [8]

```
                                        20.622   9.7242   19.623
                     90.000  90.000  90.000    SPGR =  1 P 1         OPT = 1
 192   0
    0 ITE         : ITE
  1  Si    0.32018  0.95700  0.17010      0 0 0 0 0 0 0 0 0.00
  2  Si    0.32018  0.04300  0.82990      0 0 0 0 0 0 0 0 0.00
  3  Si    0.67982  0.95700  0.32990      0 0 0 0 0 0 0 0 0.00
  4  Si    0.67982  0.04300  0.67010      0 0 0 0 0 0 0 0 0.00
  5  Si    0.67982  0.04300  0.82990      0 0 0 0 0 0 0 0 0.00
  6  Si    0.67982  0.95700  0.17010      0 0 0 0 0 0 0 0 0.00
  7  Si    0.32018  0.04300  0.67010      0 0 0 0 0 0 0 0 0.00
  8  Si    0.32018  0.95700  0.32990      0 0 0 0 0 0 0 0 0.00
  9  Si    0.82018  0.45700  0.17010      0 0 0 0 0 0 0 0 0.00
 10  Si    0.82018  0.54300  0.82990      0 0 0 0 0 0 0 0 0.00
 11  Si    0.17982  0.45700  0.32990      0 0 0 0 0 0 0 0 0.00
 12  Si    0.17982  0.54300  0.67010      0 0 0 0 0 0 0 0 0.00
 13  Si    0.17982  0.54300  0.82990      0 0 0 0 0 0 0 0 0.00
 14  Si    0.17982  0.45700  0.17010      0 0 0 0 0 0 0 0 0.00
 15  Si    0.82018  0.54300  0.67010      0 0 0 0 0 0 0 0 0.00
 16  Si    0.82018  0.45700  0.32990      0 0 0 0 0 0 0 0 0.00
 17  Si    0.07561  0.40670  0.05610      0 0 0 0 0 0 0 0 0.00
 18  Si    0.07561  0.59330  0.94390      0 0 0 0 0 0 0 0 0.00
 19  Si    0.92439  0.40670  0.44390      0 0 0 0 0 0 0 0 0.00
 20  Si    0.92439  0.59330  0.55610      0 0 0 0 0 0 0 0 0.00
 21  Si    0.92439  0.59330  0.94390      0 0 0 0 0 0 0 0 0.00
 22  Si    0.92439  0.40670  0.05610      0 0 0 0 0 0 0 0 0.00
 23  Si    0.07561  0.59330  0.55610      0 0 0 0 0 0 0 0 0.00
 24  Si    0.07561  0.40670  0.44390      0 0 0 0 0 0 0 0 0.00
 25  Si    0.57561  0.90670  0.05610      0 0 0 0 0 0 0 0 0.00
 26  Si    0.57561  0.09330  0.94390      0 0 0 0 0 0 0 0 0.00
 27  Si    0.42439  0.90670  0.44390      0 0 0 0 0 0 0 0 0.00
 28  Si    0.42439  0.09330  0.55610      0 0 0 0 0 0 0 0 0.00
 29  Si    0.42439  0.09330  0.94390      0 0 0 0 0 0 0 0 0.00
 30  Si    0.42439  0.90670  0.05610      0 0 0 0 0 0 0 0 0.00
```

```
31  Si    0.57561  0.09330  0.55610      0 0 0 0 0 0 0 0 0.00
32  Si    0.57561  0.90670  0.44390      0 0 0 0 0 0 0 0 0.00
33  Si    0.26410  0.22550  0.11210      0 0 0 0 0 0 0 0 0.00
34  Si    0.26410  0.77450  0.88790      0 0 0 0 0 0 0 0 0.00
35  Si    0.73590  0.22550  0.38790      0 0 0 0 0 0 0 0 0.00
36  Si    0.73590  0.77450  0.61210      0 0 0 0 0 0 0 0 0.00
37  Si    0.73590  0.77450  0.88790      0 0 0 0 0 0 0 0 0.00
38  Si    0.73590  0.22550  0.11210      0 0 0 0 0 0 0 0 0.00
39  Si    0.26410  0.77450  0.61210      0 0 0 0 0 0 0 0 0.00
40  Si    0.26410  0.22550  0.38790      0 0 0 0 0 0 0 0 0.00
41  Si    0.76410  0.72550  0.11210      0 0 0 0 0 0 0 0 0.00
42  Si    0.76410  0.27450  0.88790      0 0 0 0 0 0 0 0 0.00
43  Si    0.23590  0.72550  0.38790      0 0 0 0 0 0 0 0 0.00
44  Si    0.23590  0.27450  0.61210      0 0 0 0 0 0 0 0 0.00
