

Supporting information

Reaction Network of layer-to-tunnel transition of MnO₂

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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-to-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 .

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

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. The procedure is described below briefly.

Pathway collection In SSW pathway sampling, firstly, we start from one single phase (δ -MnO₂ 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. δ -MnO₂) and the FS (e.g. α -MnO₂, β -MnO₂ and R-MnO₂) 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 δ -MnO₂, 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 and 10^5 for force filed approach) are explored, which produce a database including a large number of IS/FS pairs.

Pathway screening Secondly, we use Euclidian distance between IS/FS pairs as an important quantity to screen out the candidate pathways from the database. For the crystal systems, we need to utilize a generalized coordinate $\{\mathbf{L}_r, \mathbf{q}'\}$ to define the structure, including both the lattice and the atom degrees of freedom, as defined in the following equations.

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

$$\mathbf{G}_r = (\mathbf{G}_{\text{IS}} + \mathbf{G}_{\text{FS}})/2 \quad (3)$$

$$\mathbf{S} = \mathbf{G}_r^{1/2} \quad (4)$$

$$\mathbf{q}' = \mathbf{S} \mathbf{q} \quad (5)$$

Where \mathbf{L} is the lattice vector in real distance units, e.g., in Å, \mathbf{G} is a rotational invariant matrix, \mathbf{S} is scaling matrix, which is defined as the square root of the metric tensor \mathbf{G}_r . The fractional coordinate \mathbf{q} can then be transformed to a new set of scaled coordinate, \mathbf{q}' which is compatible with the lattice length. Then we can use the generalized coordinate $\{\mathbf{L}_r, \mathbf{q}'\}$ 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) method³ 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.

Table S1. Lattice parameters using DFT+U calculations for four MnO₂ polymorphs.

structure	calculated				experimental ⁵⁻⁹			
	a (Å)	b (Å)	c (Å)	V(Å ³)	a (Å)	b (Å)	c (Å)	V (Å ³)
δ-MnO₂	5.07	2.93	5.00	70.13	5.17	2.85	7~10 [#]	-
R-MnO₂	9.43	2.93	4.62	127.43	9.27	2.86	4.52	120.09
β-MnO₂	4.47	2.96	4.47	59.22	4.40	2.87	4.40	55.48
α-MnO₂	9.91	2.93	9.91	287.75	9.90	2.87	9.87	279.55

[#]The experimental value for the c length of hydrated δ -MnO₂ varies from 7Å to 10Å, depending on the number of water layers separating MnO₂ sheets, while no dehydrated δ -MnO₂ structure was reported.

Table S2. Bulk modulus (B), shear modulus (G) and B/G ratio for δ -, α -, β -, R-MnO₂

	B (GPa)	G (GPa)	B/G
δ -MnO ₂	8.2	55.8	0.15
α -MnO ₂	70.6	61.8	1.14
β -MnO ₂	161.9	110.1	1.47
R-MnO ₂	89.7	76.6	1.17

