Supporting information

Subnano Pt Particles from First Principles Stochastic Surface Walking Global Search

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SSW Method

The SSW algorithm[1,2] features with an automated climbing mechanism to manipulate one minimum to a high energy configuration along one random direction, which is inherited from the bias-potential driven constrained-Broyden-dimer (BP-CBD) method for TS location developed in the group[3]. The method has been successfully utilized for predicting the structure of finite clusters with complex PES, such as C_{100} fullerene, and the detail of the algorithm can be found in our previous papers[1,2]. Here we briefly outline the central idea of the SSW method and an illustration of the SSW method is shown in Figure S1.

In one particular SSW step, labeled as *i*, a modified PES $V_{m\text{-}to\text{-}H}$, as shown in Eq. S1, is utilized for moving from the current minimum, $\mathbf{R}_i^m$ to a high energy configuration $\mathbf{R}_i^H$, in which a series of bias Gaussian potential v_n (*n* is the index of the bias potential, n=1,2$\cdots H$) is added one by one consecutively along the direction $\mathbf{N}_i^n$.

$$V_{m-to-H} = V_{real} + \sum_{n=1}^{H} v_n = V_{real} + \sum_{n=1}^{H} w_n \times \exp\left[-\left((\mathbf{R}^t - \mathbf{R}_t^{n-1})\cdot \mathbf{N}_i^n\right)^2 \Big/ \left(2\times ds^2\right)\right] \quad \text{(S1)}$$

$$\mathbf{F}_{\mathbf{tot}} = \mathbf{F}_{\mathbf{real}} + \sum_n w_n \cdot \exp\left[-\frac{\left((\mathbf{R}^t - \mathbf{R}_t^{n-1})\cdot \mathbf{N}_i^n\right)^2}{2\times ds^2}\right] \cdot \frac{(\mathbf{R}^t - \mathbf{R}_t^{n-1})\cdot \mathbf{N}_i^n}{ds^2} \cdot \mathbf{N}_i^n \quad \text{(S2)}$$

where **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 (see Figure S1). The PES at $\mathbf{R}_t^n$ is thus defined by $V_{m-to-n} = V_{real} + \sum_{k=1}^{n} v_k$. 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 $\mathbf{N}^n$.

$\mathbf{N}^n$ should desirably be one eigenstate of Hessian matrix (normal mode) with low eigenvalues. Since the computation of Hessian is expensive, SSW method optimizes $\mathbf{N}^n$ iteratively from the initial random direction $\mathbf{N}^0$ using the biased CBD rotation method[1,3], which is utilized practically to fast locate one soft eigenvector of Hessian matrix. It should be noticed that as inherited from CBD rotation[4], the biased CBD rotation does not compute the whole Hessian matrix but aims to find one vector close to a soft eigenvector of Hessian using the numerical approach. Owing to the extra bias added in the CBD rotation[5,6], the biased CBD rotation distinguishes from other existing eigenvector updating schemes as utilized in

single-ended TS searching method like dimer[7], CBD[4], hybrid eigenvector-following[8] and GAD[9,10], the rotation does not necessarily converges to the softest eigenvector or even any eigenvector of Hessian exactly, but to a vector that mimics the initial random direction $\mathbf{N}^0$ and at the meantime is close to a soft eigenvector of Hessian. In short, the biased CBD method is able to follow up one particular moving direction to escape the basin region, which is not always the softest mode direction (e.g. frustrated translational/rotational modes). More details on the random mode generation and optimization can be found in our previous works.[1,3]

Overall, the movement from $\mathbf{R}_i^m$ to $\mathbf{R}_i^H$ (see Figure S1) is a repeated procedure containing (i) the update of the direction $\mathbf{N}_i^n$ at $\mathbf{R}_t^{n-1}$; (ii) the adding of a new Gaussian function v_n and the displacement of $\mathbf{R}_t^{n-1}$ along the direction $\mathbf{N}_i^n$ by a magnitude of ds ($\mathbf{R}_t^{n-1} + \mathbf{N}_i^n \cdot ds$); and (iii) the local relaxation to $\mathbf{R}_t^n$ on the modified PES (the energy minimization is constrained by the added potentials). The force for the local optimization on the modified PES can be evaluated according to Eq. S2. After reaching the high energy structure $\mathbf{R}_i^H$, we remove all the added bias potentials and relax fully until a new minimum is found.

