Supplementary Information

Mechanism and Microstructures in Ga_2O_3 Pseudomartensitic Solid Phase Transition

Sheng-Cai Zhu, Shu-Hui Guan, Zhi-Pan Liu*

Collaborative Innovation Center of Chemistry for Energy Material, Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Key Laboratory of Computational Physical Science (Ministry of Education), Department of Chemistry, Fudan University, Shanghai 200433, China * email: zpliu@fudan.edu.cn

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1. Theoretical Methods

Stochastic Surface Walking (SSW) pathway sampling

The SSW algorithm has an automated climbing mechanism to manipulate a structure configuration from a minimum to a high-energy configuration along one random mode direction, inherits the idea of bias-potential driven constrained-Broyden-dimer (BP-CBD) method for TS location.[1] 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 $\mathbf{N}_i^n$.

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

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. The procedure is described below briefly.

Pathway collection In SSW pathway sampling, firstly, we start from one single phase (α-Ga_2O_3 in this paper), and utilize the SSW method to explore all the likely phases nearby the phase. A structure selection module is utilized to decide whether to accept/refuse once a new minimum is reached. If the new phase different from the starting phase is identified by the SSW crystal method, we record/output the IS (i.e. α-Ga_2O_3) and the FS (e.g. β-Ga_2O_3) of the current SSW step. Then, the program will return back to the IS by rejecting the new minimum to continue the phase exploration; On the other hand, if the new minimum identified by SSW is still α-Ga_2O_3, but with a permutation isomer with varied lattice, the program will accept the new isomeric phase and start the phase exploration from this phase. We repeat this procedure until a certain number of minima (>10^3 for first principle calculation) are explored, which produce a database including a large number of IS/FS pairs (>100 for first principle calculation).

Pathway screening Secondly, we use Euclidian distance between IS/FS pairs as an important quantity to screen out the candidate pathways from the database. The Euclidian distance is defined as

$$\boldsymbol{G} = \boldsymbol{L}^{\mathrm{T}}\boldsymbol{L} \quad (2)$$

$$\boldsymbol{G_r} = (\mathbf{G_{IS}} + \mathbf{G_{FS}})/2 \quad \textbf{(3)}$$

$$\boldsymbol{S} = \mathbf{G_r}^{1/2} \quad \textbf{(4)}$$

$$\boldsymbol{q}' = \boldsymbol{Sq} \quad \textbf{(5)}$$

Where $\boldsymbol{L}$ is the lattice vector in real distance units, e.g., in Å, $\boldsymbol{G}$ is a rotational invariant matrix, S is scaling matrix, which is defined as the square root of the metric tensor $\boldsymbol{G}_{\mathbf{r}}$. The fractional coordinate $\boldsymbol{q}$ can then be transformed to a new set of scaled coordinate, $\boldsymbol{q}'$ which is compatible with the lattice length. Then we can use the generalized coordinate $\{\boldsymbol{L}_{\mathrm{r}}, \boldsymbol{q}'\}$ to calculate the Euclidian distance between IS/FS pairs. According to our previous studies of phase transition on various materials, it have shown that the lowest energy pathway usually has the shortest Euclidian distance between IS/FS pairs, indicating a good structure match between IS and FS is a general requirement for low energy pathways.[2] Thus here we use Euclidian distance between IS and FS as an important quantity to screen out the low energy pathways from the large number of IS/FS pairs.

Lowest energy pathway determination Thirdly, we utilize the variable-cell double-ended surface walking (DESW) method[3] to establish the pseudopathway connecting IS to FS for all IS/FS pairs. The approximate barrier is obtained according to DESW pseudopathway, where the maximum energy point along the pathway is generally a good estimate for the true TS. It might be mentioned that at this stage, we generally examined thoroughly all the pathways we identified. Basically, even before we locate exactly the TS, we can have the following important information, including the approximate barrier, the pattern of lattice and atom movement from IS to FS, the habit plane and the OR for the pathways, From these, we can safely rule out the similar pathways and focus on the selected, distinct and low energy pathways. Next, the candidate lowest energy pathways are selected to locate exactly the "true" TS by using DESW TS-search method.[4] By sorting the exact barrier calculated, the energy difference between the TS and the IS, the lowest energy pathways can be finally obtained. All the lowest energy pathways will be further confirmed by extrapolating TS towards IS and FS.

2. Experimental details

2.1 Preparation of α-Ga_2O_3/β-Ga_2O_3 bicrystalline material

We have synthesized GaOOH using two different methods: (1) the precipitation method and (2) the hydrothermal method. These two methods produce Ga_2O_3 in different morphology. The hydrothermal method has been described in detail in the

main text. Here we describe the precipitation method in the following, which is used to produce large Ga_2O_3 spheres as shown in Figure 1b. The precipitation method used in this work is similar to that described previously.[5-7] The aqueous ammonia solution (5 wt%) was slowly added to a gallium nitrate solution ($Ga(NO_3)_3$, 10 wt%) under continuous stirring until the pH value of the mixture reaches 8.0. The resulting precipitate was filtered, washed with water, and dried in an oven at 80℃ for 24 h to yield a white powder, GaOOH. The α-Ga_2O_3 phase is then synthesized by calcinating GaOOH at 450℃ for 2 h. The α-Ga_2O_3/β- Ga_2O_3 bicrystalline material was prepared by calcinating α-Ga_2O_3 at elevated temperatures (500-650℃) for 2 h (SEM images in Figure 1).

3. XRD, SEM, HRTEM

3.1 XRD

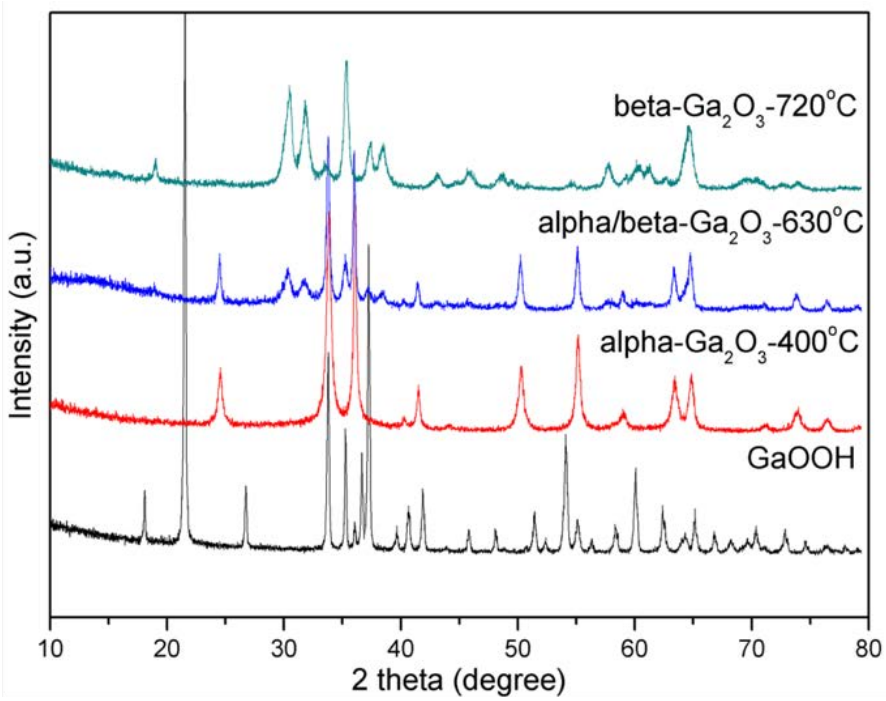

Figure S1. XRD pattern of GaOOH, α-Ga_2O_3, α- Ga_2O_3/β-Ga_2O_3 and β-Ga_2O_3 samples obtained at different calcination temperatures. GaOOH is prepared using the hydrothermal method[8]. XRD uses Cu Kα radiation with λ= 1.5406 Å (see main text Section 2.3 for discussion on XRD peaks).

