Supporting Information

Pressure-induced Silica Quartz Amorphization Studied by Iterative Stochastic Surface Walking Reaction Sampling

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I. SSW-RS method for reaction pathway search

A. Stochastic Surface Walking (SSW) method

The SSW algorithm[1] has an automated climbing mechanism to manipulate a structure configuration from a minimum to a high-energy configuration along one random mode direction. The method was initially developed for aperiodic systems, such as molecules and clusters[2], and has been extended to periodic crystals[3]. For solid phase transitions, this is to identify the one-to-one correspondence for lattice ($\mathbf{L}(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)$, $\mathbf{e}_i$ being the lattice vector) and atom ($\mathbf{q}_i$, i=1,..3N, N is the number of atom in cell) from one crystal phase (the initial state, IS) to another (the final state, FS), which constitutes the reaction coordinates of the reaction, i.e. $\mathbf{Q}_{IS}(\mathbf{L},\mathbf{q})\rightarrow\mathbf{Q}_{FS}(\mathbf{L},\mathbf{q})$, from initial state (IS) to final state (FS).

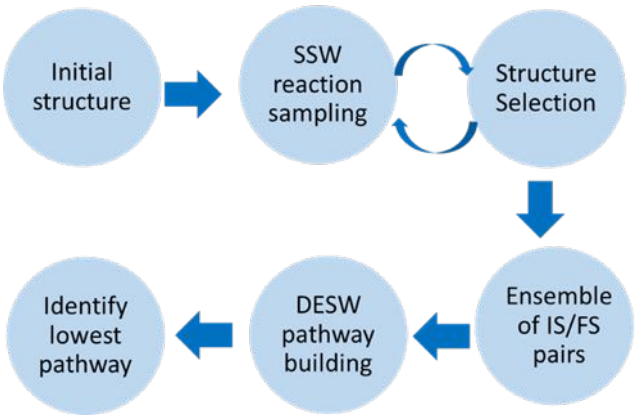
The SSW method inherits the idea of bias-potential driven constrained-Broyden-dimer (BP-CBD) method for TS location[4]. In one particular SSW step, labeled as *i*, a modified PES $V_{m\text{-}to\text{-}n}$ (*n* is the index of the bias potential, n=1,2$\cdots H$), as shown in Eq. 1, is utilized for moving from the current minimum, $\mathbf{R}_i^m$ to a high energy configuration $\mathbf{R}_i^H$ (the climbing), in which a series of bias Gaussian potential v_n is added one by one consecutively along the direction $\mathbf{N}_i^n$.

$$V_{m-to-H} = V_{real} + \sum_{n=1}^{NG} v_n = V_{real} + \sum_{n=1}^{NG} w_n \times \exp\left[-\left((\mathbf{R}^t - \mathbf{R}_t^{n-1}) \bullet \mathbf{N}_i^n \right)^2 \Big/ \left(2 \times ds^2 \right) \right] \quad (1)$$

where $\mathbf{R}$ is the coordination vector of the structure and V_{real} represents the unmodified PES; $\mathbf{R}_t^n$ are the n^{th} local minima along the movement trajectory on the modified PES that is created after adding *n* Gaussian functions. The Gaussian function is controlled by its height *w* and its width *ds*, and is always

added along one particular walking direction as defined by $\mathbf{N}^n$. Once the $\mathbf{R}_i^H$ is reached, all bias potential are removed and the local optimization is performed to quench the structure to a new minimum (These stationary points found were assumed to be minima, i.e. given the large number of structures the frequency calculations are not performed in general during SSW structural search). The applications of SSW method can be found in our previous publications (http://homepage.fudan.edu.cn/fdzpliu/publication/).

B. SSW reaction sampling (SSW-RS) algorithm



Scheme S1. The flow chart of SSW-RS method[5]

Here we outline the SSW-RS method briefly. More details on the methodology can be found in our previous works[6-10]. SSW-RS explores the pathways nearby a predefined initial state and can find the lowest energy pathway linking to these nearby phases. In our implementation, the SSW-RS is fully automated and divided into three stages in simulation, namely, (i) pathway collection via extensive SSW global search; (ii) pathway screening via fast variable-cell double-ended surface walking (VC-DESW) pathway building[5, 11, 12]; (iii) lowest energy pathway determination via VC-DESW [11] TS search. The first stage is the most important and most time-consuming part, which generates all the likely pairs of reaction coordinates linking different crystal phases to ensure the identification of the best reaction coordinate, the one corresponding to the lowest energy pathway..