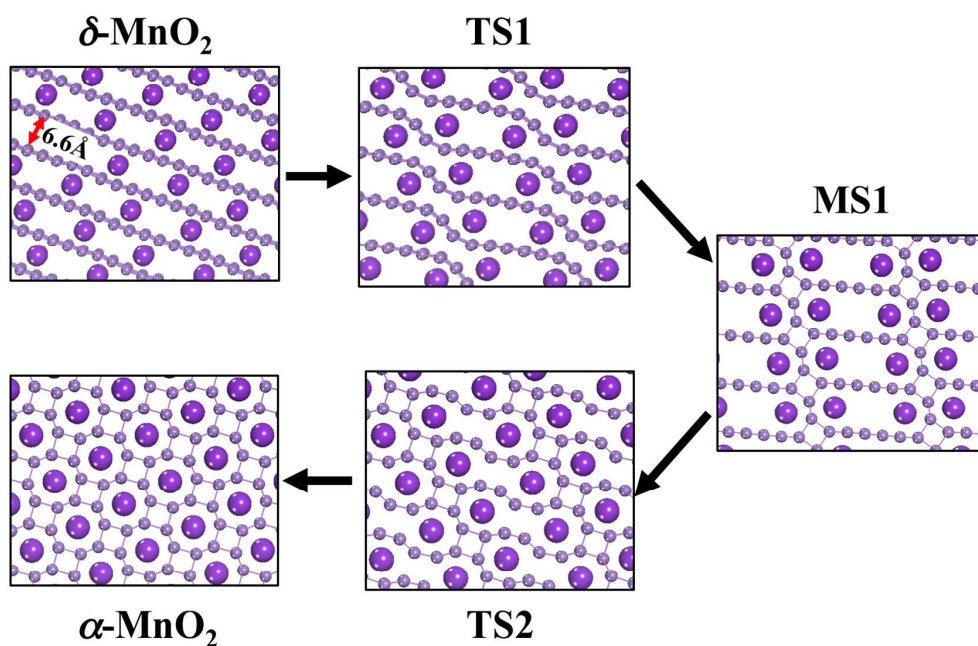


Figure S1. The atomic displacement pattern from K intercalated δ phase to α phase. The small purple balls and sticks represent Mn sublattice, while the large purple balls are intercalated K^+ .

References

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$\delta \rightarrow \alpha$

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PBC=ON

δ

!DATE

PBC	7.7881	2.9275	16.9403	94.9810	74.1326	55.5985		
O	6.560551432	0.000988936	0.345801315	CORE	1 O O	0.0000	1	
O	5.600960085	0.647432024	3.643242967	CORE	2 O O	0.0000	2	
O	3.636279480	-1.555055782	6.166963284	CORE	3 O O	0.0000	3	
O	8.733331375	0.287130712	2.285826501	CORE	4 O O	0.0000	4	
O	5.809197084	-1.268330252	8.107183915	CORE	5 O O	0.0000	5	
O	10.983834417	-3.036648962	11.404951161	CORE	6 O O	0.0000	6	
O	10.673094794	-2.823762259	13.928753810	CORE	7 O O	0.0000	7	
O	7.981846100	-0.981580722	10.047741756	CORE	8 O O	0.0000	8	
O	7.541022672	-2.464028953	15.285468330	CORE	9 O O	0.0000	9	
O	8.500682099	-3.110354530	11.988017641	CORE	10 O O	0.0000	10	
O	10.465089636	-0.907866856	9.464257697	CORE	11 O O	0.0000	11	
O	5.368049454	-2.750190674	13.345421360	CORE	12 O O	0.0000	12	
O	8.292397891	-1.194507234	7.524002064	CORE	13 O O	0.0000	13	
O	3.117776600	0.573733100	4.226312129	CORE	14 O O	0.0000	14	
O	3.428324790	0.360748116	1.702481496	CORE	15 O O	0.0000	15	
O	6.119559880	-1.481340991	5.583431299	CORE	16 O O	0.0000	16	
Mn	7.310105173	-2.295743932	8.785817328	CORE	17 Mn Mn	0.0000	17	
Mn	2.446076300	-0.740472802	2.964358624	CORE	18 Mn Mn	0.0000	18	
Mn	1.927384134	1.388602306	1.023893322	CORE	19 Mn Mn	0.0000	19	
Mn	9.482915849	-2.009111105	10.726125361	CORE	20 Mn Mn	0.0000	20	
Mn	6.791378732	-0.167077104	6.845279738	CORE	21 Mn Mn	0.0000	21	
Mn	11.655429941	-1.722439832	12.666791955	CORE	22 Mn Mn	0.0000	22	
Mn	12.174075804	-3.851587862	14.607269544	CORE	23 Mn Mn	0.0000	23	
Mn	4.618570505	-0.453748106	4.905012726	CORE	24 Mn Mn	0.0000	24	

end
end

TS1

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PBC	7.7130	2.9423	17.0966	94.8802	73.3330	55.1646		
O	6.499162652	0.074934589	0.257564833	CORE	1 O O	0.0000	1	
O	5.294686813	0.925582799	4.138959146	CORE	2 O O	0.0000	2	
O	3.081939695	-1.118394407	6.600254821	CORE	3 O O	0.0000	3	
O	8.506613352	0.471440951	2.337490286	CORE	4 O O	0.0000	4	
O	6.205459289	-1.497741751	8.547896709	CORE	5 O O	0.0000	5	
O	11.632257060	-3.478925101	11.241188331	CORE	6 O O	0.0000	6	
O	11.072708874	-3.088933755	13.690356501	CORE	7 O O	0.0000	7	
O	8.791749536	-1.504909482	9.525036900	CORE	8 O O	0.0000	8	