3.2 SEM

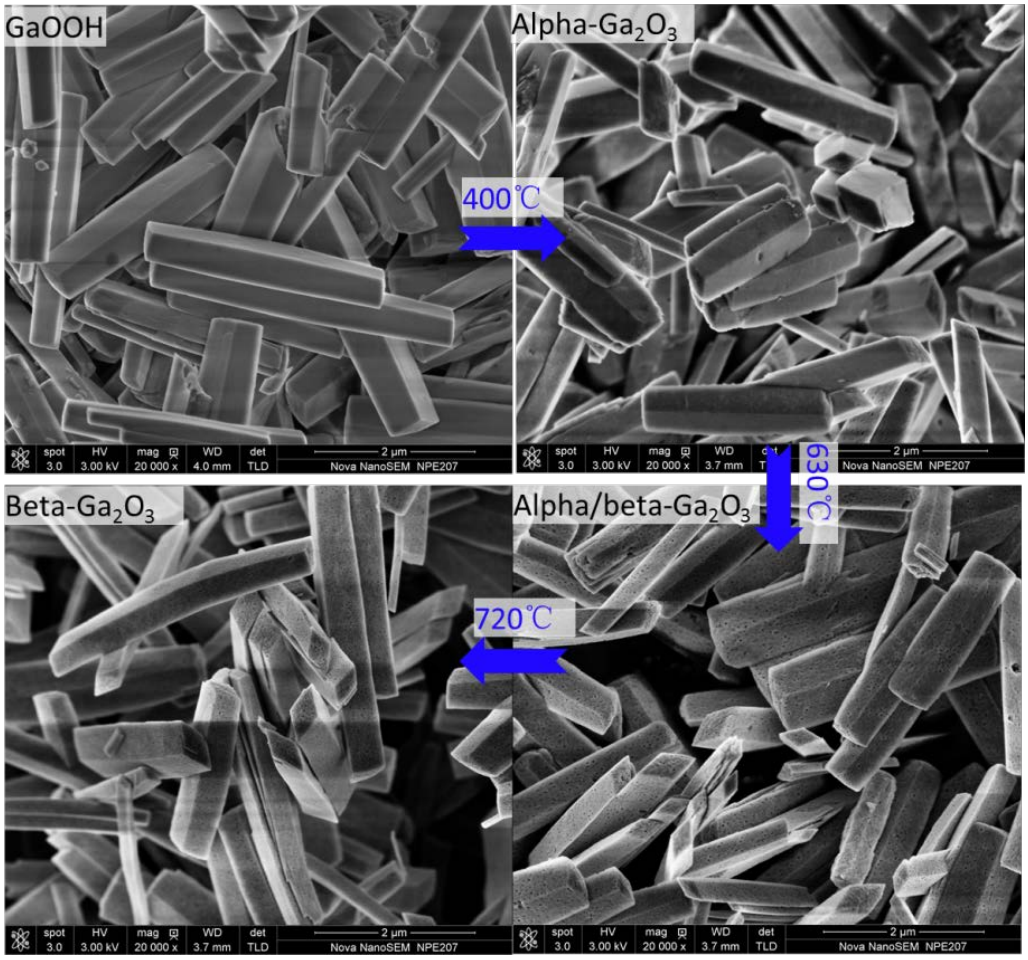

Figure S2. SEM images of GaOOH, α-Ga_2O_3, α-Ga_2O_3/β-Ga_2O_3 and β-Ga_2O_3 samples obtained at different calcination temperatures. GaOOH is prepared using the hydrothermal method[8]. The Ga_2O_3 nanostructures are uniform nanorods with ~3 μm in length and 500 nm in width. There are pores on α-Ga_2O_3 and β-Ga_2O_3 surfaces due to the dehydration of GaOOH[6]. In the phase transition, the morphology of Ga_2O_3 can be preserved as that of GaOOH without particle aggregation and fusion.

3.3 HRTEM from different zone axes

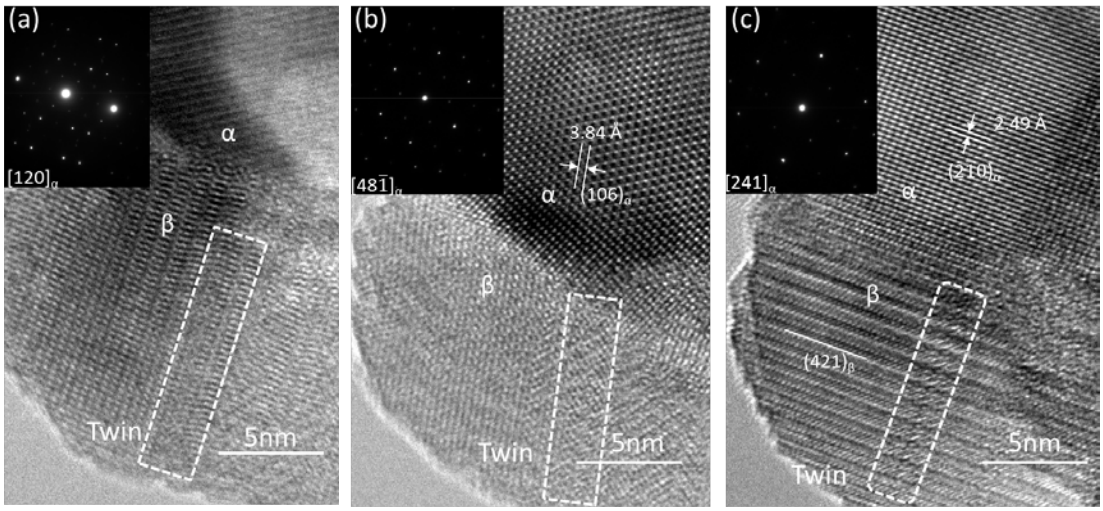

Figure S3. HRTEM of a same α-Ga_2O_3/β-Ga_2O_3 biphase junction at three different zone axes. Part of **(a)** is already shown in Figure 6i. (**b-c)** are the images at the other two zone axes by rotating the samples.

4. The biphase junction models

From the lowest energy pathway (shown in Figure 4), it is possible to identify the lowest strain interface (strain-invariant plane) based on the classic phenomenological theory of Martensitic transition[9-13] (the detail of the procedure can be found in our previous publications[14-16]). In this work, we have constructed two likely models of the interfaces using the superlattice approach, Model A and Model B, which are shown in Figure S4. The two models share the same strain-invariant line, $[120]_\alpha//[1\bar{3}2]_\beta$, the close-packed O rows, but differ in the interface planes. Model A turns out to be the one with the lowest strain and the best atomic match, which is presented in the main text. The OR of Model A is $(001)_\alpha//(20\ \bar{1}\ )_\beta+[120]_\alpha//[1\ \bar{3}\ 2]_\beta$ (or $(0001)_{hcp}//(111)_{fcc}+[11\bar{2}0]_{hcp}//[1\bar{1}0]_{fcc}$ in the notation of O sublattice). The smallest and best-matched unit cells of the two interface planes are as follows. $(001)_\alpha$: **a**=8.72 Å; **b**=8.76 Å; angle= 60.09°; and $(20\bar{1})_\beta$: **a**=8.79 Å, **b**=8.78 Å, angle= 63.31°. This interface has been discussed in the main text and the OR is proved by experiment.

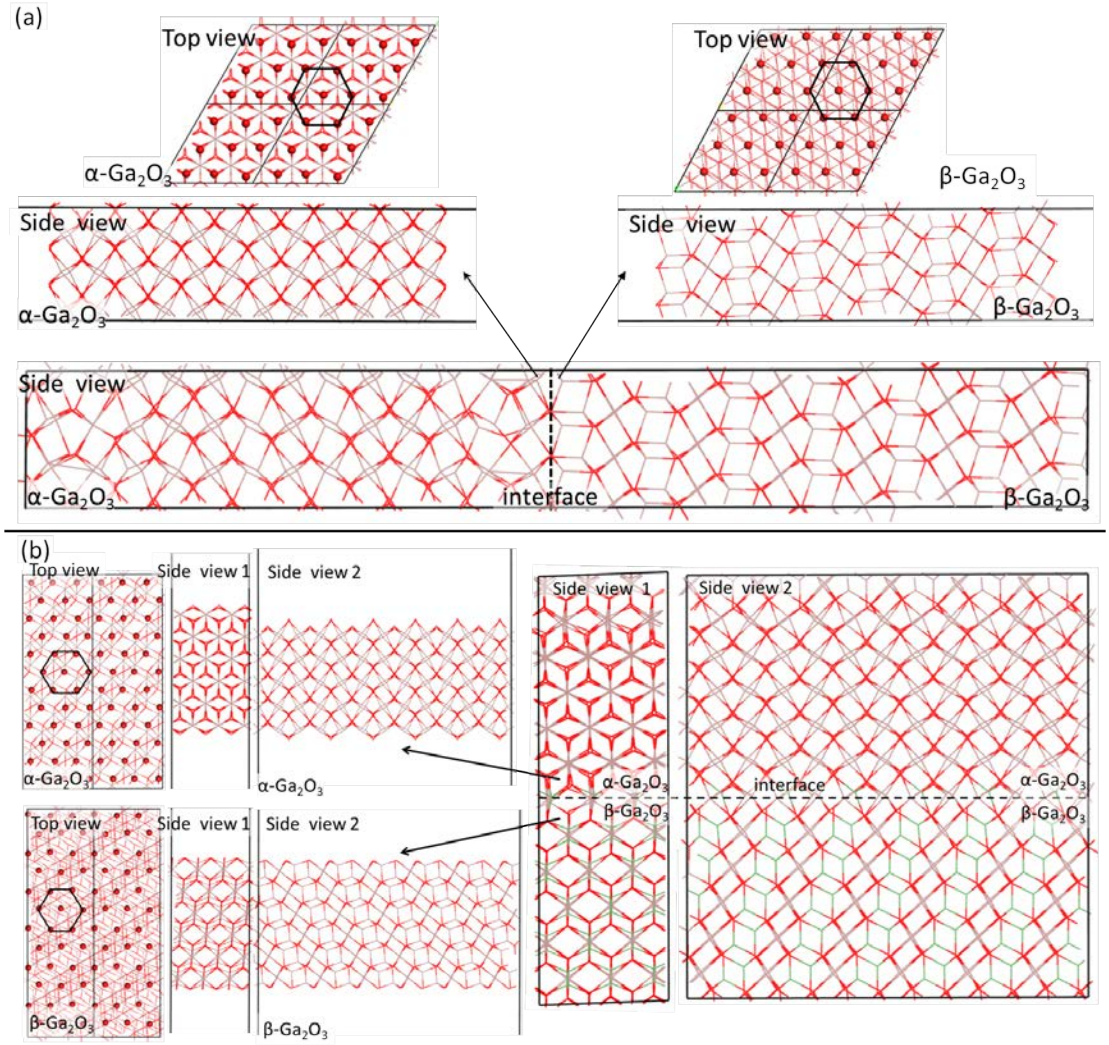

Figure S4. Two likely bi-phase junction models constructed according to the lowest energy pathway. (a) Model A with OR: $(001)_\alpha//(20\bar{1})_\beta + [120]_\alpha//[1\bar{3}2]_\beta$; (b) Model B with OR: $(2\bar{1}0)_\alpha//(3\bar{1}0)_\beta + [120]_\alpha//[1\bar{3}2]_\beta$.