The scheme, as shown in **Scheme** S1, describes the procedure of SSW-RS and is explained as follows.

(i) Input an initial structure of reactant (IS).

(ii) Perform SSW reaction sampling to identify a new minimum (FS).

(iii) Use the structure selection module to determine whether the new minimum is accepted/refused. If the reaction occurs, output the IS/FS pair when necessary and set the current structure to the IS; otherwise, replace the IS by the FS.

(iv) Repeat (ii-iii) until an ensemble of enough number of IS/FS pairs is obtained.

(v) Use VC-DESW to build the pseudo pathways from the IS/FS pairs, from which the low energy pathways are selected.

(vi) Locate the TSs of all the low energy pathways and identify the lowest energy pathways.

II. Comparison between theoretical and experimental results

Table S1 Enthalpy difference between stishovite (H_{St}) and quartz (H_Q) at different external pressures. The energy unit is in eV per formula unit (eV/f.u.)*

Pressure / GPa	Expt. *	DFT (GGA-PBE)	BKS**
0	0.38	0.55	-0.88
5	0.02	0.12	-1.31
10	-0.24	-0.22	-1.63
15	-0.45	-0.51	-0.78
20	-0.62	-0.75	-0.84
25	-0.78	-0.96	-0.89
30	-0.92	-1.14	-0.94

*The experimental data is taken from Ref. [13]

** BKS stands for the classical van Beest, Kramer, van Santen potential in Ref. [14]

III. Comparison between BKS and DFT results for important structures under 15 GPa

Table S2 The lattice parameters and Si-O bond lengths of important silica phases using DFT and BKS potential. All the length is in Å and the angle is in °

Silica phase		Lattice parameters*			Lattice error**	Average Si-O length	Bond length error**
QII	BKS	5.8550	4.6827	6.5097	1.1%	1.748	0.1%
		83.93	114.10	75.39			
	DFT	5.8671	4.6160	6.3738		1.746	
		86.50	113.49	73.82			
MI	BKS	6.4661	4.1325	6.9023	0.8%	1.780	0.4%
		90.00	99.22	129.72			
	DFT	6.4349	4.0543	6.8649		1.772	
		90.00	99.16	129.05			
St	BKS	4.9537	4.9526	6.4619	0.3%	1.777	0.5%
		71.75	71.7221	72.82			
	DFT	4.9306	4.9337	6.4441		1.768	
		71.46	71.50	72.99			
MII	BKS	5.0170	8.5482	5.0155	0.8%	1.771	0.06%
		50.06	114.80	97.53			
	DFT	4.9706	8.4876	4.9713		1.772	
		50.17	115.19	97.81			

* Upper line: lattice length **a**, **b**, **c**; lower line: lattice angle **alpha**, **beta**, **gamma**

** the error of BKS results with respect to DFT results

IV. Reaction pathway from QII to MI calculated by DFT and BKS

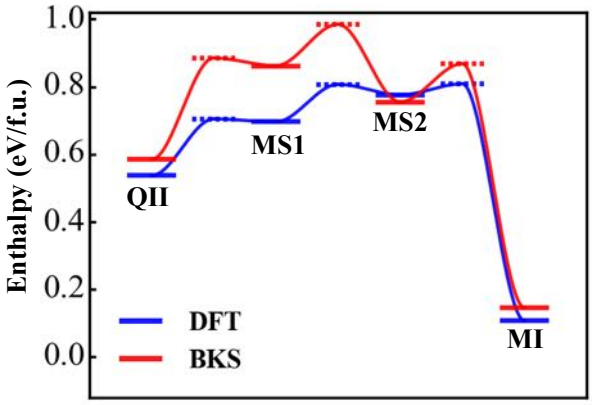


Figure S1. Reaction pathway from QII to MI calculated by BKS and DFT. The enthalpy of stishovite is set as zero in each calculation.

