

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 algorithm¹ 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 clusters², and has been extended to periodic crystals³. 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 ($\mathbf{q}_i$, $i=1, \dots, 3N$, 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. $\mathbf{Q}_{\text{IS}}(\mathbf{L}, \mathbf{q}) \rightarrow \mathbf{Q}_{\text{FS}}(\mathbf{L}, \mathbf{q})$, from initial state (IS) to final state (FS).

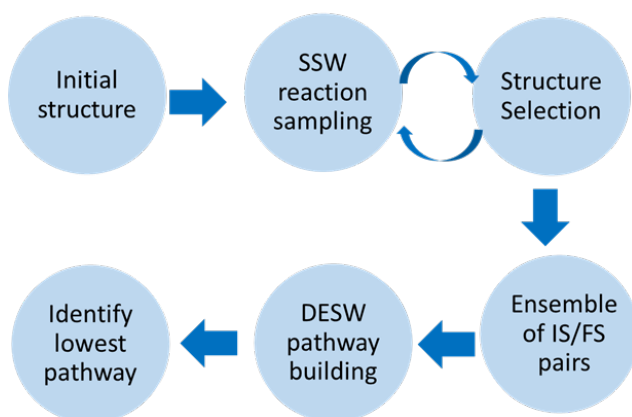
The SSW method inherits the idea of bias-potential driven constrained-Broyden-dimer (BP-CBD) method for TS location⁴. In one particular SSW step, labeled as i , a modified PES V_{m-to-n} (n is the index of the bias potential, $n=1, 2, \dots, H$), as shown in Eq. 1, is utilized for moving from the current 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 $\mathbf{N}_i^n$.

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

where $\mathbf{R}$ is the coordination vector of the structure and V_{real} represents the unmodified PES; $\mathbf{R}_i^n$ 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 method⁵

Here we outline the SSW-RS method briefly. More details on the methodology can be found in our previous works⁶⁻¹⁰. 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-DESW¹¹ 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

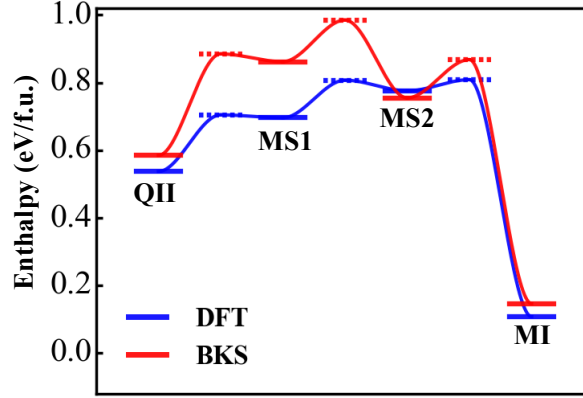


Figure S1. Reaction pathway from QII to MI calculated by BKS and DFT. The enthalpy of stishovite is set as zero in each calculation.

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 $\mathbf{R}$ and the lattice matrix $\mathbf{L}$, the fractional coordinate $\mathbf{q}$ can be calculated as

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

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

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

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

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

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

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

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

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

VI. Phase transition pathways from QII to St and MII

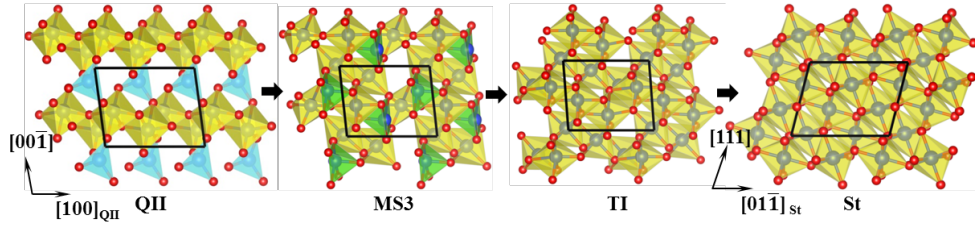


Figure S2. Reaction snapshots along the pathway from QII to St (also see Fig. 2 for energy profile). Polyhedron representation is used for all structures: yellow: $[\text{SiO}_6]$, green: $[\text{SiO}_5]$, light blue: $[\text{SiO}_4]$.