Model B has a larger strain and, importantly, has poorer atomic match at the interface. The OR of Model B can be written as $(2\bar{1}0)_\alpha//(3\bar{1}0)_\beta + [120]_\alpha//[1\bar{3}2]_\beta$, which is 19.5 degrees from the OR of Model A. The smallest and best-matched unit cell of the two interface planes can be taken as follows: $(2\bar{1}0)_\alpha$: **a**=8.76 Å; **b**=26.85 Å; angle= 89.9°; and $(3\bar{1}0)_\beta$: **a**=8.78 Å; **b**=30.12 Å; angle= 90.1°. With ~12% stretch in the **b** axis, the strain energy of this interface is found to be larger than that of Model A based on finite strain theory [14-16]. In addition, although the O-terminated planes of $(2\bar{1}0)_\alpha$ and $(3\bar{1}0)_\beta$ form the similar hexagon patterns, the O-terminated plane of $(2\bar{1}0)_\alpha$ is highly

corrugated while that of $(3\bar{1}0)_\beta$ is flat. This indicates a poor atomic match at the interface. We did not find experimental evidence for this OR in this work. We therefore disregard the possibility of this OR as the preferential OR for the phase transition.

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5. Supporting data from theory

XYZ coordinates in .arc format

10-atom pathway

α-Ga_2O_3

PBC	5.0587	5.0585	5.3966	90.0109	62.0475	120.0048			
O	1.760333631	2.781769880	1.135631902	CORE	1 O	O	0.0000	1
O	-0.769132487	4.508196786	1.135717368	CORE	2 O	O	0.0000	2
O	4.059174041	1.454711670	1.135722318	CORE	3 O	O	0.0000	3
O	3.292970044	3.047687475	3.404698215	CORE	4 O	O	0.0000	4
O	5.822395774	1.321297133	3.404738970	CORE	5 O	O	0.0000	5
O	0.994136701	4.374734751	3.404703803	CORE	6 O	O	0.0000	6
Ga	2.526695512	1.454335732	2.576397695	CORE	7 Ga	Ga	0.0000	7
Ga	5.055927795	2.914553911	4.233179890	CORE	8 Ga	Ga	0.0000	8
Ga	2.526395623	4.375082671	1.964192645	CORE	9 Ga	Ga	0.0000	9
Ga	-0.002836120	2.914850552	0.307345606	CORE	10 Ga	Ga	0.0000	10

β-Ga_2O_3

PBC	3.0831	7.6362	6.4125	55.5469	76.0777	101.6386			
O	1.540420357	6.597704759	1.121313503	CORE	1 O	O	0.0000	1
O	1.540453933	1.608640958	1.347317491	CORE	2 O	O	0.0000	2
O	-0.000304710	4.046280508	1.337349487	CORE	3 O	O	0.0000	3
O	1.541723135	4.885331949	3.631941103	CORE	4 O	O	0.0000	4
O	1.541857819	9.874955200	3.405440790	CORE	5 O	O	0.0000	5
O	3.082555815	7.437255766	3.415597309	CORE	6 O	O	0.0000	6
Ga	1.541509602	3.380541814	2.361491093	CORE	7 Ga	Ga	0.0000	7
Ga	3.083328009	5.755122323	4.206914229	CORE	8 Ga	Ga	0.0000	8
Ga	1.540755624	8.103569325	2.391333371	CORE	9 Ga	Ga	0.0000	9
Ga	-0.001268467	5.728086228	0.545643164	CORE	10 Ga	Ga	0.0000	10

60-atom pathway

α-Ga_2O_3

PBC	9.5314	8.7619	8.7571	59.9887	81.2314	72.2188			
O	10.479350270	6.889094644	6.724589479	CORE	1 O	O	0.0000	1
O	8.740010621	1.453980486	1.435216529	CORE	2 O	O	0.0000	2
O	7.051451223	11.060749035	6.724685058	CORE	3 O	O	0.0000	3
O	4.907368285	4.358123204	4.195460373	CORE	4 O	O	0.0000	4
O	5.312257575	5.625526520	1.435291656	CORE	5 O	O	0.0000	5
O	11.010807884	8.529823992	4.195419870	CORE	6 O	O	0.0000	6
O	9.671983252	4.358197280	6.723196099	CORE	7 O	O	0.0000	7

O	10.481202382	6.889099532	1.669260048	CORE	8 O	O	0.0000	8
O	6.244126023	8.529714718	6.723123330	CORE	9 O	O	0.0000	9
O	6.649122626	9.797226296	3.963074033	CORE	10 O	O	0.0000	10
O	4.377685300	2.717428685	1.669344066	CORE	11 O	O	0.0000	11
O	10.076940488	5.625562606	3.963038566	CORE	12 O	O	0.0000	12
O	11.413845889	9.797256225	6.490634759	CORE	13 O	O	0.0000	13
O	9.673856573	4.358245994	1.667771621	CORE	14 O	O	0.0000	14
O	5.310313392	5.625538656	6.490507103	CORE	15 O	O	0.0000	15
O	5.714659227	6.888982315	4.196892861	CORE	16 O	O	0.0000	16
O	6.245986505	8.529863922	1.667771757	CORE	17 O	O	0.0000	17
O	9.142365055	2.717415303	4.197017293	CORE	18 O	O	0.0000	18
O	8.766773384	8.976238998	5.725488135	CORE	19 O	O	0.0000	19
O	7.024527936	3.538337645	0.904185736	CORE	20 O	O	0.0000	20
O	2.663580321	4.804503199	5.725519805	CORE	21 O	O	0.0000	21
O	3.191759316	6.443826405	3.196879193	CORE	22 O	O	0.0000	22
O	3.596481672	7.709943174	0.904169298	CORE	23 O	O	0.0000	23
O	6.619631096	2.272131211	3.197035874	CORE	24 O	O	0.0000	24
O	7.022606239	3.538215740	5.959449809	CORE	25 O	O	0.0000	25
O	7.958419282	6.443911885	0.669302548	CORE	26 O	O	0.0000	26
O	3.594690143	7.709774139	5.959575257	CORE	27 O	O	0.0000	27
O	4.002448569	8.976258675	3.197802288	CORE	28 O	O	0.0000	28
O	1.854932226	2.272204713	0.669226588	CORE	29 O	O	0.0000	29
O	7.430184431	4.804638442	3.197892699	CORE	30 O	O	0.0000	30
O	7.956443972	6.443831291	5.724760840	CORE	31 O	O	0.0000	31
O	6.093118741	0.633153832	0.670014399	CORE	32 O	O	0.0000	32
O	4.528665826	10.615429937	5.724626727	CORE	33 O	O	0.0000	33
O	2.257866064	3.538330139	3.431923625	CORE	34 O	O	0.0000	34
O	2.665448333	4.804635220	0.670196827	CORE	35 O	O	0.0000	35
O	8.361311850	7.709837575	3.431753765	CORE	36 O	O	0.0000	36
Ga	11.072452438	11.440329437	7.487958357	CORE	37 Ga	Ga	0.0000	37
Ga	8.398599185	3.096864857	2.432740135	CORE	38 Ga	Ga	0.0000	38
Ga	4.968836064	7.268473020	7.488009323	CORE	39 Ga	Ga	0.0000	39
Ga	3.940547901	6.067293272	4.959918028	CORE	40 Ga	Ga	0.0000	40
Ga	4.970895123	7.268552729	2.432677959	CORE	41 Ga	Ga	0.0000	41
Ga	10.043965355	10.238995090	4.959909060	CORE	42 Ga	Ga	0.0000	42
Ga	6.991744469	8.152847723	4.959667069	CORE	43 Ga	Ga	0.0000	43
Ga	8.705218188	6.067513020	7.487565306	CORE	44 Ga	Ga	0.0000	44
Ga	10.419685920	3.981216313	4.959622186	CORE	45 Ga	Ga	0.0000	45
Ga	1.918883205	5.181445116	2.432704654	CORE	46 Ga	Ga	0.0000	46
Ga	5.277346131	10.239074940	7.487646865	CORE	47 Ga	Ga	0.0000	47
Ga	8.022495872	9.353199529	2.432659751	CORE	48 Ga	Ga	0.0000	48
Ga	9.735462916	7.268536572	4.960314558	CORE	49 Ga	Ga	0.0000	49
Ga	1.916941672	5.181533992	7.488049349	CORE	50 Ga	Ga	0.0000	50
Ga	3.632102936	3.096843541	4.960439902	CORE	51 Ga	Ga	0.0000	51

Ga	2.603651208	1.895813057	2.432306267	CORE	52	Ga	Ga	0.0000	52
Ga	8.020479085	9.353154644	7.488049969	CORE	53	Ga	Ga	0.0000	53
Ga	8.707100875	6.067402604	2.432132797	CORE	54	Ga	Ga	0.0000	54
Ga	11.756492362	8.152917387	7.487334374	CORE	55	Ga	Ga	0.0000	55
Ga	11.758502873	8.152892494	2.431882264	CORE	56	Ga	Ga	0.0000	56
Ga	8.328749130	12.324563154	7.487316998	CORE	57	Ga	Ga	0.0000	57
Ga	6.683617271	5.181449408	4.960377727	CORE	58	Ga	Ga	0.0000	58
Ga	5.654811367	3.981239351	2.431942945	CORE	59	Ga	Ga	0.0000	59
Ga	3.255837005	9.353140435	4.960409735	CORE	60	Ga	Ga	0.0000	60