V. Formula to calculate the distance between two crystal phases

We utilize the generalized coordinate for crystals Q(L,q) as described in our previous work to measure the distance between two crystal phases. The approach is described as follows. For a crystal with the Cartesian coordinate **R** and the lattice matrix **L**, the fractional coordinate **q** can be calculated as

$$\mathbf{q} = \mathbf{L}^{-1}\mathbf{R} \qquad (2)$$

To measure the distance for $Q_{IS}(L,q) \rightarrow Q_{FS}(L,q)$, we need to choose the same scaling matrix **S** to rescale the fractional coordinate for IS and FS phases. The scaling matrix **S** can be obtained by the Cholesky decomposition of a metric tensor **G.** The **G** tensor can be obtained from the lattice matrix of the IS and FS, as shown in the eq. 3-6.

$$\mathbf{G} = \mathbf{L}^{T}\mathbf{L} \qquad (3)$$

$$\mathbf{G}_r = (\mathbf{G}_{IS} + \mathbf{G}_{FS})/2 \qquad (4)$$

$$\mathbf{S} = \mathbf{G}^{1/2} \qquad (5)$$

$$\mathbf{q}' = \mathbf{S}\mathbf{q} \qquad (6)$$

The distance is given by the Euclidean distance between the generalized coordinates of IS and FS.

$$\mathbf{Q}_{IS} = \{\mathbf{L}_{IS}, \mathbf{q}'_{IS}\}, \mathbf{Q}_{FS} = \{\mathbf{L}_{FS}, \mathbf{q}'_{FS}\} \qquad (7)$$

$$d = \| \mathbf{Q}_{IS} - \mathbf{Q}_{FS} \| \qquad (8)$$

VI. Phase transition pathways from QII to St and MII

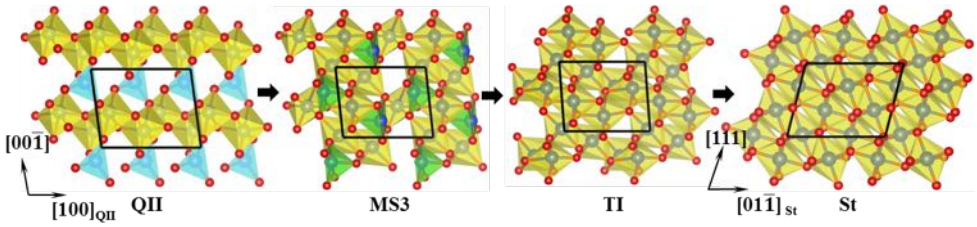


Figure S2. Reaction snapshots along the pathway from QII to St (also see Fig. 2 for energy profile). Polyhedron representation is used for all structures: yellow: [SiO_6], green: [SiO_5], light blue: [SiO_4].

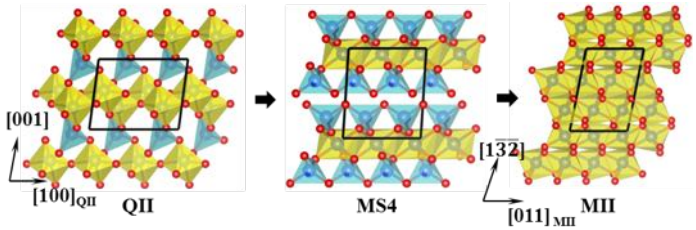


Figure S3. Reaction snapshots along the pathway from QII to MII (also see Fig. 2 for energy profile). Polyhedron representation is used for all structures: yellow: [SiO_6], green: [SiO_5], light blue: [SiO_4].

VII. Simulated XRD pattern

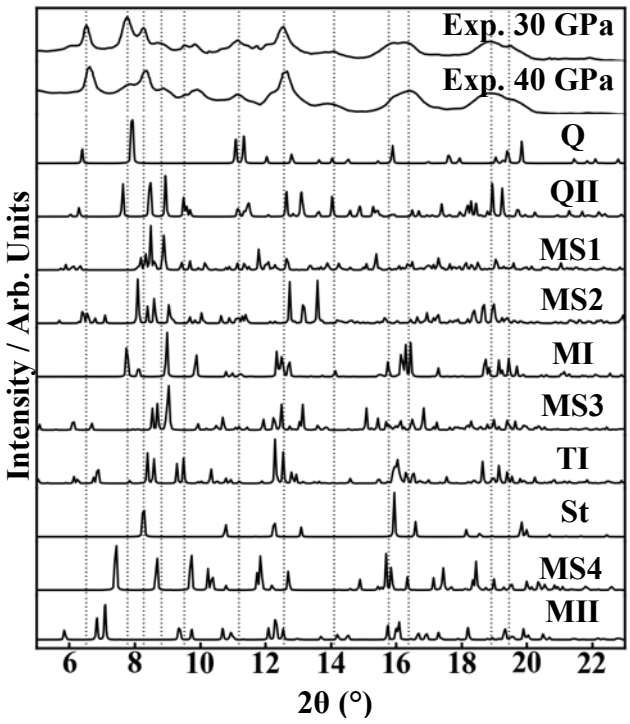


Figure S4. Simulated XRD for all possible structures (optimized with DFT under 30 GPa) from the reaction pathways, which are compared with experiment data under 30 GPa and under 40 GPa (reported in reference [15]).