It might be noticed that the purpose of adding bias potential in SSW method is quite different from the MD-based metadynamics[6] method. In SSW method, the bias potential is for driving the structure across the TS and will be removed before the full energy minimization. In metadynamics, the bias potentials are kept during the simulation to gradually fill the basins. Special reaction coordinate, i.e. collective variables, needs to be designed in order to fill only those related basins and drive the simulation to the target state. In contrast, the bias potential in SSW method is imposed simply using the Cartesian coordinate, the direction of which is obtained from the biased CBD rotation. There is no need for guessing the reaction coordinate.

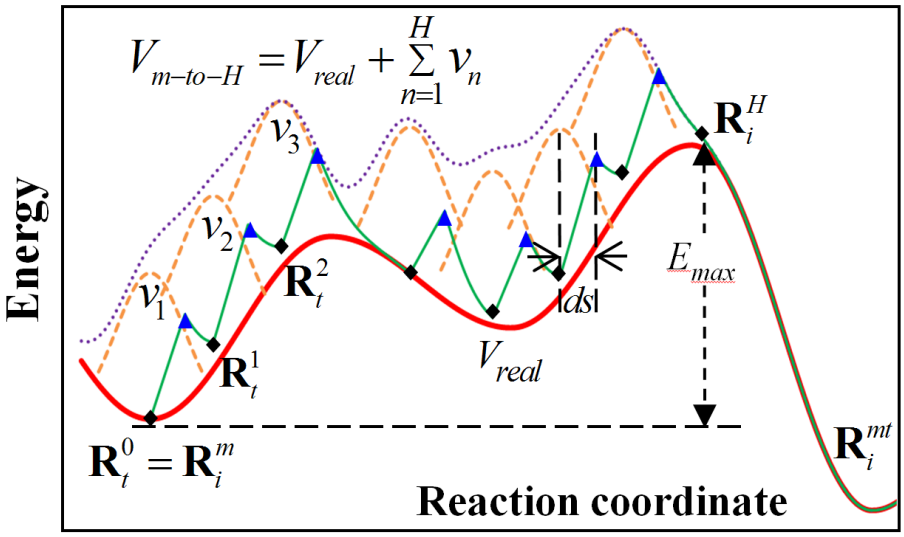

Figure S1. The illustration of the SSW method. The real PES is described by the red curve showing separated minima. one SSW step from one minimum to another, where the bias Gaussian potentials are imposed only on the atom degrees of freedom[1,2]. The green curve represents the subsequent atom relaxation.

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Table S1 The comparison of the bond number (BN) and average bond length (BL) of the GM and SLM

Atom Number (N)	Bond Number of GM (BN_a)	Bond Number of SLM (BN_b)	ΔBN*	ΔBL** (Å)
12	25	25	0	0.002
13	29	33	-4	-0.030
14	36	36	0	-0.011
15	39	38	1	-0.014
16	39	37	2	0.000
17	37	35	2	0.019
18	39	37	2	0.017
19	42	40	2	0.015
20	48	47	1	-0.003
21	59	62	-3	-0.021
22	65	65	0	-0.011
23	72	72	0	0.004
24	75	57	18	0.067
25	57	50	7	0.052
26	55	81	-26	-0.125
27	54	54	0	-0.010
28	58	88	-30	-0.128
29	90	63	27	0.104
30	96	98	-2	-0.007
31	104	102	2	0.009
32	103	103	0	-0.004
33	111	108	3	0.000
34	108	110	-2	-0.004
35	110	110	0	-0.002
36	111	111	0	-0.002
37	121	128	-7	-0.017
38	125	120	5	0.014
39	132	139	-7	-0.027
40	152	148	4	0.008
41	141	138	3	0.006
42	160	160	0	0.001
43	164	150	14	0.038
44	168	146	22	0.055
45	153	166	-13	-0.041
46	157	159	-2	-0.012

*: $\Delta BN(= BN_a - BN_b)$ is the difference of the bond number (BN) between the GM and SLM.

**: ΔBL is the difference of the average Pt-Pt bond length (BL) between the GM and SLM.

The trends of ΔBN is same as the average coordination number shown in Fig. 4. And the ΔBL of most Pt_N is very small (< 0.05 Å). As listed in Table 1, for only 3 clusters (Pt_{26}, Pt_{28} and Pt_{29}), the absolute values of ΔBL are larger than 0.10 Å. The large difference is due to the presence of the simple cubic packing local structure, which has much smaller BN and shorter BL.