MS-A

PBC	9.7353	8.6550	8.7499	62.1837	81.6273	74.6936

O	10.309463360	6.739310259	6.948193877	CORE	1	O	O	0.0000	1
O	8.981739708	1.379376250	1.580576938	CORE	2	O	O	0.0000	2
O	6.584554916	10.913161112	6.948198813	CORE	3	O	O	0.0000	3
O	4.909600842	4.170962353	4.239985767	CORE	4	O	O	0.0000	4
O	5.256430077	5.553479845	1.580595019	CORE	5	O	O	0.0000	5
O	10.919634257	8.344844928	4.239612555	CORE	6	O	O	0.0000	6
O	9.677394280	4.165502388	6.822812454	CORE	7	O	O	0.0000	7
O	10.434064021	6.817725323	1.693974935	CORE	8	O	O	0.0000	8
O	5.951981595	8.339686624	6.822655938	CORE	9	O	O	0.0000	9
O	6.450191849	9.637871104	4.055271619	CORE	10	O	O	0.0000	10
O	4.423724942	2.643615975	1.693664198	CORE	11	O	O	0.0000	11
O	10.175545211	5.464180961	4.055293195	CORE	12	O	O	0.0000	12
O	11.103931960	9.635537196	6.616792752	CORE	13	O	O	0.0000	13
O	9.691240066	4.225673145	1.788256126	CORE	14	O	O	0.0000	14
O	5.093568159	5.461674333	6.617143400	CORE	15	O	O	0.0000	15
O	5.564635017	6.700187675	4.297865644	CORE	16	O	O	0.0000	16
O	5.966043897	8.399434348	1.788491449	CORE	17	O	O	0.0000	17
O	9.289453220	2.526068438	4.297511374	CORE	18	O	O	0.0000	18
O	8.328644076	9.072527772	5.873926732	CORE	19	O	O	0.0000	19
O	7.046081494	3.575009620	0.762850838	CORE	20	O	O	0.0000	20
O	2.318715338	4.898810575	5.874053897	CORE	21	O	O	0.0000	21
O	3.000376635	6.279325686	3.209067488	CORE	22	O	O	0.0000	22
O	3.320801486	7.749030976	0.762815627	CORE	23	O	O	0.0000	23
O	6.725389850	2.105652889	3.208539712	CORE	24	O	O	0.0000	24
O	6.839409493	3.192070930	5.799052197	CORE	25	O	O	0.0000	25
O	8.027241115	6.112584274	0.738202680	CORE	26	O	O	0.0000	26
O	3.113991976	7.366441128	5.798907090	CORE	27	O	O	0.0000	27
O	3.752168011	8.806446824	3.263150317	CORE	28	O	O	0.0000	28
O	2.016627364	1.938817046	0.738281945	CORE	29	O	O	0.0000	29
O	7.477553668	4.632066115	3.263130557	CORE	30	O	O	0.0000	30
O	7.716923290	6.221960503	5.796435707	CORE	31	O	O	0.0000	31
O	6.295108781	0.612572813	0.637317374	CORE	32	O	O	0.0000	32

O	3.991990844	10.396074840	5.796323867 CORE	33 O	O	0.0000	33
O	2.086834380	3.453197556	3.403094841 CORE	34 O	O	0.0000	34
O	2.569742060	4.786927401	0.637427607 CORE	35 O	O	0.0000	35
O	8.096833268	7.626912731	3.403044762 CORE	36 O	O	0.0000	36
Ga	10.753977530	11.262729057	7.748698284 CORE	37 Ga	Ga	0.0000	37
Ga	8.507177715	2.930013901	2.613914723 CORE	38 Ga	Ga	0.0000	38
Ga	4.743395664	7.088940215	7.748549855 CORE	39 Ga	Ga	0.0000	39
Ga	3.932318734	5.773724024	5.018579394 CORE	40 Ga	Ga	0.0000	40
Ga	4.781769393	7.103885710	2.613968694 CORE	41 Ga	Ga	0.0000	41
Ga	9.942364458	9.947616565	5.018447615 CORE	42 Ga	Ga	0.0000	42
Ga	6.961755605	7.871139837	5.038916157 CORE	43 Ga	Ga	0.0000	43
Ga	8.516566698	5.835619657	7.421148588 CORE	44 Ga	Ga	0.0000	44
Ga	10.687297786	3.697279055	5.038998318 CORE	45 Ga	Ga	0.0000	45
Ga	1.754152198	4.992114759	2.341464792 CORE	46 Ga	Ga	0.0000	46
Ga	4.791595706	10.009608174	7.421265444 CORE	47 Ga	Ga	0.0000	47
Ga	7.764239199	9.165970595	2.341500249 CORE	48 Ga	Ga	0.0000	48
Ga	11.060005979	6.676954463	5.199630138 CORE	49 Ga	Ga	0.0000	49
Ga	1.588696292	5.073085272	7.731540784 CORE	50 Ga	Ga	0.0000	50
Ga	5.049924124	2.502636992	5.199784284 CORE	51 Ga	Ga	0.0000	51
Ga	2.753082377	1.850211450	2.715781189 CORE	52 Ga	Ga	0.0000	52
Ga	7.598987906	9.246960646	7.731557368 CORE	53 Ga	Ga	0.0000	53
Ga	8.763058983	6.023864165	2.715826541 CORE	54 Ga	Ga	0.0000	54
Ga	10.301221676	8.415724617	7.818790132 CORE	55 Ga	Ga	0.0000	55
Ga	11.746064141	8.052450507	2.415386927 CORE	56 Ga	Ga	0.0000	56
Ga	6.575553769	12.589871333	7.819128944 CORE	57 Ga	Ga	0.0000	57
Ga	6.665175637	4.916330231	5.022326990 CORE	58 Ga	Ga	0.0000	58
Ga	5.735796895	3.878284325	2.415140955 CORE	59 Ga	Ga	0.0000	59
Ga	2.939966778	9.090660995	5.022381471 CORE	60 Ga	Ga	0.0000	60

MS-B

PBC	9.7845	8.7604	9.0992	60.2706	82.0251	86.4217

O	9.699141261	6.908969994	7.017589670 CORE	1 O	O	0.0000	1
O	8.918327228	0.799287813	1.472391219 CORE	2 O	O	0.0000	2
O	5.080854516	11.506753744	7.030959558 CORE	3 O	O	0.0000	3
O	4.612247860	4.210686373	4.192324648 CORE	4 O	O	0.0000	4
O	4.408027462	5.624054754	1.587786213 CORE	5 O	O	0.0000	5
O	9.626696450	8.258331446	4.099332056 CORE	6 O	O	0.0000	6
O	9.529983951	4.002098541	6.784698302 CORE	7 O	O	0.0000	7
O	8.949649678	6.877683945	1.732575774 CORE	8 O	O	0.0000	8
O	4.733677937	8.430446385	6.686940164 CORE	9 O	O	0.0000	9
O	4.871719968	10.142123532	4.062166298 CORE	10 O	O	0.0000	10
O	3.880696909	2.858905084	1.812749373 CORE	11 O	O	0.0000	11
O	9.586183818	5.593095303	4.139926933 CORE	12 O	O	0.0000	12
O	9.841722635	9.867150026	6.611523436 CORE	13 O	O	0.0000	13

O	9.074086384	4.160828448	1.781428159	CORE	14	O	O	0.0000	14
O	4.863155991	5.637980197	6.572683205	CORE	15	O	O	0.0000	15
O	4.619409041	7.040148041	4.359385837	CORE	16	O	O	0.0000	16
O	4.372904342	8.653453531	1.748783944	CORE	17	O	O	0.0000	17
O	9.204197581	2.724359422	4.455130209	CORE	18	O	O	0.0000	18
O	6.894691405	9.927065591	5.869167830	CORE	19	O	O	0.0000	19
O	6.334058022	4.132368602	0.482296856	CORE	20	O	O	0.0000	20
O	1.909531485	5.498094588	5.899153717	CORE	21	O	O	0.0000	21
O	1.956223180	6.874928170	2.818975592	CORE	22	O	O	0.0000	22
O	1.747120664	8.260752332	0.407507595	CORE	23	O	O	0.0000	23
O	6.469264684	2.630749245	2.872919177	CORE	24	O	O	0.0000	24
O	6.864096415	3.763744318	5.505805529	CORE	25	O	O	0.0000	25
O	6.855228138	6.780734019	0.215601954	CORE	26	O	O	0.0000	26
O	2.100497693	8.095993768	5.620370624	CORE	27	O	O	0.0000	27
O	2.000257974	9.750658575	3.304589787	CORE	28	O	O	0.0000	28
O	1.733089651	2.137572298	0.237677944	CORE	29	O	O	0.0000	29
O	6.968627989	5.318996870	3.281123325	CORE	30	O	O	0.0000	30
O	7.152121486	6.919279263	5.588971432	CORE	31	O	O	0.0000	31
O	6.198213832	0.959946142	0.603737781	CORE	32	O	O	0.0000	32
O	2.474651083	11.127407950	5.624056845	CORE	33	O	O	0.0000	33
O	1.782375102	3.940247890	3.408550435	CORE	34	O	O	0.0000	34
O	1.613445989	5.175686186	0.639786127	CORE	35	O	O	0.0000	35
O	6.812671120	8.353247838	3.328868223	CORE	36	O	O	0.0000	36
Ga	8.128349653	8.352634043	0.714469554	CORE	37	Ga	Ga	0.0000	37
Ga	8.036820651	3.606037526	3.274422215	CORE	38	Ga	Ga	0.0000	38
Ga	2.764204133	3.696426372	0.551702871	CORE	39	Ga	Ga	0.0000	39
Ga	3.516381632	6.905697348	5.984966953	CORE	40	Ga	Ga	0.0000	40
Ga	3.821954549	7.088941640	2.663900356	CORE	41	Ga	Ga	0.0000	41
Ga	8.792623648	11.411352241	6.152475938	CORE	42	Ga	Ga	0.0000	42
Ga	5.924891056	8.446746100	5.089347316	CORE	43	Ga	Ga	0.0000	43
Ga	7.879084303	6.910176233	7.376053885	CORE	44	Ga	Ga	0.0000	44
Ga	10.663626877	4.013088711	5.141230434	CORE	45	Ga	Ga	0.0000	45
Ga	0.821991324	5.283803733	2.427271060	CORE	46	Ga	Ga	0.0000	46
Ga	3.234514575	11.044223909	7.321598688	CORE	47	Ga	Ga	0.0000	47
Ga	5.960568602	9.758834145	2.367887331	CORE	48	Ga	Ga	0.0000	48
Ga	10.441270893	6.939356898	5.248926948	CORE	49	Ga	Ga	0.0000	49
Ga	11.080462911	5.769426626	7.758172079	CORE	50	Ga	Ga	0.0000	50
Ga	5.857802943	11.433612525	5.132935504	CORE	51	Ga	Ga	0.0000	51
Ga	2.768069327	2.334819961	3.370101384	CORE	52	Ga	Ga	0.0000	52
Ga	6.489580761	10.246220019	7.719006062	CORE	53	Ga	Ga	0.0000	53
Ga	8.121555247	6.962490069	3.527179043	CORE	54	Ga	Ga	0.0000	54
Ga	8.097512397	5.223041597	0.578221054	CORE	55	Ga	Ga	0.0000	55
Ga	10.699658013	8.449850890	2.421349009	CORE	56	Ga	Ga	0.0000	56
Ga	2.947134074	0.263737827	0.146958706	CORE	57	Ga	Ga	0.0000	57