45  Si    0.23590  0.27450  0.88790      0 0 0 0 0 0 0 0 0.00
46  Si    0.23590  0.72550  0.11210      0 0 0 0 0 0 0 0 0.00
47  Si    0.76410  0.27450  0.61210      0 0 0 0 0 0 0 0 0.00
48  Si    0.76410  0.72550  0.38790      0 0 0 0 0 0 0 0 0.00
49  Si    0.15302  0.15510  0.00360      0 0 0 0 0 0 0 0 0.00
50  Si    0.15302  0.84490  0.99640      0 0 0 0 0 0 0 0 0.00
51  Si    0.84698  0.15510  0.49640      0 0 0 0 0 0 0 0 0.00
52  Si    0.84698  0.84490  0.50360      0 0 0 0 0 0 0 0 0.00
53  Si    0.84698  0.84490  0.99640      0 0 0 0 0 0 0 0 0.00
54  Si    0.84698  0.15510  0.00360      0 0 0 0 0 0 0 0 0.00
55  Si    0.15302  0.84490  0.50360      0 0 0 0 0 0 0 0 0.00
56  Si    0.15302  0.15510  0.49640      0 0 0 0 0 0 0 0 0.00
57  Si    0.65302  0.65510  0.00360      0 0 0 0 0 0 0 0 0.00
58  Si    0.65302  0.34490  0.99640      0 0 0 0 0 0 0 0 0.00
59  Si    0.34698  0.65510  0.49640      0 0 0 0 0 0 0 0 0.00
60  Si    0.34698  0.34490  0.50360      0 0 0 0 0 0 0 0 0.00
61  Si    0.34698  0.34490  0.99640      0 0 0 0 0 0 0 0 0.00
62  Si    0.34698  0.65510  0.00360      0 0 0 0 0 0 0 0 0.00
63  Si    0.65302  0.34490  0.50360      0 0 0 0 0 0 0 0 0.00
64  Si    0.65302  0.65510  0.49640      0 0 0 0 0 0 0 0 0.00
65  O     0.34270  0.94190  0.25000      0 0 0 0 0 0 0 0 0.00
66  O     0.34270  0.05810  0.75000      0 0 0 0 0 0 0 0 0.00
67  O     0.65730  0.94190  0.25000      0 0 0 0 0 0 0 0 0.00
68  O     0.65730  0.05810  0.75000      0 0 0 0 0 0 0 0 0.00
69  O     0.84270  0.44190  0.25000      0 0 0 0 0 0 0 0 0.00
70  O     0.84270  0.55810  0.75000      0 0 0 0 0 0 0 0 0.00
71  O     0.15730  0.44190  0.25000      0 0 0 0 0 0 0 0 0.00
72  O     0.15730  0.55810  0.75000      0 0 0 0 0 0 0 0 0.00
73  O     0.26750  0.85150  0.14910      0 0 0 0 0 0 0 0 0.00
74  O     0.26750  0.14850  0.85090      0 0 0 0 0 0 0 0 0.00
75  O     0.73250  0.85150  0.35090      0 0 0 0 0 0 0 0 0.00
76  O     0.73250  0.14850  0.64910      0 0 0 0 0 0 0 0 0.00
77  O     0.73250  0.14850  0.85090      0 0 0 0 0 0 0 0 0.00
```

78	0	0.73250	0.85150	0.14910	0	0	0	0	0	0	0	0	0.00
79	0	0.26750	0.14850	0.64910	0	0	0	0	0	0	0	0	0.00
80	0	0.26750	0.85150	0.35090	0	0	0	0	0	0	0	0	0.00
81	0	0.76750	0.35150	0.14910	0	0	0	0	0	0	0	0	0.00
82	0	0.76750	0.64850	0.85090	0	0	0	0	0	0	0	0	0.00
83	0	0.23250	0.35150	0.35090	0	0	0	0	0	0	0	0	0.00
84	0	0.23250	0.64850	0.64910	0	0	0	0	0	0	0	0	0.00
85	0	0.23250	0.64850	0.85090	0	0	0	0	0	0	0	0	0.00
86	0	0.23250	0.35150	0.14910	0	0	0	0	0	0	0	0	0.00
87	0	0.76750	0.64850	0.64910	0	0	0	0	0	0	0	0	0.00
88	0	0.76750	0.35150	0.35090	0	0	0	0	0	0	0	0	0.00
89	0	0.09960	0.50000	0.00000	0	0	0	0	0	0	0	0	0.00
90	0	0.90040	0.50000	0.50000	0	0	0	0	0	0	0	0	0.00
91	0	0.90040	0.50000	0.00000	0	0	0	0	0	0	0	0	0.00
92	0	0.09960	0.50000	0.50000	0	0	0	0	0	0	0	0	0.00
93	0	0.59960	0.00000	0.00000	0	0	0	0	0	0	0	0	0.00
94	0	0.40040	0.00000	0.50000	0	0	0	0	0	0	0	0	0.00