O	7.899092188	-2.661427348	15.412193453	CORE	9	O	O	0.0000	9
O	9.102922062	-3.511961709	11.531657283	CORE	10	O	O	0.0000	10
O	11.315765192	-1.468145596	9.070459915	CORE	11	O	O	0.0000	11
O	5.891401645	-3.057804500	13.332144851	CORE	12	O	O	0.0000	12
O	8.192093551	-1.088995201	7.122371823	CORE	13	O	O	0.0000	13
O	2.765424681	0.892647715	4.428944593	CORE	14	O	O	0.0000	14
O	3.325297904	0.502456508	1.979966328	CORE	15	O	O	0.0000	15
O	5.605835650	-1.081638034	6.145192926	CORE	16	O	O	0.0000	16
Mn	7.793835917	-2.603659943	8.293346544	CORE	17	Mn	Mn	0.0000	17
Mn	2.214454672	-0.516549408	3.211889016	CORE	18	Mn	Mn	0.0000	18
Mn	1.898743295	1.494518208	1.109464849	CORE	19	Mn	Mn	0.0000	19
Mn	10.235837370	-2.508200613	10.301196252	CORE	20	Mn	Mn	0.0000	20
Mn	6.603776860	0.016949490	7.376925769	CORE	21	Mn	Mn	0.0000	21
Mn	12.183303003	-2.069841925	12.458302644	CORE	22	Mn	Mn	0.0000	22
Mn	12.499494302	-4.080970817	14.560291240	CORE	23	Mn	Mn	0.0000	23
Mn	4.161695249	-0.078151805	5.369358278	CORE	24	Mn	Mn	0.0000	24
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MS1

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PBC	8.1493	2.9281	16.7698	95.0018	74.4019	57.3398			
O	6.892936982	-0.018009353	0.234776297	CORE	1	O	O	0.0000	1
O	5.042449890	1.162223140	4.398132823	CORE	2	O	O	0.0000	2
O	2.465870527	-0.664232638	6.620634819	CORE	3	O	O	0.0000	3
O	8.840800772	0.472263457	2.314065733	CORE	4	O	O	0.0000	4
O	6.349812822	-1.410827902	8.715822473	CORE	5	O	O	0.0000	5
O	11.759608000	-3.134900986	11.165224862	CORE	6	O	O	0.0000	6
O	11.023757038	-2.663464527	13.545621182	CORE	7	O	O	0.0000	7
O	9.095537990	-1.429914037	8.955390622	CORE	8	O	O	0.0000	8
O	7.366103457	-2.064783560	15.346647833	CORE	9	O	O	0.0000	9
O	9.215869082	-3.243444146	11.185051536	CORE	10	O	O	0.0000	10
O	11.792363944	-1.416935048	8.962606987	CORE	11	O	O	0.0000	11
O	5.417734185	-2.554402925	13.267262038	CORE	12	O	O	0.0000	12
O	7.908726684	-0.670287969	6.867664866	CORE	13	O	O	0.0000	13
O	2.498613647	1.053089801	4.417354647	CORE	14	O	O	0.0000	14
O	3.234796209	0.581232101	2.037107385	CORE	15	O	O	0.0000	15
O	5.162789818	-0.651036030	6.628267865	CORE	16	O	O	0.0000	16
Mn	7.799289370	-2.338618686	7.856226034	CORE	17	Mn	Mn	0.0000	17
Mn	2.112751614	-0.438471200	3.258602518	CORE	18	Mn	Mn	0.0000	18
Mn	1.788453630	1.508255835	1.102023928	CORE	19	Mn	Mn	0.0000	19
Mn	10.460030904	-2.302342667	10.009111340	CORE	20	Mn	Mn	0.0000	20
Mn	6.459327770	0.257629831	7.727244050	CORE	21	Mn	Mn	0.0000	21
Mn	12.145468407	-1.643362539	12.323967022	CORE	22	Mn	Mn	0.0000	22