In order to verify the presence of the intermediate structures in PIA as determined from the lowest energy pathway in Figure 2, we also simulated the X-ray diffraction (XRD) pattern for these structures and the results are shown in Fig. S4. All the possible structures, including Q, QII, MS1, MS2, MI, MS3, TI, MS4 and MII, have been optimized at 30 GPa and their XRD were simulated using the synchrotron with a wavelength of 0.41693 Å. The experimental results from Ref. [18] are also shown in figure for comparison.

As shown, the experimental XRD peaks are quite broad, suggesting the presence of amorphous structures. It is clearly that the peaks from experiment cannot be attributed only to the known crystalline phases, Q, QII, MI and St. For example, the peak at 6.5° increases from 30 to 40 GPa, implying it cannot be only due to Q phase. From the figure, we observe that the MS1 and MS2 structure have the similar diffraction pattern with experiment at the peaks of 6.5°, 8.3°, 8.8° and 12.56°; TI phase also matches the peaks at 8.8° and 12.56°. These results suggest that MS1, MS2 and TI phases are all likely components in PIA products.

VIII. Phonon spectrum of α-quartz under 15 GPa calculated by DFT

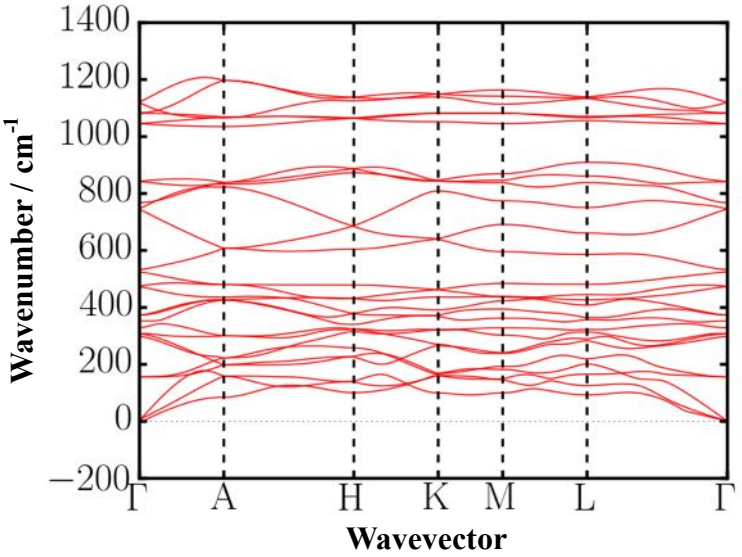


Figure S5. Phonon dispersion of α-quartz under 15 GPa calculated with DFT.

References

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IX. XYZ structure coordinates for the states along the lowest energy pathways

All structures were optimized using DFT under 15 GPa. The format of the structures below is Cartesian Coordinate Archive File (.arc).

α-quartz (Q)

!BIOSYM archive 2
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!DATE
PBC 6.9205 4.5519 6.9250 109.1586 110.5199 70.8007
O 0.379390935 -0.817227064 5.852052898 CORE 1 O O 0.0000 1
O 5.974706667 0.045216076 0.935400503 CORE 2 O O 0.0000 2
O 3.697009204 0.838395864 1.965991037 CORE 3 O O 0.0000 3
O 5.801834162 2.112736474 2.704594517 CORE 4 O O 0.0000 4
O 2.049165334 1.413937989 4.082852154 CORE 5 O O 0.0000 5
O -0.228525124 2.207120906 5.113447086 CORE 6 O O 0.0000 6
O 3.105432470 3.624485504 1.551719483 CORE 7 O O 0.0000 7
O 2.688328194 0.788636141 6.490902208 CORE 8 O O 0.0000 8
O 4.243615916 3.229882501 4.496688131 CORE 9 O O 0.0000 9
O 4.603519820 0.694503153 4.699175295 CORE 10 O O 0.0000 10
O -0.306671081 -0.580106337 3.343448088 CORE 11 O O 0.0000 11
O 1.248620840 1.861165745 1.349214326 CORE 12 O O 0.0000 12
Si 1.223859330 2.710789940 4.598287976 CORE 13 Si Si 0.0000 13
Si 5.149410720 1.342064374 1.450827435 CORE 14 Si Si 0.0000 14
Si 1.519776562 3.385111699 1.791427750 CORE 15 Si Si 0.0000 15
Si 3.017879063 0.455131960 4.938909508 CORE 16 Si Si 0.0000 16
Si 5.337523499 2.057214449 4.256940709 CORE 17 Si Si 0.0000 17
Si 2.342523794 0.688491353 1.109455317 CORE 18 Si Si 0.0000 18
end
end