Ga	5.956898603	5.403956633	5.023693353 CORE	58 Ga	Ga	0.0000	58	
Ga	5.318517512	4.121033648	2.396933690 CORE	59 Ga	Ga	0.0000	59	
Ga	1.203713714	9.694807469	5.076816738 CORE	60 Ga	Ga	0.0000	60	
MS-C								
PBC	9.8933	8.7506	8.9391	61.0048	84.3176	91.1316		
O	9.422558071	6.880637993	6.706102616 CORE	1 O	O	0.0000	1	
O	8.692701618	9.617505329	1.370901530 CORE	2 O	O	0.0000	2	
O	4.265706729	11.144196089	6.870245171 CORE	3 O	O	0.0000	3	
O	4.046009754	3.714486840	4.117394210 CORE	4 O	O	0.0000	4	
O	3.920646973	5.154051662	1.449122988 CORE	5 O	O	0.0000	5	
O	9.084098448	8.267857436	4.109559706 CORE	6 O	O	0.0000	6	
O	9.267477057	3.935684759	6.646238653 CORE	7 O	O	0.0000	7	
O	8.421651748	7.000160178	1.699290030 CORE	8 O	O	0.0000	8	
O	4.373814034	8.194235302	6.730197159 CORE	9 O	O	0.0000	9	
O	4.124169435	9.753969278	4.083521814 CORE	10 O	O	0.0000	10	
O	3.420860016	2.508603195	1.714294169 CORE	11 O	O	0.0000	11	
O	9.096649932	5.503410320	3.989830716 CORE	12 O	O	0.0000	12	
O	9.164012768	9.846032162	6.574713116 CORE	13 O	O	0.0000	13	
O	8.827365635	4.169780206	1.612072880 CORE	14 O	O	0.0000	14	
O	4.268572412	5.307492665	6.727354710 CORE	15 O	O	0.0000	15	
O	3.969600425	6.982290148	4.341433787 CORE	16 O	O	0.0000	16	
O	3.699916741	8.564129868	1.779818759 CORE	17 O	O	0.0000	17	
O	8.945113635	2.644389143	4.305884449 CORE	18 O	O	0.0000	18	
O	6.287339268	9.847622202	5.706121074 CORE	19 O	O	0.0000	19	
O	6.209408654	4.188735562	0.360263785 CORE	20 O	O	0.0000	20	
O	1.474086162	5.438712002	5.702752119 CORE	21 O	O	0.0000	21	
O	1.199763702	6.945345309	2.894586012 CORE	22 O	O	0.0000	22	
O	1.051213410	8.418224213	0.472707349 CORE	23 O	O	0.0000	23	
O	6.211060218	2.580881126	2.733945235 CORE	24 O	O	0.0000	24	
O	6.617548193	3.681093063	5.374049918 CORE	25 O	O	0.0000	25	
O	6.320214245	6.808496184	0.146304462 CORE	26 O	O	0.0000	26	
O	1.713774577	8.095337777	5.308753393 CORE	27 O	O	0.0000	27	
O	1.380497042	9.652466092	3.215855116 CORE	28 O	O	0.0000	28	
O	1.451562518	2.362865548	0.103638765 CORE	29 O	O	0.0000	29	
O	6.642075830	5.186203614	2.948482105 CORE	30 O	O	0.0000	30	
O	6.699148541	6.774873357	5.555538668 CORE	31 O	O	0.0000	31	
O	6.159700870	1.019353334	0.263673141 CORE	32 O	O	0.0000	32	
O	1.567696032	11.148183133	5.525171630 CORE	33 O	O	0.0000	33	
O	1.318341599	3.910246218	3.277141801 CORE	34 O	O	0.0000	34	
O	1.246805424	5.300111256	0.549573928 CORE	35 O	O	0.0000	35	
O	6.283350165	8.259040076	3.228307617 CORE	36 O	O	0.0000	36	
Ga	7.413682280	8.369207735	0.616276712 CORE	37 Ga	Ga	0.0000	37	
Ga	7.820831999	3.608345740	3.130423637 CORE	38 Ga	Ga	0.0000	38	
Ga	2.597776158	3.937264783	0.646047971 CORE	39 Ga	Ga	0.0000	39	

Ga	3.092951828	6.707166103	5.992640692 CORE	40 Ga Ga	0.0000	40
Ga	2.737622494	8.097325562	3.422694815 CORE	41 Ga Ga	0.0000	41
Ga	7.844503065	11.136274679	5.967752991 CORE	42 Ga Ga	0.0000	42
Ga	5.337038626	8.244837969	4.977527106 CORE	43 Ga Ga	0.0000	43
Ga	7.698251853	7.088558663	7.206003468 CORE	44 Ga Ga	0.0000	44
Ga	10.349688918	3.899940102	5.015685104 CORE	45 Ga Ga	0.0000	45
Ga	0.420837834	5.234578266	2.293805881 CORE	46 Ga Ga	0.0000	46
Ga	2.452933235	11.191256771	7.269865985 CORE	47 Ga Ga	0.0000	47
Ga	5.203183377	9.627838121	2.384041475 CORE	48 Ga Ga	0.0000	48
Ga	10.183726865	6.821215421	4.879430436 CORE	49 Ga Ga	0.0000	49
Ga	10.645922548	5.680957052	7.530280416 CORE	50 Ga Ga	0.0000	50
Ga	4.934590560	11.224172350	5.082274611 CORE	51 Ga Ga	0.0000	51
Ga	2.623742867	2.560040884	3.492756987 CORE	52 Ga Ga	0.0000	52
Ga	5.653981611	9.929779206	7.578759095 CORE	53 Ga Ga	0.0000	53
Ga	7.540852988	6.816711741	3.526660267 CORE	54 Ga Ga	0.0000	54
Ga	7.725035954	5.384266284	0.663231529 CORE	55 Ga Ga	0.0000	55
Ga	-0.005851424	8.405858882	2.290837367 CORE	56 Ga Ga	0.0000	56
Ga	2.741707875	0.917112466	0.745541646 CORE	57 Ga Ga	0.0000	57
Ga	6.026230082	5.118331647	6.323779266 CORE	58 Ga Ga	0.0000	58
Ga	5.054924155	4.199272275	2.577599436 CORE	59 Ga Ga	0.0000	59
Ga	10.345014354	9.552910954	5.116488490 CORE	60 Ga Ga	0.0000	60

MS-D

PBC	9.7939	8.8926	9.0158	59.8194	81.1759	88.1659			
O	9.874345375	6.957064208	6.960075914 CORE	1 O	O	0.0000	1
O	8.773736189	0.837942633	1.334137477 CORE	2 O	O	0.0000	2
O	5.113490691	11.394413253	6.964456438 CORE	3 O	O	0.0000	3
O	4.278320963	3.855098772	4.047422176 CORE	4 O	O	0.0000	4
O	4.021250677	5.270257218	1.334884621 CORE	5 O	O	0.0000	5
O	9.321468420	8.305340310	4.048615631 CORE	6 O	O	0.0000	6
O	9.610013385	3.853779647	6.387338794 CORE	7 O	O	0.0000	7
O	8.701611643	6.910005285	1.586192036 CORE	8 O	O	0.0000	8
O	4.855852703	8.295612230	6.388171211 CORE	9 O	O	0.0000	9
O	4.729298403	10.134836051	4.044628615 CORE	10 O	O	0.0000	10
O	3.663724557	2.448180974	1.588449353 CORE	11 O	O	0.0000	11
O	9.475840296	5.696150977	4.041471242 CORE	12 O	O	0.0000	12
O	9.958026323	9.923093806	6.563999000 CORE	13 O	O	0.0000	13
O	8.897953957	4.204869419	1.757134672 CORE	14 O	O	0.0000	14
O	4.920667678	5.474395267	6.557865450 CORE	15 O	O	0.0000	15
O	4.227754137	6.875805480	3.979564605 CORE	16 O	O	0.0000	16
O	4.143364856	8.639934386	1.755842372 CORE	17 O	O	0.0000	17
O	8.981056311	2.436042523	3.982867913 CORE	18 O	O	0.0000	18
O	6.958707469	10.126914361	5.623796995 CORE	19 O	O	0.0000	19
O	6.393488707	4.271883295	0.206513732 CORE	20 O	O	0.0000	20