Mn	12.470584636	-3.590808177	14.479435915	CORE	23 Mn Mn	0.0000	23
Mn	3.798201048	0.221089806	5.574121611	CORE	24 Mn Mn	0.0000	24

end
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TS2

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PBC	8.2095	2.9292	16.6064	95.0347	67.4808	57.6980		
O	7.046396949	-0.190018617	0.695272414	CORE	1 O O	0.0000	1	
O	5.854428516	0.573517960	3.491587947	CORE	2 O O	0.0000	2	
O	11.514655333	-1.279116621	5.736669592	CORE	3 O O	0.0000	3	
O	9.575548036	-0.054115685	1.760049511	CORE	4 O O	0.0000	4	
O	7.224740148	-2.026980952	7.817706350	CORE	5 O O	0.0000	5	
O	4.287128613	-3.632640913	10.434738992	CORE	6 O O	0.0000	6	
O	11.393225025	-2.935687601	12.567402492	CORE	7 O O	0.0000	7	
O	9.989316017	-2.044787045	7.985047085	CORE	8 O O	0.0000	8	
O	7.309208310	-5.535496695	13.528796139	CORE	9 O O	0.0000	9	
O	9.964981937	-3.764054233	10.191240631	CORE	10 O O	0.0000	10	
O	4.517173291	-2.045213269	8.109227975	CORE	11 O O	0.0000	11	
O	5.868266622	-2.896180251	12.633748419	CORE	12 O O	0.0000	12	
O	8.752083412	-1.261724174	5.949503964	CORE	13 O O	0.0000	13	
O	11.534823744	0.439777399	3.570258730	CORE	14 O O	0.0000	14	
O	3.862453625	0.099697388	1.107610691	CORE	15 O O	0.0000	15	
O	6.003102957	-1.254068966	5.751369968	CORE	16 O O	0.0000	16	
Mn	8.671258676	-2.943800390	6.919398506	CORE	17 Mn Mn	0.0000	17	
Mn	2.885521691	-1.014958477	2.383043290	CORE	18 Mn Mn	0.0000	18	
Mn	2.043606992	1.250063129	0.517063875	CORE	19 Mn Mn	0.0000	19	
Mn	11.325517853	-2.891767402	9.106019377	CORE	20 Mn Mn	0.0000	20	
Mn	5.741143170	-2.821333871	6.845060468	CORE	21 Mn Mn	0.0000	21	
Mn	12.709792961	-2.034733947	11.553628727	CORE	22 Mn Mn	0.0000	22	
Mn	13.717222184	-4.400082405	13.758811505	CORE	23 Mn Mn	0.0000	23	
Mn	4.637704501	-0.389417583	4.682307486	CORE	24 Mn Mn	0.0000	24	

end
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PBC	8.3127	2.9265	15.9010	95.2901	68.9019	58.1181		
O	7.608959725	-0.394277622	1.000210313	CORE	1 O O	0.0000	1	
O	5.906448435	0.664144952	3.762760123	CORE	2 O O	0.0000	2	
O	11.247903890	-0.934213336	5.625065604	CORE	3 O O	0.0000	3	
O	10.400780888	-0.407134370	0.986002789	CORE	4 O O	0.0000	4	
O	7.081140063	-1.790376067	7.932360025	CORE	5 O O	0.0000	5	
O	3.841936786	-3.224606386	10.688993833	CORE	6 O O	0.0000	6	
O	10.732417735	-2.340202239	12.554208166	CORE	7 O O	0.0000	7	