Quartz II (QII)

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PBC 5.8671 4.6160 6.3738 86.4996 113.4868 73.8160
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O 4.871800447 0.548031403 0.623075097 CORE 2 O O 0.0000 2
O 3.061559176 1.749275731 1.916349005 CORE 3 O O 0.0000 3
O 4.919246114 3.557866215 2.371840166 CORE 4 O O 0.0000 4

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O          2.523553419     4.288491003     1.477860882 CORE     7 O    O      0.0000      7
O          1.753289531     3.812789130     5.693084612 CORE     8 O    O      0.0000      8
O          3.011254069     5.206071891     3.996364540 CORE     9 O    O      0.0000      9
O          3.543709113     2.643171559     4.344325386 CORE    10 O    O      0.0000     10
O         -0.553471897     1.025014135     2.826586663 CORE    11 O    O      0.0000     11
O          0.704502238     2.418279172     1.129867925 CORE    12 O    O      0.0000     12
Si         1.107531172     4.842854058     4.427038862 CORE    13 Si Si      0.0000     13
Si         4.667913970     2.055082665     1.560553659 CORE    14 Si Si      0.0000     14
Si         0.936851271     3.951105077     1.888864867 CORE    15 Si Si      0.0000     15
Si         1.957050621     2.305782948     4.755341390 CORE    16 Si Si      0.0000     16
Si         4.194102486     4.012973391     3.827275043 CORE    17 Si Si      0.0000     17
Si         1.887318377     1.225174752     0.960827645 CORE    18 Si Si      0.0000     18
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end
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Monoclinic I (MI)

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O          2.370748011     1.336602591     0.632939563 CORE     2 O    O      0.0000      2
O          0.098586050     1.918066474     5.852205424 CORE     3 O    O      0.0000      3
O          2.194743056     1.174386903     5.121913772 CORE     4 O    O      0.0000      4
O          1.216707510     0.469412798     2.871007481 CORE     5 O    O      0.0000      5
O          0.335773232    -0.499933892     5.121919008 CORE     6 O    O      0.0000      6
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O         -1.025103640     1.191861554     3.622074278 CORE    10 O    O      0.0000     10
O          4.512000256     0.444035541     5.852193924 CORE    11 O    O      0.0000     11
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Si        -1.524362042     1.989522773     2.127508413 CORE    13 Si Si      0.0000     13
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Stishovite (St)

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O          1.572818945     1.173207588     2.091900564 CORE    10 O    O      0.0000    10
O          5.402451659     2.581389255     3.850548120 CORE    11 O    O      0.0000    11
O          0.550593733     1.836310427    -0.099578864 CORE    12 O    O      0.0000    12
Si         5.441779736     4.034492386     2.862152702 CORE    13 Si Si      0.0000    13
Si         5.441938192     0.383255222     0.888918114 CORE    14 Si Si      0.0000    14
Si         1.533442236     1.142084511     3.848817153 CORE    15 Si Si      0.0000    15
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Monoclinic II (MII)

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Si         2.178437172      9.769840057      2.220414404 CORE    17 Si Si      0.0000     17
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end
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MS1