95	0	0.40040	0.00000	0.00000	0	0	0	0	0	0	0	0	0.00
96	0	0.59960	0.00000	0.50000	0	0	0	0	0	0	0	0	0.00
97	0	0.09780	0.25160	0.02870	0	0	0	0	0	0	0	0	0.00
98	0	0.09780	0.74840	0.97130	0	0	0	0	0	0	0	0	0.00
99	0	0.90220	0.25160	0.47130	0	0	0	0	0	0	0	0	0.00
100	0	0.90220	0.74840	0.52870	0	0	0	0	0	0	0	0	0.00
101	0	0.90220	0.74840	0.97130	0	0	0	0	0	0	0	0	0.00
102	0	0.90220	0.25160	0.02870	0	0	0	0	0	0	0	0	0.00
103	0	0.09780	0.74840	0.52870	0	0	0	0	0	0	0	0	0.00
104	0	0.09780	0.25160	0.47130	0	0	0	0	0	0	0	0	0.00
105	0	0.59780	0.75160	0.02870	0	0	0	0	0	0	0	0	0.00
106	0	0.59780	0.24840	0.97130	0	0	0	0	0	0	0	0	0.00
107	0	0.40220	0.75160	0.47130	0	0	0	0	0	0	0	0	0.00
108	0	0.40220	0.24840	0.52870	0	0	0	0	0	0	0	0	0.00
109	0	0.40220	0.24840	0.97130	0	0	0	0	0	0	0	0	0.00
110	0	0.40220	0.75160	0.02870	0	0	0	0	0	0	0	0	0.00
111	0	0.59780	0.24840	0.52870	0	0	0	0	0	0	0	0	0.00
112	0	0.59780	0.75160	0.47130	0	0	0	0	0	0	0	0	0.00
113	0	0.00000	0.41050	0.07180	0	0	0	0	0	0	0	0	0.00
114	0	0.00000	0.58950	0.92820	0	0	0	0	0	0	0	0	0.00
115	0	0.00000	0.41050	0.42820	0	0	0	0	0	0	0	0	0.00
116	0	0.00000	0.58950	0.57180	0	0	0	0	0	0	0	0	0.00
117	0	0.50000	0.91050	0.07180	0	0	0	0	0	0	0	0	0.00
118	0	0.50000	0.08950	0.92820	0	0	0	0	0	0	0	0	0.00
119	0	0.50000	0.91050	0.42820	0	0	0	0	0	0	0	0	0.00
120	0	0.50000	0.08950	0.57180	0	0	0	0	0	0	0	0	0.00
121	0	0.21480	0.15870	0.05690	0	0	0	0	0	0	0	0	0.00
122	0	0.21480	0.84130	0.94310	0	0	0	0	0	0	0	0	0.00
123	0	0.78520	0.15870	0.44310	0	0	0	0	0	0	0	0	0.00
124	0	0.78520	0.84130	0.55690	0	0	0	0	0	0	0	0	0.00

```
125  0     0.78520  0.84130  0.94310      0 0 0 0 0 0 0 0 0.00
126  0     0.78520  0.15870  0.05690      0 0 0 0 0 0 0 0 0.00
127  0     0.21480  0.84130  0.55690      0 0 0 0 0 0 0 0 0.00
128  0     0.21480  0.15870  0.44310      0 0 0 0 0 0 0 0 0.00
129  0     0.71480  0.65870  0.05690      0 0 0 0 0 0 0 0 0.00
130  0     0.71480  0.34130  0.94310      0 0 0 0 0 0 0 0 0.00
131  0     0.28520  0.65870  0.44310      0 0 0 0 0 0 0 0 0.00
132  0     0.28520  0.34130  0.55690      0 0 0 0 0 0 0 0 0.00
133  0     0.28520  0.34130  0.94310      0 0 0 0 0 0 0 0 0.00
134  0     0.28520  0.65870  0.05690      0 0 0 0 0 0 0 0 0.00
135  0     0.71480  0.34130  0.55690      0 0 0 0 0 0 0 0 0.00
136  0     0.71480  0.65870  0.44310      0 0 0 0 0 0 0 0 0.00
137  0     0.38700  0.93720  0.12880      0 0 0 0 0 0 0 0 0.00
138  0     0.38700  0.06280  0.87120      0 0 0 0 0 0 0 0 0.00
139  0     0.61300  0.93720  0.37120      0 0 0 0 0 0 0 0 0.00
140  0     0.61300  0.06280  0.62880      0 0 0 0 0 0 0 0 0.00
141  0     0.61300  0.06280  0.87120      0 0 0 0 0 0 0 0 0.00
142  0     0.61300  0.93720  0.12880      0 0 0 0 0 0 0 0 0.00
143  0     0.38700  0.06280  0.62880      0 0 0 0 0 0 0 0 0.00
144  0     0.38700  0.93720  0.37120      0 0 0 0 0 0 0 0 0.00
145  0     0.88700  0.43720  0.12880      0 0 0 0 0 0 0 0 0.00
146  0     0.88700  0.56280  0.87120      0 0 0 0 0 0 0 0 0.00