O	1.920847004	5.678807981	5.619463910 CORE	21 O	O	0.0000	21
O	1.842373371	6.855340350	2.300038970 CORE	22 O	O	0.0000	22
O	1.633059163	8.708802324	0.200531106 CORE	23 O	O	0.0000	23
O	6.596359680	2.419253916	2.298716137 CORE	24 O	O	0.0000	24
O	6.975210553	3.772276931	5.138262302 CORE	25 O	O	0.0000	25
O	6.637875422	6.916233291	0.015383612 CORE	26 O	O	0.0000	26
O	2.222505822	8.210494601	5.136407163 CORE	27 O	O	0.0000	27
O	1.959007700	9.841068550	2.888439039 CORE	28 O	O	0.0000	28
O	1.603603914	2.462911985	0.014684930 CORE	29 O	O	0.0000	29
O	6.714211696	5.403049559	2.889709967 CORE	30 O	O	0.0000	30
O	7.215759198	6.923535423	5.290256349 CORE	31 O	O	0.0000	31
O	6.185736229	0.835578685	0.209897176 CORE	32 O	O	0.0000	32
O	2.467597867	11.352480140	5.294213523 CORE	33 O	O	0.0000	33
O	1.627831749	3.971117575	3.172477009 CORE	34 O	O	0.0000	34
O	1.429180665	5.269553665	0.214935831 CORE	35 O	O	0.0000	35
O	6.666233964	8.427164805	3.163935812 CORE	36 O	O	0.0000	36
Ga	7.941349793	8.335148765	0.518941698 CORE	37 Ga	Ga	0.0000	37
Ga	7.692851069	3.711788598	3.213037147 CORE	38 Ga	Ga	0.0000	38
Ga	2.905836678	3.880605878	0.518585042 CORE	39 Ga	Ga	0.0000	39
Ga	3.664039720	6.767992523	5.800333979 CORE	40 Ga	Ga	0.0000	40
Ga	2.937769412	8.149388171	3.210375164 CORE	41 Ga	Ga	0.0000	41
Ga	8.699078352	11.214177353	5.802905044 CORE	42 Ga	Ga	0.0000	42
Ga	6.138341828	8.505806956	5.004111935 CORE	43 Ga	Ga	0.0000	43
Ga	8.433739903	7.043873459	8.148313501 CORE	44 Ga	Ga	0.0000	44
Ga	10.905562619	4.047922416	5.015553886 CORE	45 Ga	Ga	0.0000	45
Ga	0.588493155	5.345652613	2.355780970 CORE	46 Ga	Ga	0.0000	46
Ga	3.671661324	11.480847202	8.148641244 CORE	47 Ga	Ga	0.0000	47
Ga	5.622012272	9.798592826	2.346735231 CORE	48 Ga	Ga	0.0000	48
Ga	10.301631860	7.118797615	5.128856221 CORE	49 Ga	Ga	0.0000	49
Ga	11.282397037	5.781462942	7.553846971 CORE	50 Ga	Ga	0.0000	50
Ga	5.545008947	11.567105775	5.135388863 CORE	51 Ga	Ga	0.0000	51
Ga	2.903227747	2.498730156	3.423873740 CORE	52 Ga	Ga	0.0000	52
Ga	6.527783308	10.226148670	7.557481586 CORE	53 Ga	Ga	0.0000	53
Ga	7.943030413	6.956083819	3.423550151 CORE	54 Ga	Ga	0.0000	54
Ga	7.885202663	5.396297446	0.664130784 CORE	55 Ga	Ga	0.0000	55
Ga	9.863983661	9.767949877	3.060472575 CORE	56 Ga	Ga	0.0000	56
Ga	2.845289558	0.937242302	0.657073306 CORE	57 Ga	Ga	0.0000	57
Ga	6.714672230	5.360912051	6.155917946 CORE	58 Ga	Ga	0.0000	58
Ga	4.826240363	5.317621494	3.061068018 CORE	59 Ga	Ga	0.0000	59
Ga	1.956493120	9.792788087	6.162924556 CORE	60 Ga	Ga	0.0000	60

MS-E

PBC	9.7094	8.7071	8.8887	61.2757	83.1385	89.4050

O	9.474565547	6.581712291	6.937043185 CORE	1 O	O	0.0000	1

O	8.623603884	0.864260320	1.386505404	CORE	2	O	O	0.0000	2
O	4.663586761	10.932331587	6.938685983	CORE	3	O	O	0.0000	3
O	4.102205414	3.653879481	4.031973473	CORE	4	O	O	0.0000	4
O	3.812729063	5.223310959	1.390885524	CORE	5	O	O	0.0000	5
O	8.999653452	8.008518594	4.030349213	CORE	6	O	O	0.0000	6
O	9.355036879	3.737136528	6.680900022	CORE	7	O	O	0.0000	7
O	8.537029101	6.591429918	1.656283071	CORE	8	O	O	0.0000	8
O	4.545995228	8.087807107	6.687124660	CORE	9	O	O	0.0000	9
O	4.395136226	9.604118210	4.041390143	CORE	10	O	O	0.0000	10
O	3.637526022	2.241260708	1.659043967	CORE	11	O	O	0.0000	11
O	9.205178452	5.252046299	4.042145629	CORE	12	O	O	0.0000	12
O	9.482342342	9.603072641	6.542327027	CORE	13	O	O	0.0000	13
O	8.560025219	3.926012811	1.679444501	CORE	14	O	O	0.0000	14
O	4.581866131	5.251564581	6.545822403	CORE	15	O	O	0.0000	15
O	4.075661615	6.805154832	4.133624072	CORE	16	O	O	0.0000	16
O	3.748223232	8.279658956	1.680786390	CORE	17	O	O	0.0000	17
O	8.886558506	2.451779438	4.128924519	CORE	18	O	O	0.0000	18
O	6.544308576	9.781316866	5.511772375	CORE	19	O	O	0.0000	19
O	6.240884044	4.041955683	0.175023837	CORE	20	O	O	0.0000	20
O	1.646266377	5.429206838	5.513755958	CORE	21	O	O	0.0000	21
O	1.657755031	6.709026804	2.479742458	CORE	22	O	O	0.0000	22
O	1.432035442	8.395572469	0.174514575	CORE	23	O	O	0.0000	23
O	6.474850193	2.344618453	2.476294671	CORE	24	O	O	0.0000	24
O	6.758320217	3.685778464	5.238613720	CORE	25	O	O	0.0000	25
O	6.397341286	6.679208186	0.008575960	CORE	26	O	O	0.0000	26
O	1.947447146	8.040715817	5.240617547	CORE	27	O	O	0.0000	27
O	1.636856207	9.632820753	2.924061662	CORE	28	O	O	0.0000	28
O	1.494354476	2.329588470	0.016046169	CORE	29	O	O	0.0000	29
O	6.445293782	5.276035087	2.924210898	CORE	30	O	O	0.0000	30
O	6.759655677	6.826166212	5.160157338	CORE	31	O	O	0.0000	31
O	6.071731963	0.942405974	0.237225760	CORE	32	O	O	0.0000	32
O	1.952641724	11.178501004	5.163580324	CORE	33	O	O	0.0000	33
O	1.596845018	3.858191796	2.558383145	CORE	34	O	O	0.0000	34
O	1.262498299	5.296774367	0.241968611	CORE	35	O	O	0.0000	35
O	6.490670017	8.199775327	2.540414366	CORE	36	O	O	0.0000	36
Ga	7.421282087	8.150348409	0.789700503	CORE	37	Ga	Ga	0.0000	37
Ga	7.499357490	3.700397594	3.326763351	CORE	38	Ga	Ga	0.0000	38
Ga	2.520111966	3.798989919	0.797820272	CORE	39	Ga	Ga	0.0000	39
Ga	3.272099057	6.547342932	5.918448632	CORE	40	Ga	Ga	0.0000	40
Ga	2.690676765	8.057231794	3.331460540	CORE	41	Ga	Ga	0.0000	41
Ga	8.173754518	10.899466310	5.912891728	CORE	42	Ga	Ga	0.0000	42
Ga	5.464046508	8.221227952	4.995016264	CORE	43	Ga	Ga	0.0000	43
Ga	7.233552920	2.495007196	0.692017696	CORE	44	Ga	Ga	0.0000	44
Ga	0.568392272	3.868303680	4.989512184	CORE	45	Ga	Ga	0.0000	45