O	9.872778317	-1.803341882	7.921967428	CORE	8 O O	0.0000	8
O	6.432330679	-4.835945105	12.933162368	CORE	9 O O	0.0000	9
O	9.674484948	-3.404320972	10.176422082	CORE	10 O O	0.0000	10
O	4.327196709	-1.802155393	8.308818919	CORE	11 O O	0.0000	11
O	5.186747203	-2.338352253	12.946557199	CORE	12 O O	0.0000	12
O	8.495748712	-0.946739862	6.005194065	CORE	13 O O	0.0000	13
O	11.741162093	0.482650134	3.242653502	CORE	14 O O	0.0000	14
O	4.856276867	-0.405567851	1.382515892	CORE	15 O O	0.0000	15
O	5.703661101	-0.933612636	6.016197031	CORE	16 O O	0.0000	16
Mn	8.489014386	-2.665587025	6.913774124	CORE	17 Mn Mn	0.0000	17
Mn	3.332204356	-1.180915146	2.239807229	CORE	18 Mn Mn	0.0000	18
Mn	2.248422953	1.216379882	-0.020364695	CORE	19 Mn Mn	0.0000	19
Mn	11.120203251	-2.580366845	9.170981955	CORE	20 Mn Mn	0.0000	20
Mn	5.542456584	-2.556713423	7.023622873	CORE	21 Mn Mn	0.0000	21
Mn	12.253900986	-1.563061981	11.694373515	CORE	22 Mn Mn	0.0000	22
Mn	13.338312090	-3.961376070	13.953844520	CORE	23 Mn Mn	0.0000	23
Mn	4.457705472	-0.157890489	4.765643448	CORE	24 Mn Mn	0.0000	24
end							
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δ

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PBC	9.7955	5.8529	5.2651	90.0090	101.6760	89.9950		
O	8.294224972	1.462828157	0.895175145	CORE	1 O O	0.0000	1	
O	3.684199434	2.926459996	0.393772457	CORE	2 O O	0.0000	2	
O	0.681286668	2.925879786	2.184228887	CORE	3 O O	0.0000	3	
O	5.866765919	4.389503854	1.682834015	CORE	4 O O	0.0000	4	
O	2.863950993	4.388924532	3.473162493	CORE	5 O O	0.0000	5	
O	8.048814597	-0.000388274	2.971961414	CORE	6 O O	0.0000	6	
O	5.046648825	5.851972462	4.762235806	CORE	7 O O	0.0000	7	
O	0.436023956	1.462668653	4.261016301	CORE	8 O O	0.0000	8	
O	0.436253266	4.389133762	4.261026589	CORE	9 O O	0.0000	9	
O	5.046405919	2.925510648	4.762233995	CORE	10 O O	0.0000	10	
O	8.049054096	2.926090305	2.971970317	CORE	11 O O	0.0000	11	
O	2.863675389	1.462458053	3.473174266	CORE	12 O O	0.0000	12	
O	5.866536274	1.463037609	1.682824313	CORE	13 O O	0.0000	13	
O	0.681526189	5.852341268	2.184238314	CORE	14 O O	0.0000	14	
O	3.683956289	-0.000018646	0.393770911	CORE	15 O O	0.0000	15	
O	8.294500220	4.389293127	0.895163946	CORE	16 O O	0.0000	16	
Mn	7.080751828	5.852654231	1.289002505	CORE	17 Mn Mn	0.0000	17	
Mn	9.262838418	1.462734686	2.578133017	CORE	18 Mn Mn	0.0000	18	
Mn	1.649969334	2.925778436	3.867097752	CORE	19 Mn Mn	0.0000	19	