The XYZ coordinates for the GM of Pt_N clusters

12

Pt	11.338200	10.252740	9.994580
Pt	10.088000	9.626160	14.222640
Pt	10.823480	8.584800	12.045220
Pt	7.798440	9.969820	13.070600
Pt	6.621280	10.506740	10.820900
Pt	11.025740	12.712480	10.477920
Pt	9.783440	11.269760	12.239420
Pt	8.904420	10.001320	9.337440
Pt	8.483860	12.254160	10.328040
Pt	9.218420	7.497460	8.989800
Pt	8.421420	8.383860	11.240240
Pt	11.583180	7.730220	9.780140

13

Pt	8.90361	8.34517	11.05539
Pt	11.10054	8.61645	9.43356
Pt	13.10709	9.77233	10.47145
Pt	9.48723	13.08749	10.33148
Pt	8.07504	10.55390	10.16763
Pt	9.20232	9.26654	13.40187
Pt	8.84429	11.58825	12.32561
Pt	8.04796	9.72503	7.79018
Pt	11.79435	11.96928	10.11230
Pt	8.94522	7.49197	8.65416
Pt	8.07464	12.34459	8.21797
Pt	10.18615	10.80453	8.57285
Pt	10.91147	10.26066	11.74278

14

Pt	12.92784	12.60233	10.16370
Pt	12.12270	7.77398	11.32302
Pt	10.98864	8.64396	9.21236
Pt	12.55388	10.22499	10.92003
Pt	7.98434	13.47713	10.50049
Pt	9.66425	8.23101	11.64359
Pt	7.17463	8.63670	11.61493
Pt	7.58533	11.09581	11.22896
Pt	11.42555	11.28284	8.58372
Pt	10.47574	13.08889	10.50613
Pt	8.72744	11.76566	8.76302
Pt	9.69134	9.85220	7.37763
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Pt	10.08924	10.70189	11.26818

15

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Pt	10.43770	11.45050	12.57377
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16

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Pt	9.89725	11.06005	11.16046
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Pt	7.80563	11.98518	10.08569
Pt	13.39781	11.32581	10.41659
Pt	11.16109	9.39988	6.33295
Pt	11.29949	12.50405	9.64302
Pt	10.05544	11.40873	7.39168
Pt	12.37301	10.21350	8.39194
Pt	9.24282	13.49268	8.56397
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17

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Pt	8.70768	9.97272	5.34673
Pt	7.91830	7.87686	8.12661
Pt	9.13613	10.94825	12.84625
Pt	12.70686	10.93207	9.22356
Pt	11.97477	8.88244	12.10037
Pt	9.86094	12.99631	9.96792
Pt	7.59667	9.44275	11.48031
Pt	8.34906	11.56187	8.50306
Pt	10.53782	7.30905	10.70761
Pt	11.29123	9.42685	7.73208
Pt	8.09265	12.96481	11.75718
Pt	13.71536	8.88296	10.28333
Pt	6.60017	11.50130	10.35125
Pt	12.28781	7.37280	8.86196
Pt	11.62482	12.94868	8.17271
Pt	10.18168	8.89579	13.86542
Pt	10.96814	10.98950	11.08132
Pt	10.17316	11.48440	6.72690
Pt	8.71822	7.38303	12.48395
Pt	9.44170	9.43385	9.60521

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Pt	7.50345	12.91246	9.49932
Pt	7.46472	7.79893	9.52935
Pt	7.50804	10.35263	6.97224
Pt	7.49348	10.35979	12.04465
Pt	7.50182	12.87533	12.04430
Pt	7.48672	7.83498	7.00598
Pt	7.48013	7.81591	12.04547
Pt	7.54198	12.86049	6.97357
Pt	7.41073	10.36151	9.50718
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Pt	12.58389	10.30266	6.97146
Pt	12.55567	7.78445	9.53140
Pt	12.63442	12.82996	9.48888
Pt	10.02943	10.34725	12.13308
Pt	10.06360	12.96273	9.48919
Pt	10.00273	7.70570	9.53078
Pt	10.04594	10.32706	6.89234
Pt	12.57450	12.83127	12.02147
Pt	12.54046	7.78974	7.00384
Pt	10.04772	12.89907	12.04850
Pt	10.01266	7.79771	6.97927
Pt	12.60870	12.81557	6.95343
Pt	12.51823	7.80476	12.05771
Pt	12.65242	10.31321	9.51116
Pt	10.07400	12.84466	6.91906
Pt	9.99520	7.78324	12.06809
Pt	10.03830	10.34601	9.50656
Pt	8.77285	14.91969	10.78993