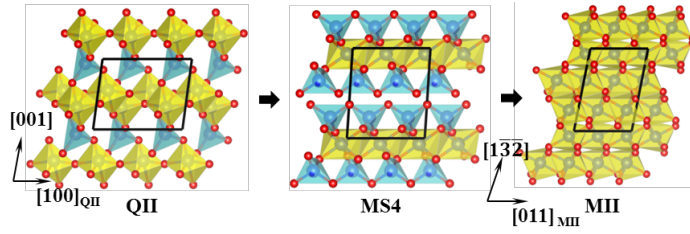


Figure S3. Reaction snapshots along the pathway from QII to MII (also see Fig. 2 for energy profile). Polyhedron representation is used for all structures: yellow: $[\text{SiO}_6]$, green: $[\text{SiO}_5]$, light blue: $[\text{SiO}_4]$.

VII. Simulated XRD pattern

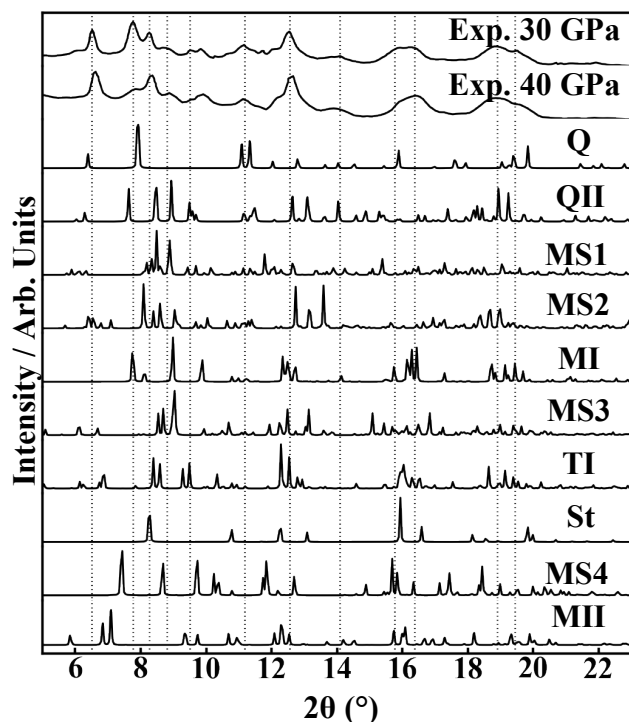


Figure S4. Simulated XRD for all possible structures (optimized with DFT under 30 GPa) from the reaction pathways, which are compared with experiment data under 30 GPa and under 40 GPa (reported in reference ¹⁵).

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

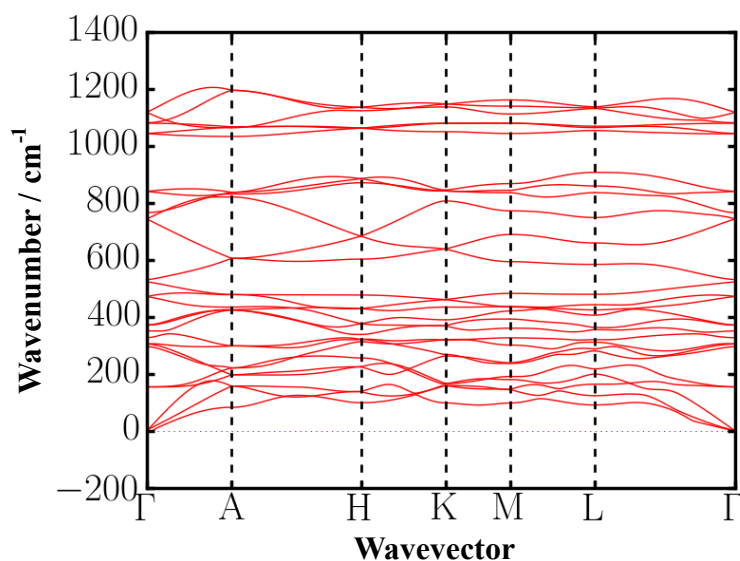


Figure S5. Phonon dispersion of α -quartz under 15 GPa calculated with DFT.