Ga	0.343657886	5.307267443	2.232633363 CORE	46 Ga Ga	0.0000	46		
Ga	2.425797608	6.850383336	0.696925962 CORE	47 Ga Ga	0.0000	47		
Ga	5.244819184	9.656644373	2.231112582 CORE	48 Ga Ga	0.0000	48		
Ga	9.988116303	6.889500597	5.177993340 CORE	49 Ga Ga	0.0000	49		
Ga	1.035519225	5.203812578	7.474213429 CORE	50 Ga Ga	0.0000	50		
Ga	5.180350798	11.243362080	5.181291714 CORE	51 Ga Ga	0.0000	51		
Ga	2.653524496	2.489584397	3.382197569 CORE	52 Ga Ga	0.0000	52		
Ga	5.935872629	9.557465356	7.476336663 CORE	53 Ga Ga	0.0000	53		
Ga	7.550648827	6.843869398	3.377948135 CORE	54 Ga Ga	0.0000	54		
Ga	7.658859169	5.233756848	0.580006237 CORE	55 Ga Ga	0.0000	55		
Ga	9.486380560	9.567529301	3.107558776 CORE	56 Ga Ga	0.0000	56		
Ga	2.756961112	0.883162296	0.583760663 CORE	57 Ga Ga	0.0000	57		
Ga	6.400716924	5.316000822	6.222493320 CORE	58 Ga Ga	0.0000	58		
Ga	4.586029954	5.215630116	3.111738153 CORE	59 Ga Ga	0.0000	59		
Ga	1.592061320	9.669352289	6.225814525 CORE	60 Ga Ga	0.0000	60		

MS-F

PBC	9.7339	8.8048	9.1418	60.0137	81.9922	85.6169		
O	9.947182541	6.913767117	7.101542689 CORE	1 O	O	0.0000	1	
O	8.668801019	0.990962110	1.501233355 CORE	2 O	O	0.0000	2	
O	5.162028347	11.176707260	7.099718153 CORE	3 O	O	0.0000	3	
O	4.319966119	3.605685824	4.039098320 CORE	4 O	O	0.0000	4	
O	4.207896518	5.152264265	1.342013650 CORE	5 O	O	0.0000	5	
O	9.432530719	8.196632020	4.143371750 CORE	6 O	O	0.0000	6	
O	9.480086646	3.914648963	6.781944094 CORE	7 O	O	0.0000	7	
O	8.920056827	6.765476233	1.606411829 CORE	8 O	O	0.0000	8	
O	4.878960876	8.048788420	6.719648916 CORE	9 O	O	0.0000	9	
O	4.834103555	9.494441471	3.961186501 CORE	10 O	O	0.0000	10	
O	3.856755536	2.077388116	1.661312686 CORE	11 O	O	0.0000	11	
O	9.337132431	5.592168466	4.078337531 CORE	12 O	O	0.0000	12	
O	10.134090960	9.905124444	6.647401610 CORE	13 O	O	0.0000	13	
O	8.959339149	4.085656037	1.749086101 CORE	14 O	O	0.0000	14	
O	4.926663749	5.206895394	6.556779481 CORE	15 O	O	0.0000	15	
O	4.325263511	6.696560910	4.105282771 CORE	16 O	O	0.0000	16	
O	3.998817910	8.057338934	1.564737015 CORE	17 O	O	0.0000	17	
O	8.873292603	2.502280018	4.162538360 CORE	18 O	O	0.0000	18	
O	6.988257981	10.196746073	5.648894024 CORE	19 O	O	0.0000	19	
O	6.644710442	4.274617223	0.087013519 CORE	20 O	O	0.0000	20	
O	2.015047797	5.588747349	5.515269172 CORE	21 O	O	0.0000	21	
O	1.906749549	6.752409472	2.495748558 CORE	22 O	O	0.0000	22	
O	1.805497823	8.472878710	-0.040565034 CORE	23 O	O	0.0000	23	
O	6.604485047	2.638786490	2.406635111 CORE	24 O	O	0.0000	24	
O	6.984141251	3.982360697	5.312372090 CORE	25 O	O	0.0000	25	
O	6.856888555	6.887150782	-0.081316077 CORE	26 O	O	0.0000	26	

O	2.364621568	8.100382346	5.271831952 CORE	27 O	O	0.0000	27
O	2.187554208	9.729627597	2.977412184 CORE	28 O	O	0.0000	28
O	1.821809391	2.241645212	0.050333048 CORE	29 O	O	0.0000	29
O	6.746182990	5.437882453	2.947369907 CORE	30 O	O	0.0000	30
O	7.071731805	7.150027972	5.156286444 CORE	31 O	O	0.0000	31
O	6.221236998	1.105737815	0.060992346 CORE	32 O	O	0.0000	32
O	2.742981653	11.177713202	5.307925477 CORE	33 O	O	0.0000	33
O	1.975760479	3.848689081	2.491254719 CORE	34 O	O	0.0000	34
O	1.656973800	5.252924434	0.173870767 CORE	35 O	O	0.0000	35
O	7.057450686	8.453849978	2.426155300 CORE	36 O	O	0.0000	36
Ga	8.024447566	8.315379643	0.736793937 CORE	37 Ga	Ga	0.0000	37
Ga	7.795434728	3.866839317	3.329174758 CORE	38 Ga	Ga	0.0000	38
Ga	2.893249298	3.797430825	0.754645329 CORE	39 Ga	Ga	0.0000	39
Ga	3.650866358	6.657228947	5.906369862 CORE	40 Ga	Ga	0.0000	40
Ga	3.180803464	8.072595814	3.322719618 CORE	41 Ga	Ga	0.0000	41
Ga	8.982592972	11.323911346	5.976791052 CORE	42 Ga	Ga	0.0000	42
Ga	5.938523237	8.655954608	5.293609059 CORE	43 Ga	Ga	0.0000	43
Ga	7.269129570	2.601446799	0.599695088 CORE	44 Ga	Ga	0.0000	44
Ga	11.220132616	3.927679106	6.143246897 CORE	45 Ga	Ga	0.0000	45
Ga	10.416199981	5.270218726	2.495995317 CORE	46 Ga	Ga	0.0000	46
Ga	2.673248574	6.843981859	0.741197060 CORE	47 Ga	Ga	0.0000	47
Ga	6.044282535	10.013119585	2.535259561 CORE	48 Ga	Ga	0.0000	48
Ga	10.338510892	6.917691378	5.212094824 CORE	49 Ga	Ga	0.0000	49
Ga	11.186611889	5.889792999	8.068031867 CORE	50 Ga	Ga	0.0000	50
Ga	5.914333534	11.906770170	5.573823235 CORE	51 Ga	Ga	0.0000	51
Ga	2.754144461	2.423326126	3.469779401 CORE	52 Ga	Ga	0.0000	52
Ga	6.652221741	10.151172895	7.733251678 CORE	53 Ga	Ga	0.0000	53
Ga	7.981181283	6.997592977	3.386873030 CORE	54 Ga	Ga	0.0000	54
Ga	8.157417581	5.362335583	0.552339161 CORE	55 Ga	Ga	0.0000	55
Ga	10.045330913	9.703241932	3.278759777 CORE	56 Ga	Ga	0.0000	56
Ga	3.033896764	0.755318318	0.514662817 CORE	57 Ga	Ga	0.0000	57
Ga	6.770941279	5.652535735	6.211446629 CORE	58 Ga	Ga	0.0000	58
Ga	4.886809733	5.189729649	3.110279475 CORE	59 Ga	Ga	0.0000	59
Ga	2.203420386	9.656735924	6.308385530 CORE	60 Ga	Ga	0.0000	60

MS-G

PBC	9.7205	8.6645	8.7402	62.1374	81.9728	74.6336

O	10.308920655	5.724819024	6.833382548 CORE	1 O	O	0.0000	1
O	8.601535390	0.588656124	1.433315579 CORE	2 O	O	0.0000	2
O	6.583450586	9.890353357	6.818014776 CORE	3 O	O	0.0000	3
O	4.478969968	3.058207423	3.907115759 CORE	4 O	O	0.0000	4
O	4.894225427	4.758611500	1.431093991 CORE	5 O	O	0.0000	5
O	10.472703145	7.235522794	3.918324426 CORE	6 O	O	0.0000	6
O	9.456180051	2.829539440	6.631105242 CORE	7 O	O	0.0000	7