Mn	3.832642115	4.388855543	5.156069590	CORE	20	Mn Mn	0.0000	20
Mn	1.650220356	5.852285696	3.867095220	CORE	21	Mn Mn	0.0000	21
Mn	9.263090606	4.389229503	2.578130685	CORE	22	Mn Mn	0.0000	22
Mn	7.080497017	2.926149588	1.288999655	CORE	23	Mn Mn	0.0000	23
Mn	3.832388739	1.462370481	5.156069411	CORE	24	Mn Mn	0.0000	24

end
end

TS3

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PBC	9.7627	5.8602	4.7365	89.9972	90.4686	90.0017		
O	8.361775036	1.467607731	0.113977983	CORE	1	O O	0.0000	1
O	3.783007964	2.932236042	0.663167534	CORE	2	O O	0.0000	2
O	1.233738313	2.932297439	2.442500618	CORE	3	O O	0.0000	3
O	6.203758217	4.397732800	1.412199585	CORE	4	O O	0.0000	4
O	3.507852741	4.397813837	3.337637945	CORE	5	O O	0.0000	5
O	8.483805151	0.001959881	2.302734967	CORE	6	O O	0.0000	6
O	5.928882949	5.862835141	4.086389736	CORE	7	O O	0.0000	7
O	1.347268153	1.467402395	4.631840511	CORE	8	O O	0.0000	8
O	1.351150347	4.397697690	4.638486030	CORE	9	O O	0.0000	9
O	5.928919995	2.932961694	4.086460288	CORE	10	O O	0.0000	10
O	8.483784076	2.932937040	2.302657170	CORE	11	O O	0.0000	11
O	3.507950973	1.467536831	3.337826708	CORE	12	O O	0.0000	12
O	6.203828602	1.467435312	1.412432864	CORE	13	O O	0.0000	13
O	1.233720524	5.863224321	2.442410211	CORE	14	O O	0.0000	14
O	3.783044551	0.002386793	0.663228448	CORE	15	O O	0.0000	15
O	8.365727568	4.397875210	0.120632874	CORE	16	O O	0.0000	16
Mn	7.321761966	5.863362702	0.754114041	CORE	17	Mn Mn	0.0000	17
Mn	9.739568283	1.467478609	2.375626890	CORE	18	Mn Mn	0.0000	18
Mn	2.389466349	2.933061167	3.995744219	CORE	19	Mn Mn	0.0000	19
Mn	4.836316695	4.397786667	4.742786534	CORE	20	Mn Mn	0.0000	20
Mn	2.389424930	5.862335496	3.995698870	CORE	21	Mn Mn	0.0000	21
Mn	9.741870563	4.397720130	2.354812772	CORE	22	Mn Mn	0.0000	22
Mn	7.321800995	2.932189556	0.754160009	CORE	23	Mn Mn	0.0000	23
Mn	4.836123908	1.467541243	4.742479540	CORE	24	Mn Mn	0.0000	24

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PBC	9.3319	5.8674	4.6486	89.9996	83.8682	90.0000		
O	8.038862515	1.466731190	-0.672241850	CORE	1	O O	0.0000	1
O	3.733700454	2.933559572	0.865948170	CORE	2	O O	0.0000	2
O	1.305406366	2.933575770	2.969080341	CORE	3	O O	0.0000	3
O	6.260882952	4.400409513	1.095202157	CORE	4	O O	0.0000	4

O	3.568284675	4.400453018	3.527311327 CORE	5 O O	0.0000	5
O	8.523535731	-0.000104239	1.651816332 CORE	6 O O	0.0000	6
O	6.093988149	5.867298768	3.757226674 CORE	7 O O	0.0000	7
O	1.788683250	1.466758148	5.292897741 CORE	8 O O	0.0000	8
O	1.788623109	4.400428891	5.292841404 CORE	9 O O	0.0000	9
O	6.093983454	2.933617404	3.757224993 CORE	10 O O	0.0000	10
O	8.523473116	2.933567582	1.651865079 CORE	11 O O	0.0000	11
O	3.568273569	1.466752335	3.527302221 CORE	12 O O	0.0000	12
O	6.260873338	1.466718855	1.095205390 CORE	13 O O	0.0000	13
O	1.305385879	5.867266342	2.969093163 CORE	14 O O	0.0000	14
O	3.733705638	-0.000113564	0.865953105 CORE	15 O O	0.0000	15
O	8.038909785	4.400416590	-0.672202038 CORE	16 O O	0.0000	16
Mn	7.206336479	5.867212605	0.225417718 CORE	17 Mn Mn	0.0000	17
Mn	9.580304698	1.466746928	2.310601518 CORE	18 Mn Mn	0.0000	18
Mn	2.622223321	2.933601677	4.396196124 CORE	19 Mn Mn	0.0000	19
Mn	5.162436423	4.400438340	4.622853634 CORE	20 Mn Mn	0.0000	20
Mn	2.622225136	5.867297352	4.396197285 CORE	21 Mn Mn	0.0000	21
Mn	9.580301769	4.400417278	2.310613465 CORE	22 Mn Mn	0.0000	22
Mn	7.206333820	2.933593786	0.225413947 CORE	23 Mn Mn	0.0000	23
Mn	5.162412771	1.466763073	4.622809576 CORE	24 Mn Mn	0.0000	24