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Pt	11.71117	11.26063	9.71202
Pt	10.74990	8.59269	11.55507
Pt	9.10662	6.59177	11.39707
Pt	12.15126	8.03327	13.75820
Pt	7.01544	12.02026	9.75944
Pt	13.48355	7.43657	11.49512
Pt	9.62275	12.87890	10.20459
Pt	9.84049	9.83790	13.62522
Pt	7.47572	8.09656	9.95722
Pt	9.14011	6.46642	8.76931
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Pt	12.24641	10.36725	7.31221
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Pt	8.28526	13.66597	8.13675
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Pt	6.12494	9.97879	11.13523
Pt	12.26211	10.60845	14.17975
Pt	10.77579	8.30877	7.89992
Pt	9.59848	7.18761	13.91482
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Pt	8.42547	11.05087	11.76656
Pt	12.88417	10.03659	11.72352
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Pt	11.50053	6.73939	9.90353
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Pt	13.12204	8.71623	12.34651
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Pt	8.88420	11.53264	7.06551
Pt	7.53420	9.71650	8.35697
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Pt	7.02795	12.29089	8.88809
Pt	12.79420	13.27924	12.56919
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Pt	8.85599	6.43988	7.89617
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Pt	7.73192	8.22652	6.38400
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Pt	7.73241	12.75856	12.74289
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Pt	8.06183	12.38852	8.18491
Pt	9.45151	10.50938	11.05539
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Pt	9.55297	10.50313	6.00648
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Pt	6.17586	10.37044	8.90263
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Pt	7.23578	12.77084	9.32034
Pt	11.66255	11.84944	9.92716
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Pt	9.16056	11.34132	13.25374
Pt	11.83989	9.46299	5.27579
Pt	7.71239	8.89907	7.04256

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Pt	11.82220	10.18582	12.98440
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Pt	9.83659	11.50201	11.43669
Pt	8.95777	10.54007	9.17742
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Pt	11.74574	12.84850	10.13977
Pt	10.84518	11.87810	7.81003
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Pt	9.83177	8.92873	14.06365
Pt	8.04323	6.98532	9.54628
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Pt	10.49606	6.43650	10.17441
Pt	12.49618	7.82870	8.77803
Pt	13.01639	6.34983	10.86738

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Pt	6.64189	12.37022	11.71488
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Pt	9.89138	13.16712	8.62429
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Pt	7.38247	9.02119	7.78258
Pt	8.70686	8.70308	13.62225
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Pt	9.10009	9.54727	5.82061
Pt	12.50731	9.73827	8.90573
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Pt	9.48190	11.08424	10.20108
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Pt	9.09905	6.25773	12.18188
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Pt	10.71845	11.31962	6.88264
Pt	11.78753	7.18765	8.73664
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Pt	7.29474	6.44402	8.10650
Pt	11.66289	8.73937	6.48531
Pt	9.22689	8.64205	11.03711
Pt	12.43904	12.38981	8.56744
Pt	9.63703	7.11844	6.97135

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Pt	13.24842	8.64669	7.68398
Pt	9.86832	10.77788	5.41666
Pt	10.94129	11.32081	8.75602
Pt	9.56582	11.94214	10.88058
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Pt	8.82826	13.99100	9.40970
Pt	9.29969	6.70038	7.19151
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Pt	7.75501	10.24263	6.95863
Pt	10.48133	6.63405	9.65154
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Pt	14.45076	10.88371	8.34988
Pt	11.15028	14.03947	10.89590
Pt	12.02209	11.82459	12.08253
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Pt	13.51540	13.12354	7.24851
Pt	15.24964	8.61147	9.42086
Pt	12.80652	9.57233	13.19579
Pt	13.08946	12.62088	9.80175