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

PBC=ON

!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)

!BIOSYM archive 2

PBC=ON

!DATE

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PBC      5.8671      4.6160      6.3738   86.4996  113.4868   73.8160
O         0.072272302    1.912529599    5.238345521 CORE    1 O   O    0.0000    1
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
```

O	1.311403931	3.335808732	3.489571938 CORE	5 O O	0.0000	5
O	-0.498811193	4.537093750	4.782817833 CORE	6 O O	0.0000	6
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
end						
end						

Monoclinic I (MI)

BIOSYM archive 2

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PBC	6.4349	4.0543	6.8649	89.9994	99.1595	129.0547		
O	4.724044448	0.361279126	1.384028917 CORE	1 O O	0.0000	1		
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		
O	-2.023654496	2.787179000	0.632946817 CORE	7 O O	0.0000	7		
O	3.324899781	1.836567874	2.870973689 CORE	8 O O	0.0000	8		
O	1.015407379	2.642452515	3.622069059 CORE	9 O O	0.0000	9		
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		
O	0.061326990	2.142523504	1.384027815 CORE	12 O O	0.0000	12		
Si	-1.524362042	1.989522773	2.127508413 CORE	13 Si Si	0.0000	13		
Si	1.693095312	1.989526357	2.127509337 CORE	14 Si Si	0.0000	14		
Si	-0.392061518	2.924252385	-0.119201254 CORE	15 Si Si	0.0000	15		
Si	1.748364429	2.018324793	6.599932806 CORE	16 Si Si	0.0000	16		
Si	3.778198612	1.054785997	4.374197396 CORE	17 Si Si	0.0000	17		
Si	0.545008831	1.074168207	4.374201297 CORE	18 Si Si	0.0000	18		
end								
end								

Stishovite (St)

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PBC	4.9306	4.9337	6.4441	71.4578	71.5042	72.9945			
O	3.015902487		2.240000609	0.118620026	CORE	1 O O	0.0000	1	
O	5.402403579		6.232722741	5.823840123	CORE	2 O O	0.0000	2	
O	6.503223367		4.824476094	4.065224384	CORE	3 O O	0.0000	3	
O	2.937148350		2.177698333	3.632499610	CORE	4 O O	0.0000	4	
O	4.038129534		0.769564793	1.873769190	CORE	5 O O	0.0000	5	
O	4.037861159		4.420718198	3.846976941	CORE	6 O O	0.0000	6	
O	4.380293259		3.244522245	1.659177289	CORE	7 O O	0.0000	7	
O	6.845636653		3.648196508	1.877347849	CORE	8 O O	0.0000	8	
O	2.937078665		5.829016085	5.605747969	CORE	9 O O	0.0000	9	
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	
Si	2.976552036		2.208861553	1.875539747	CORE	16 Si Si	0.0000	16	
Si	6.463932857		4.793359055	5.822114088	CORE	17 Si Si	0.0000	17	
Si	3.998693711		2.967724965	4.835447532	CORE	18 Si Si	0.0000	18	
end									
end									

Monoclinic II (MII)

!BIOSYM archive 2

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!DATE

PBC	4.9706	8.4876	4.9713	50.1670	115.1864	97.8071			
O	0.894765742		4.580245102	1.502474123	CORE	1 O O	0.0000	1	
O	-0.355553750		6.550524909	2.938372023	CORE	2 O O	0.0000	2	
O	0.837662053		1.290156794	0.211896002	CORE	3 O O	0.0000	3	
O	-2.648323573		6.042276063	3.211815322	CORE	4 O O	0.0000	4	
O	3.187536407		5.088487009	1.229027090	CORE	5 O O	0.0000	5	
O	2.265169224		2.752189065	1.921240719	CORE	6 O O	0.0000	6	
O	-0.647719903		7.239759169	0.516788629	CORE	7 O O	0.0000	7	
O	-0.240614255		2.428958117	2.214719649	CORE	8 O O	0.0000	8	
O	-1.726019672		8.378501351	2.519659161	CORE	9 O O	0.0000	9	
O	0.779784858		8.701798162	2.226134684	CORE	10 O O	0.0000	10	

O	3.302481528	0.966927633	0.505375951 CORE	11 O O	0.0000	11
O	1.817081131	6.916466737	0.810322172 CORE	12 O O	0.0000	12
Si	2.254502671	4.378691454	2.615173650 CORE	13 Si Si	0.0000	13
Si	0.826981944	2.916639470	0.905824494 CORE	14 Si Si	0.0000	14
Si	-1.715331276	6.752077350	1.825622716 CORE	15 Si Si	0.0000	15
Si	-0.287830280	8.214118277	3.534971500 CORE	16 Si Si	0.0000	16
Si	2.178437172	9.769840057	2.220414404 CORE	17 Si Si	0.0000	17
Si	0.750905319	8.307785758	0.511045335 CORE	18 Si Si	0.0000	18

end
end

MS1

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PBC	6.3310	4.6434	6.0694	113.7972	86.4672	109.7787		
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O	2.872320746	3.942546582	0.936477467 CORE	1 O O	0.0000	1
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		
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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		
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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

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						