O	10.016775604	6.002792209	1.652876979 CORE	8	O	O	0.0000	8
O	5.736850376	7.001008281	6.616912916 CORE	9	O	O	0.0000	9
O	6.014590153	8.821119095	4.020557141 CORE	10	O	O	0.0000	10
O	4.016792567	1.820812234	1.645569009 CORE	11	O	O	0.0000	11
O	9.749932407	4.636617164	4.035368320 CORE	12	O	O	0.0000	12
O	11.089606771	8.616037294	6.494733605 CORE	13	O	O	0.0000	13
O	9.261180508	3.122559260	1.473492277 CORE	14	O	O	0.0000	14
O	5.088790718	4.431731647	6.477914133 CORE	15	O	O	0.0000	15
O	5.193093199	5.916003932	4.126508493 CORE	16	O	O	0.0000	16
O	5.526869044	7.301093294	1.444412966 CORE	17	O	O	0.0000	17
O	8.911580608	1.723457859	4.150925656 CORE	18	O	O	0.0000	18
O	8.410597440	9.534611723	4.974232454 CORE	19	O	O	0.0000	19
O	7.326079569	4.089896525	-0.098760946 CORE	20	O	O	0.0000	20
O	2.408526853	5.356115980	4.984595141 CORE	21	O	O	0.0000	21
O	2.979828484	6.828914150	2.448041491 CORE	22	O	O	0.0000	22
O	4.809440468	12.166047528	7.603039728 CORE	23	O	O	0.0000	23
O	6.711915696	2.658004386	2.456307100 CORE	24	O	O	0.0000	24
O	7.101521697	3.723249991	4.932996541 CORE	25	O	O	0.0000	25
O	9.354374937	10.460621552	7.567610310 CORE	26	O	O	0.0000	26
O	3.366131402	7.895120706	4.937887890 CORE	27	O	O	0.0000	27
O	3.746773873	9.355494718	2.496143628 CORE	28	O	O	0.0000	28
O	2.138972334	2.368648937	-0.151240320 CORE	29	O	O	0.0000	29
O	7.459956735	5.192484835	2.494101433 CORE	30	O	O	0.0000	30
O	7.867304595	6.682119275	5.087501495 CORE	31	O	O	0.0000	31
O	6.466853483	1.051811687	-0.077200523 CORE	32	O	O	0.0000	32
O	4.167051606	10.844830550	5.094688561 CORE	33	O	O	0.0000	33
O	2.340916177	3.821203224	2.316462379 CORE	34	O	O	0.0000	34
O	2.748338480	5.214246285	-0.078325253 CORE	35	O	O	0.0000	35
O	8.344906708	8.007879634	2.311768242 CORE	36	O	O	0.0000	36
Ga	9.503891156	7.763747654	0.689097943 CORE	37	Ga	Ga	0.0000	37
Ga	8.457739783	3.401008810	3.304143690 CORE	38	Ga	Ga	0.0000	38
Ga	3.502717968	3.580940546	0.693094505 CORE	39	Ga	Ga	0.0000	39
Ga	4.102692633	6.112330271	5.703031578 CORE	40	Ga	Ga	0.0000	40
Ga	4.725733853	7.582773126	3.278796387 CORE	41	Ga	Ga	0.0000	41
Ga	10.104331221	10.285563438	5.716171660 CORE	42	Ga	Ga	0.0000	42
Ga	6.960969398	8.257643081	5.710537501 CORE	43	Ga	Ga	0.0000	43
Ga	7.505452151	2.371970952	0.691381947 CORE	44	Ga	Ga	0.0000	44
Ga	0.993285778	4.074483517	5.747241388 CORE	45	Ga	Ga	0.0000	45
Ga	11.405516176	5.430895711	3.009009974 CORE	46	Ga	Ga	0.0000	46
Ga	3.770725645	6.550529692	0.679464398 CORE	47	Ga	Ga	0.0000	47
Ga	7.702771472	9.623387679	2.998969024 CORE	48	Ga	Ga	0.0000	48
Ga	11.112725882	6.936103747	5.632290308 CORE	49	Ga	Ga	0.0000	49
Ga	0.510163263	1.514816300	0.707901829 CORE	50	Ga	Ga	0.0000	50
Ga	7.396985789	11.105949903	5.626745096 CORE	51	Ga	Ga	0.0000	51

Ga	2.678383254	2.288069181	3.386013618 CORE	52 Ga Ga	0.0000	52
Ga	7.729693120	9.587372776	8.419881536 CORE	53 Ga Ga	0.0000	53
Ga	8.682330336	6.474776154	3.382024388 CORE	54 Ga Ga	0.0000	54
Ga	9.114803927	4.794891690	0.518296538 CORE	55 Ga Ga	0.0000	55
Ga	11.682129470	8.524934851	3.114441428 CORE	56 Ga Ga	0.0000	56
Ga	3.111889092	0.620787736	0.497952022 CORE	57 Ga Ga	0.0000	57
Ga	6.897453179	5.340508186	6.017849882 CORE	58 Ga Ga	0.0000	58
Ga	5.692197116	4.354479539	3.110624713 CORE	59 Ga Ga	0.0000	59
Ga	3.170563464	9.517174443	6.018700761 CORE	60 Ga Ga	0.0000	60

β-Ga_2O_3

PBC	9.6480	8.7973	8.7960	63.4487	82.2881	91.9380		
O	9.333299311	6.384043586	6.483133777 CORE	1 O	O	0.0000	1
O	8.347883163	9.596389555	1.311389983 CORE	2 O	O	0.0000	2
O	4.360428939	10.780515677	6.483348377 CORE	3 O	O	0.0000	3
O	4.165250693	3.594178010	3.897354234 CORE	4 O	O	0.0000	4
O	3.673267430	5.200320523	1.311358211 CORE	5 O	O	0.0000	5
O	8.840804345	7.990165782	3.897272115 CORE	6 O	O	0.0000	6
O	8.907584272	12.241537776	6.526753288 CORE	7 O	O	0.0000	7
O	8.219448065	6.661660400	1.354264372 CORE	8 O	O	0.0000	8
O	4.232564945	7.845156291	6.526465514 CORE	9 O	O	0.0000	9
O	3.739565010	9.451773655	3.940299661 CORE	10 O	O	0.0000	10
O	3.544594056	2.265446106	1.354460114 CORE	11 O	O	0.0000	11
O	8.712337391	5.055574967	3.940242928 CORE	12 O	O	0.0000	12
O	9.013027962	9.355727895	6.552976755 CORE	13 O	O	0.0000	13
O	8.325027109	3.775613378	1.380957620 CORE	14 O	O	0.0000	14
O	4.337522939	4.959096600	6.553121524 CORE	15 O	O	0.0000	15
O	3.845026657	6.565326486	3.967252521 CORE	16 O	O	0.0000	16
O	3.352390438	8.171558504	1.381375560 CORE	17 O	O	0.0000	17
O	8.520486955	10.961765364	3.967297039 CORE	18 O	O	0.0000	18
O	6.458059414	9.377050386	5.218744161 CORE	19 O	O	0.0000	19
O	6.951020727	7.770612383	7.804307048 CORE	20 O	O	0.0000	20
O	1.783157366	4.979862685	5.218077426 CORE	21 O	O	0.0000	21
O	1.290517451	6.586059219	2.632404569 CORE	22 O	O	0.0000	22
O	1.978400401	12.165676693	7.803977143 CORE	23 O	O	0.0000	23
O	6.262995493	2.190886013	2.632741717 CORE	24 O	O	0.0000	24
O	6.883427586	3.519207761	5.174235041 CORE	25 O	O	0.0000	25
O	7.078429090	10.704998835	7.760054783 CORE	26 O	O	0.0000	26
O	1.910984186	7.915140170	5.174643476 CORE	27 O	O	0.0000	27
O	1.418194106	9.521221586	2.587954313 CORE	28 O	O	0.0000	28
O	2.403473734	6.309071642	7.760206385 CORE	29 O	O	0.0000	29
O	6.390830251	5.125185920	2.588356218 CORE	30 O	O	0.0000	30
O	6.772940870	6.402339571	5.147966936 CORE	31 O	O	0.0000	31
O	7.264581891	4.795677126	7.733958276 CORE	32 O	O	0.0000	32

O	1.800294753	10.798025626	5.148227935	CORE	33	O	O	0.0000	33
O	1.604794972	3.611714570	2.562269903	CORE	34	O	O	0.0000	34
O	2.293217615	9.191802556	7.734579394	CORE	35	O	O	0.0000	35
O	6.280913526	8.008846673	2.562133523	CORE	36	O	O	0.0000	36
Ga	7.001765237	8.272382766	0.749078364	CORE	37	Ga	Ga	0.0000	37
Ga	7.608558696	3.512829321	3.195569422	CORE	38	Ga	Ga	0.0000	38
Ga	2.326836373	3.876150867	0.749440380	CORE	39	Ga	Ga	0.0000	39
Ga	3.128311904	6.302255649	5.781841573	CORE	40	Ga	Ga	0.0000	40
Ga	2.635686770	7.908344919	3.195804827	CORE	41	Ga	Ga	0.0000	41
Ga	7.803661745	10.698943184	5.781538707	CORE	42	Ga	Ga	0.0000	42
Ga	6.090755406	7.810063981	6.152808093	CORE	43	Ga	Ga	0.0000	43
Ga	5.402967637	2.229982049	0.980955156	CORE	44	Ga	Ga	0.0000	44
Ga	11.063459540	3.413486369	6.152660327	CORE	45	Ga	Ga	0.0000	45
Ga	0.922894541	5.019588922	3.566687104	CORE	46	Ga	Ga	0.0000	46
Ga	0.429978024	6.625631805	0.981009598	CORE	47	Ga	Ga	0.0000	47
Ga	5.598095725	9.416201427	3.566897624	CORE	48	Ga	Ga	0.0000	48
Ga	9.699642736	7.951878954	5.547931981	CORE	49	Ga	Ga	0.0000	49
Ga	-0.636052701	2.371796846	0.376049971	CORE	50	Ga	Ga	0.0000	50
Ga	4.727003054	12.348000000	5.548031666	CORE	51	Ga	Ga	0.0000	51
Ga	2.819403152	2.270018074	3.335028488	CORE	52	Ga	Ga	0.0000	52
Ga	4.039339346	6.768052859	0.376326781	CORE	53	Ga	Ga	0.0000	53
Ga	7.494513826	6.666261948	3.335145429	CORE	54	Ga	Ga	0.0000	54
Ga	7.116006530	5.118759474	0.609525455	CORE	55	Ga	Ga	0.0000	55
Ga	9.207111549	9.557957360	2.962099870	CORE	56	Ga	Ga	0.0000	56
Ga	2.440595381	0.722092368	0.609779311	CORE	57	Ga	Ga	0.0000	57
Ga	7.986884850	5.060302244	5.921236963	CORE	58	Ga	Ga	0.0000	58
Ga	4.531904794	5.161912620	2.962193710	CORE	59	Ga	Ga	0.0000	59
Ga	3.014493398	9.456292065	5.921475033	CORE	60	Ga	Ga	0.0000	60