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PBC	9.3174	5.8656	4.6654	90.0001	83.7535	90.0000		
O	8.537770344	1.466270029	3.966509806 CORE	1 O O	0.0000	1		
O	3.726004698	2.932673122	0.864447597 CORE	2 O O	0.0000	2		
O	1.313467827	2.932674667	2.975678423 CORE	3 O O	0.0000	3		
O	6.251962447	4.399058565	1.097656129 CORE	4 O O	0.0000	4		
O	3.573013178	4.399050382	3.539832675 CORE	5 O O	0.0000	5		
O	8.511516790	5.865442086	1.661913216 CORE	6 O O	0.0000	6		
O	6.099034104	5.865445840	3.772987908 CORE	7 O O	0.0000	7		
O	1.287214592	1.466271076	0.671062662 CORE	8 O O	0.0000	8		
O	1.287172969	4.399047789	0.671126260 CORE	9 O O	0.0000	9		
O	6.099041853	2.932661273	3.773000355 CORE	10 O O	0.0000	10		
O	8.511505302	2.932670080	1.661892469 CORE	11 O O	0.0000	11		
O	3.573014048	1.466257842	3.539908349 CORE	12 O O	0.0000	12		
O	6.251987591	1.466265420	1.097699418 CORE	13 O O	0.0000	13		
O	1.313452683	5.865436496	2.975661922 CORE	14 O O	0.0000	14		
O	3.726012207	5.865442084	0.864459362 CORE	15 O O	0.0000	15		
O	8.537767808	4.399045885	3.966489024 CORE	16 O O	0.0000	16		

Mn	7.198633820	5.865418942	0.228589480	CORE	17 Mn Mn	0.0000	17
Mn	9.571200213	1.466206612	2.318751244	CORE	18 Mn Mn	0.0000	18
Mn	2.626459178	2.932523620	4.408968599	CORE	19 Mn Mn	0.0000	19
Mn	5.166247134	4.399039426	4.637596478	CORE	20 Mn Mn	0.0000	20
Mn	2.626441868	-0.000004682	4.408955771	CORE	21 Mn Mn	0.0000	21
Mn	9.571172583	4.399110871	2.318784866	CORE	22 Mn Mn	0.0000	22
Mn	7.198616421	2.932692704	0.228577285	CORE	23 Mn Mn	0.0000	23
Mn	5.166127404	1.466271049	4.637564135	CORE	24 Mn Mn	0.0000	24