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O          3.161067166     -0.914750960      5.646289909 CORE     2 O   O      0.0000      2
O          1.718796045      1.094400139      4.595918503 CORE     3 O   O      0.0000      3
O          4.272453030      0.824615924      4.234626704 CORE     4 O   O      0.0000      4
O          2.567553334      0.692282335      2.243595533 CORE     5 O   O      0.0000      5
O          1.547923999     -1.212446707      3.688217314 CORE     6 O   O      0.0000      6
O         -0.702507054      4.153428450      0.468211812 CORE     7 O   O      0.0000      7
O          4.397332274      2.584181117      2.258828775 CORE     8 O   O      0.0000      8
O          3.980059453     -1.175777540      3.202945232 CORE     9 O   O      0.0000      9
O         -0.152787283      0.682433524      2.671675497 CORE    10 O   O      0.0000     10
O          5.816817528     -0.974532050      5.048290317 CORE    11 O   O      0.0000     11
O          0.912300280      2.620140827      1.367036952 CORE    12 O   O      0.0000     12
Si        -0.320363544      2.255663538      2.414036087 CORE    13 Si Si      0.0000     13
Si         2.679509964      2.314441714      1.684643205 CORE    14 Si Si      0.0000     14
Si         2.550168167     -0.126787269      0.521918992 CORE    15 Si Si      0.0000     15
Si         5.721873594     -0.027634491     -0.037789502 CORE    16 Si Si      0.0000     16
Si         5.413940851     -0.415870704      3.577530615 CORE    17 Si Si      0.0000     17
Si         2.700637384     -0.041946362      3.929988623 CORE    18 Si Si      0.0000     18
end
end
```

MS2

```
!BIOSYM archive 2
PBC=ON

!DATE
```

PBC 5.8653 4.4867 7.0607 99.6736 90.3958 121.2837
O 4.210233602 -0.069119626 1.242880599 CORE 1 O O 0.0000 1
O 2.292646876 1.486984573 0.596880964 CORE 2 O O 0.0000 2
O 0.813181723 1.752762007 6.098017530 CORE 3 O O 0.0000 3
O 2.855839407 1.258715123 5.143671938 CORE 4 O O 0.0000 4
O 1.597016876 0.747077227 2.891048732 CORE 5 O O 0.0000 5
O 1.140597787 -0.508266755 4.739803060 CORE 6 O O 0.0000 6
O -1.607189884 3.434185996 0.237369861 CORE 7 O O 0.0000 7
O 3.450014342 2.394599786 2.657987381 CORE 8 O O 0.0000 8
O 1.281330507 2.871367746 3.833531644 CORE 9 O O 0.0000 9
O -0.582577411 1.188650172 3.929533185 CORE 10 O O 0.0000 10
O 4.823703520 -0.211766979 6.079739079 CORE 11 O O 0.0000 11
O 0.055816426 2.467692057 1.781577956 CORE 12 O O 0.0000 12
Si -0.963449206 2.784189478 3.165158220 CORE 13 Si Si 0.0000 13
Si 1.923316308 2.252891630 2.072653460 CORE 14 Si Si 0.0000 14
Si -0.026865435 3.662642180 0.507274032 CORE 15 Si Si 0.0000 15
Si 2.669579745 2.109845720 6.706333229 CORE 16 Si Si 0.0000 16
Si 4.149513535 0.311686165 4.750921273 CORE 17 Si Si 0.0000 17
Si 1.126768358 1.129662494 4.540247852 CORE 18 Si Si 0.0000 18
end
end

MS3

!BIOSYM archive 2
PBC=ON

!DATE
PBC 5.0421 4.7900 6.7537 114.3017 102.7947 72.0823
O 1.712727957 1.597574069 0.969775561 CORE 1 O O 0.0000 1
O 4.117877678 0.041923483 5.144540200 CORE 2 O O 0.0000 2
O 1.860170347 2.577354423 4.658343271 CORE 3 O O 0.0000 3
O 1.663055982 0.268120128 5.246198661 CORE 4 O O 0.0000 4
O 0.384179336 0.482571675 3.059043103 CORE 5 O O 0.0000 5
O 4.201868589 1.417706725 1.003266927 CORE 6 O O 0.0000 6
O 2.704809919 0.499824666 3.136550434 CORE 7 O O 0.0000 7
O 4.348239628 3.916713398 0.706366418 CORE 8 O O 0.0000 8
O 5.489350987 3.034955014 2.649952505 CORE 9 O O 0.0000 9
O 2.901967286 2.808869928 2.548404540 CORE 10 O O 0.0000 10
O 1.859111570 4.096604600 0.672883881 CORE 11 O O 0.0000 11
O 4.180777807 2.594306866 4.735377308 CORE 12 O O 0.0000 12
Si 3.030530233 2.757133734 0.838169933 CORE 13 Si Si 0.0000 13
Si 4.108679415 -0.068976721 1.906621067 CORE 14 Si Si 0.0000 14
Si 1.445673095 1.755417932 2.664971699 CORE 15 Si Si 0.0000 15
Si -1.016922634 -1.411975523 5.887531947 CORE 16 Si Si 0.0000 16