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Pt	13.23910	8.64041	7.74824
Pt	9.90970	10.85315	5.45431
Pt	10.92132	11.35564	8.73528
Pt	9.56291	11.91663	10.89325
Pt	12.33329	10.83294	6.60238
Pt	6.21423	9.53129	8.88711
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Pt	9.66353	9.12708	8.49266
Pt	8.25125	9.66032	10.62489
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Pt	11.02315	8.57524	6.33260
Pt	7.76278	10.39400	6.94566
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Pt	11.74274	6.42030	7.76872
Pt	11.60429	6.53571	10.40754
Pt	7.13983	7.29375	10.05291
Pt	11.57429	7.42933	12.88017
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Pt	12.00281	11.92349	12.04037
Pt	15.28434	8.79542	9.47572
Pt	14.40041	10.98425	8.32292
Pt	11.20220	14.03256	8.24238
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Pt	12.91165	9.72919	13.15888
Pt	11.10919	14.10464	10.88543
Pt	13.48265	13.17596	7.20573
Pt	13.72389	7.91615	11.42000
Pt	13.98884	10.58584	10.90942

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Pt	12.10494	12.46912	7.87466
Pt	9.28392	14.26101	10.75150
Pt	10.81282	6.86453	8.43829
Pt	8.46306	7.39146	12.98796
Pt	9.60951	8.51829	10.92260
Pt	10.92868	10.47379	6.33796
Pt	8.28287	13.06151	12.86309
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Pt	11.49201	11.12087	12.27375
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Pt	12.14190	8.06017	6.48032
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Pt	7.95927	14.25218	8.50172
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Pt	9.91136	11.57969	14.36507
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Pt	9.59115	12.71931	6.90292
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Pt	8.03040	9.86115	13.88263
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Pt	12.24858	6.19565	10.57321
Pt	13.32996	10.22697	7.39655
Pt	11.77657	13.09141	10.45028
Pt	6.64591	10.27920	10.50152
Pt	12.47816	10.60797	9.86791
Pt	7.36143	11.66636	8.38797

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Pt	11.43445	6.99706	6.54271
Pt	12.78885	9.29720	11.13733
Pt	8.83771	7.03424	6.39317
Pt	9.42784	11.71082	5.96393
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Pt	7.93098	11.58564	12.94992
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Pt	12.06452	11.61872	6.61273
Pt	10.59277	11.29910	13.56275
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Pt	8.61081	6.18250	10.92947
Pt	9.64454	13.61987	12.72997
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Pt	8.83414	8.45949	8.58775
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Pt	8.77926	12.51833	10.50826
Pt	13.27832	11.95647	10.94315
Pt	10.21676	6.31101	8.81308
Pt	6.27238	7.52259	6.48187
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Pt	9.62164	10.41514	8.17733
Pt	8.13172	6.26469	12.08895
Pt	12.48911	10.70138	14.09314
Pt	13.13722	11.66160	9.84154
Pt	11.24355	10.65088	11.44175
Pt	11.98368	8.33128	13.00548
Pt	13.80453	9.90096	11.90425
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Pt	13.17789	12.57986	12.35777
Pt	10.94855	11.13845	5.88115
Pt	7.67932	8.78958	13.18562
Pt	9.96127	9.91027	13.91127
Pt	11.94444	8.66830	5.69432
Pt	8.91194	13.37868	9.33752
Pt	11.34206	9.02669	9.40455
Pt	5.98783	10.25218	11.78587
Pt	11.14958	13.21837	10.73115
Pt	11.21323	12.45381	8.17637
Pt	13.13363	7.63507	7.90014
Pt	10.45082	7.36543	7.47090
Pt	10.90346	6.26985	11.74531
Pt	14.49744	9.40525	9.40365
Pt	10.57476	12.42418	13.35695
Pt	8.97082	12.68785	6.76609
Pt	9.29550	9.07308	5.78846
Pt	8.84053	13.81782	11.93334
Pt	7.31720	10.62194	6.68195
Pt	8.03032	11.49545	12.95353
Pt	6.64041	12.80496	8.07080
Pt	6.52976	10.40565	9.21721
Pt	8.82720	10.95193	10.51630
Pt	11.64446	5.84349	9.24924
Pt	9.64037	8.61650	11.33056
Pt	7.98488	8.42051	8.00986
Pt	7.12349	8.18635	10.52099
Pt	9.11627	6.63277	9.62875
Pt	12.83705	10.33036	7.57800
Pt	13.08377	7.55479	10.69323
Pt	9.73882	7.26373	13.93822