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PBC	9.9274	5.8628	4.7812	90.0030	74.0997	90.0023		
O	9.608060351	1.467127862	3.788106057	CORE	1 O O	0.0000	1	
O	4.135369956	2.932745550	1.116349127	CORE	2 O O	0.0000	2	
O	1.460792959	2.932702941	2.213907007	CORE	3 O O	0.0000	3	
O	6.694059926	4.398699311	1.147502679	CORE	4 O O	0.0000	4	
O	4.654151184	4.397863998	3.808797106	CORE	5 O O	0.0000	5	
O	9.004015521	5.864151475	1.471717478	CORE	6 O O	0.0000	6	
O	7.166715210	5.864150693	3.849909285	CORE	7 O O	0.0000	7	
O	1.089428893	1.466894594	0.181040034	CORE	8 O O	0.0000	8	
O	1.089321329	4.398039353	0.181124312	CORE	9 O O	0.0000	9	
O	7.166821086	2.932780932	3.849978011	CORE	10 O O	0.0000	10	
O	9.004166272	2.932722658	1.471656062	CORE	11 O O	0.0000	11	
O	4.654234992	1.466917413	3.808702680	CORE	12 O O	0.0000	12	
O	6.694157413	1.467237835	1.147439008	CORE	13 O O	0.0000	13	
O	1.460384576	5.864165677	2.214290022	CORE	14 O O	0.0000	14	
O	4.135617147	5.864240493	1.116277959	CORE	15 O O	0.0000	15	
O	9.608003251	4.398542393	3.788164581	CORE	16 O O	0.0000	16	
Mn	7.559272251	5.864421885	0.188976236	CORE	17 Mn Mn	0.0000	17	
Mn	10.186340865	1.466927783	1.917367051	CORE	18 Mn Mn	0.0000	18	
Mn	3.654556439	2.932285965	4.628719340	CORE	19 Mn Mn	0.0000	19	
Mn	6.318664106	4.398479866	4.797983457	CORE	20 Mn Mn	0.0000	20	
Mn	3.654045282	0.000856148	4.627124279	CORE	21 Mn Mn	0.0000	21	
Mn	10.186227210	4.398465992	1.917416492	CORE	22 Mn Mn	0.0000	22	
Mn	7.559355204	2.932939899	0.188965024	CORE	23 Mn Mn	0.0000	23	
Mn	6.318813754	1.466853000	4.797909373	CORE	24 Mn Mn	0.0000	24	

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PBC	10.5031	5.8525	4.6159	90.0005	63.9287	90.0006		
O	10.326013706	1.462979775	3.003397496	CORE	1 O O	0.0000	1	

O	5.338519409	2.926118367	2.179284508 CORE	2 O O	0.0000	2
O	1.697239562	2.926137916	1.545366543 CORE	3 O O	0.0000	3
O	7.548509954	4.389254406	1.251977411 CORE	4 O O	0.0000	4
O	5.814346224	4.389232372	4.515660407 CORE	5 O O	0.0000	5
O	9.850107907	5.852337788	0.666982775 CORE	6 O O	0.0000	6
O	8.115973592	5.852314973	3.930701539 CORE	7 O O	0.0000	7
O	1.435559219	1.462977951	-0.508905760 CORE	8 O O	0.0000	8
O	1.435532359	4.389214152	-0.508906016 CORE	9 O O	0.0000	9
O	8.116003394	2.926078809	3.930702277 CORE	10 O O	0.0000	10
O	9.850134069	2.926100756	0.666982238 CORE	11 O O	0.0000	11
O	5.814377670	1.462998254	4.515661312 CORE	12 O O	0.0000	12
O	7.548536890	1.463017857	1.251978430 CORE	13 O O	0.0000	13
O	1.697210597	5.852374444	1.545368047 CORE	14 O O	0.0000	14
O	5.338492313	5.852355422	2.179281691 CORE	15 O O	0.0000	15
O	10.325983527	4.389214725	3.003401077 CORE	16 O O	0.0000	16
Mn	8.013258845	5.852352624	0.059445875 CORE	17 Mn Mn	0.0000	17
Mn	10.973714800	1.462998755	1.180547740 CORE	18 Mn Mn	0.0000	18
Mn	4.690804146	2.926101290	4.002137516 CORE	19 Mn Mn	0.0000	19
Mn	7.651210286	4.389216054	5.123205586 CORE	20 Mn Mn	0.0000	20
Mn	4.690833859	-0.000164601	4.002138968 CORE	21 Mn Mn	0.0000	21
Mn	10.973686257	4.389234422	1.180546302 CORE	22 Mn Mn	0.0000	22
Mn	8.013290930	2.926120180	0.059446132 CORE	23 Mn Mn	0.0000	23
Mn	7.651237406	1.462979317	5.123202541 CORE	24 Mn Mn	0.0000	24
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