```
Si        1.545619749    -0.740347803     3.897324566 CORE    17 Si Si    0.0000    17
Si        3.119355719     1.321348740     5.129209802 CORE    18 Si Si    0.0000    18
end
end
```

Triclinic I (TI)

```
!BIOSYM archive 2
PBC=ON

!DATE
PBC      5.0251      4.8924      6.8959   120.5317   102.1190    73.0168
O         1.620640417     1.602622299     0.996563674 CORE     1 O    O      0.0000     1
O         3.888059749    -0.775449640     4.868996577 CORE     2 O    O      0.0000     2
O         1.659948731     1.857917032     4.581192976 CORE     3 O    O      0.0000     3
O         1.601755128    -0.546413121     4.966831728 CORE     4 O    O      0.0000     4
O         0.266760074     0.466715144     2.898515465 CORE     5 O    O      0.0000     5
O         4.113975313     1.364378803     0.930362278 CORE     6 O    O      0.0000     6
O         2.746873388     0.312067006     3.051585587 CORE     7 O    O      0.0000     7
O         4.252934246     3.928872679     0.709243537 CORE     8 O    O      0.0000     8
O         5.342348996     2.998382240     2.651825789 CORE     9 O    O      0.0000     9
O         2.820480206     2.744943323     2.579087648 CORE    10 O    O      0.0000    10
O         1.770376597     4.081852218     0.660652950 CORE    11 O    O      0.0000    11
O         4.154751805     1.849194175     4.628968986 CORE    12 O    O      0.0000    12
Si        2.950129003     2.706328155     0.791758288 CORE    13 Si Si    0.0000    13
Si        4.144956223    -0.120241350     1.865925907 CORE    14 Si Si    0.0000    14
Si        1.391222616     1.635863742     2.799253092 CORE    15 Si Si    0.0000    15
Si       -0.970488144    -2.250883101     5.764575772 CORE    16 Si Si    0.0000    16
Si        2.536176189    -1.390242092     3.722614806 CORE    17 Si Si    0.0000    17
Si        2.954244449     0.697446748     4.933582785 CORE    18 Si Si    0.0000    18
end
end
```

MS4

```
!BIOSYM archive 2
PBC=ON

!DATE
PBC      6.3006      7.1079      4.9285    60.0912   122.3161   102.6260
O         1.304437428     3.542020778     1.817370367 CORE     1 O    O      0.0000     1
O        -0.640714595     5.010727660     2.978546270 CORE     2 O    O      0.0000     2
O         1.332805841     1.008283174     1.029578230 CORE     3 O    O      0.0000     3
O        -3.163250136     4.506125578     3.663342707 CORE     4 O    O      0.0000     4
O         3.826981467     4.046660216     1.132547355 CORE     5 O    O      0.0000     5
```

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O      3.165739352   1.972300698   2.875605954 CORE   6 O   O    0.0000   6
O     -0.496361973   5.561514935   0.463154145 CORE   7 O   O    0.0000   7
O     -0.672465572   2.027139900   2.486730199 CORE   8 O   O    0.0000   8
O     -2.501712282   6.580449623   1.920296619 CORE   9 O   O    0.0000   9
O      1.336547762   6.525588497   2.309117483 CORE  10 O   O    0.0000  10
O      3.795198905   1.063042752   0.640771405 CORE  11 O   O    0.0000  11
O      1.965949018   5.616368894   0.074275430 CORE  12 O   O    0.0000  12
Si     2.269938934   3.241487225   3.100264845 CORE  13 Si Si   0.0000  13
Si     0.437058458   2.277433610   1.254292241 CORE  14 Si Si   0.0000  14
Si    -1.606061265   5.311195140   1.695407295 CORE  15 Si Si   0.0000  15
Si     2.861593282   4.347137358  -0.150560580 CORE  16 Si Si   0.0000  16
Si     2.705505348   7.744405462   2.397963110 CORE  17 Si Si   0.0000  17
Si     0.872606926   6.780335153   0.551945602 CORE  18 Si Si   0.0000  18
end
end
```