147  0     0.11300  0.43720  0.37120      0 0 0 0 0 0 0 0 0.00
148  0     0.11300  0.56280  0.62880      0 0 0 0 0 0 0 0 0.00
149  0     0.11300  0.56280  0.87120      0 0 0 0 0 0 0 0 0.00
150  0     0.11300  0.43720  0.12880      0 0 0 0 0 0 0 0 0.00
151  0     0.88700  0.56280  0.62880      0 0 0 0 0 0 0 0 0.00
152  0     0.88700  0.43720  0.37120      0 0 0 0 0 0 0 0 0.00
153  0     0.29130  0.10930  0.16250      0 0 0 0 0 0 0 0 0.00
154  0     0.29130  0.89070  0.83750      0 0 0 0 0 0 0 0 0.00
155  0     0.70870  0.10930  0.33750      0 0 0 0 0 0 0 0 0.00
156  0     0.70870  0.89070  0.66250      0 0 0 0 0 0 0 0 0.00
157  0     0.70870  0.89070  0.83750      0 0 0 0 0 0 0 0 0.00
158  0     0.70870  0.10930  0.16250      0 0 0 0 0 0 0 0 0.00
159  0     0.29130  0.89070  0.66250      0 0 0 0 0 0 0 0 0.00
160  0     0.29130  0.10930  0.33750      0 0 0 0 0 0 0 0 0.00
161  0     0.79130  0.60930  0.16250      0 0 0 0 0 0 0 0 0.00
162  0     0.79130  0.39070  0.83750      0 0 0 0 0 0 0 0 0.00
163  0     0.20870  0.60930  0.33750      0 0 0 0 0 0 0 0 0.00
164  0     0.20870  0.39070  0.66250      0 0 0 0 0 0 0 0 0.00
165  0     0.20870  0.39070  0.83750      0 0 0 0 0 0 0 0 0.00
166  0     0.20870  0.60930  0.16250      0 0 0 0 0 0 0 0 0.00
167  0     0.79130  0.39070  0.66250      0 0 0 0 0 0 0 0 0.00
168  0     0.79130  0.60930  0.33750      0 0 0 0 0 0 0 0 0.00
169  0     0.32750  0.28710  0.06950      0 0 0 0 0 0 0 0 0.00
170  0     0.32750  0.71290  0.93050      0 0 0 0 0 0 0 0 0.00
171  0     0.67250  0.28710  0.43050      0 0 0 0 0 0 0 0 0.00
```

```
172  0     0.67250  0.71290  0.56950     0 0 0 0 0 0 0 0 0.00
173  0     0.67250  0.71290  0.93050     0 0 0 0 0 0 0 0 0.00
174  0     0.67250  0.28710  0.06950     0 0 0 0 0 0 0 0 0.00
175  0     0.32750  0.71290  0.56950     0 0 0 0 0 0 0 0 0.00
176  0     0.32750  0.28710  0.43050     0 0 0 0 0 0 0 0 0.00
177  0     0.82750  0.78710  0.06950     0 0 0 0 0 0 0 0 0.00
178  0     0.82750  0.21290  0.93050     0 0 0 0 0 0 0 0 0.00
179  0     0.17250  0.78710  0.43050     0 0 0 0 0 0 0 0 0.00
180  0     0.17250  0.21290  0.56950     0 0 0 0 0 0 0 0 0.00
181  0     0.17250  0.21290  0.93050     0 0 0 0 0 0 0 0 0.00
182  0     0.17250  0.78710  0.06950     0 0 0 0 0 0 0 0 0.00
183  0     0.82750  0.21290  0.56950     0 0 0 0 0 0 0 0 0.00
184  0     0.82750  0.78710  0.43050     0 0 0 0 0 0 0 0 0.00
185  0     0.13080  0.00000  0.00000     0 0 0 0 0 0 0 0 0.00
186  0     0.86920  0.00000  0.50000     0 0 0 0 0 0 0 0 0.00
187  0     0.86920  0.00000  0.00000     0 0 0 0 0 0 0 0 0.00
188  0     0.13080  0.00000  0.50000     0 0 0 0 0 0 0 0 0.00
189  0     0.63080  0.50000  0.00000     0 0 0 0 0 0 0 0 0.00
190  0     0.36920  0.50000  0.50000     0 0 0 0 0 0 0 0 0.00
191  0     0.36920  0.50000  0.00000     0 0 0 0 0 0 0 0 0.00
192  0     0.63080  0.50000  0.50000     0 0 0 0 0 0 0 0 0.00
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