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Pt	10.59347	6.31927	12.96313
Pt	10.99332	8.72192	14.34189
Pt	8.37096	5.95195	8.99512
Pt	12.85082	6.90213	14.13492
Pt	13.26484	9.04872	7.61152
Pt	11.58432	11.09010	7.22908
Pt	11.74741	13.19960	8.92718
Pt	10.97467	8.62202	6.28867
Pt	13.76116	8.99005	10.23509
Pt	11.75045	13.20302	11.60637
Pt	11.59445	11.16413	13.32345
Pt	6.86717	10.09509	12.97490
Pt	12.96536	6.74598	11.53453
Pt	7.16840	12.40863	9.05750
Pt	11.00058	8.63726	8.96714
Pt	7.21584	12.39003	11.63604
Pt	6.36614	10.15956	10.35282
Pt	9.13910	10.43272	6.25349
Pt	13.64176	11.30508	8.91351
Pt	9.51944	12.80117	12.94242
Pt	12.90824	6.75653	8.95552
Pt	11.02405	8.64853	11.62390
Pt	9.54575	12.83142	7.63739
Pt	7.29221	12.26155	6.45758
Pt	10.59962	6.35003	7.65762
Pt	9.41588	13.26189	10.31347
Pt	6.49068	7.84034	11.67396
Pt	8.54619	8.05725	13.36629
Pt	9.12961	10.51207	11.62829
Pt	13.67465	11.33820	11.59172
Pt	9.10533	10.50038	8.97091
Pt	6.44777	7.81797	8.99492
Pt	10.71264	5.88602	10.28449
Pt	13.36533	9.14713	12.91506
Pt	8.38858	5.94750	11.67492
Pt	11.38052	10.91508	10.27887
Pt	9.15007	10.52659	14.30860
Pt	8.53015	7.99030	7.27172
Pt	6.76305	10.01237	7.67196
Pt	8.74725	8.23461	10.31533

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Pt	11.08788	8.61262	11.43084
Pt	8.29966	8.44970	11.19950
Pt	13.19602	7.05014	11.09958
Pt	14.33870	10.04122	7.69752
Pt	7.87100	10.89412	11.90920
Pt	13.40312	7.69832	8.55140
Pt	9.79144	6.95828	12.95144
Pt	12.41272	6.89972	13.63604
Pt	11.39140	5.23908	11.79202
Pt	7.39696	6.83784	6.39228
Pt	10.42542	8.11094	8.96448
Pt	12.18552	13.89584	9.02652
Pt	9.78146	10.74690	6.65262
Pt	10.21202	13.75590	10.75076
Pt	9.46874	10.50600	9.24348
Pt	12.37864	11.46470	13.57252
Pt	7.44054	9.36868	6.93710
Pt	14.59926	11.36878	12.08786
Pt	13.92848	11.92198	9.55350
Pt	7.68914	7.55208	8.88392
Pt	12.01124	10.11166	9.52936
Pt	10.89816	13.70204	13.36938
Pt	9.67736	11.44838	13.91138
Pt	8.46504	9.10576	13.76584
Pt	12.68042	13.09404	11.49586
Pt	11.98068	9.24094	6.75910
Pt	11.70038	5.75834	9.19948
Pt	8.35410	13.40898	12.52098
Pt	7.79428	12.71086	10.02062
Pt	10.66376	11.18384	11.46566
Pt	9.70978	8.08890	6.32526
Pt	9.86332	12.97738	8.21366
Pt	7.50746	11.89202	7.52110
Pt	14.40798	9.33340	10.35748
Pt	11.09240	9.17326	14.05844
Pt	12.18050	11.76282	7.45600
Pt	9.22962	6.03456	10.48192
Pt	6.91860	10.09394	9.52014
Pt	11.83150	6.56068	6.71248
Pt	13.52938	9.15534	12.88230
Pt	9.41816	5.78892	7.79934

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Pt	9.41586	13.60027	9.69030
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Pt	6.45587	8.17427	8.30828
Pt	9.46421	13.14965	7.04801
Pt	9.28429	10.75155	13.69475
Pt	12.99886	7.13172	10.76445
Pt	10.57846	6.67601	6.85585
Pt	9.07237	10.87623	5.67711
Pt	6.82924	10.42564	7.07771
Pt	6.50951	8.14505	11.07590
Pt	13.75906	11.65603	10.90461
Pt	9.63780	13.15059	12.35612
Pt	9.13165	10.84646	8.33998
Pt	10.80537	6.22717	9.52069
Pt	9.18081	10.82451	10.99433
Pt	11.08522	8.98032	10.86997
Pt	12.98063	7.12509	8.17007
Pt	8.44335	6.24388	8.18755
Pt	13.33465	9.52053	6.82796
Pt	8.78637	8.54786	9.61829
Pt	7.22059	12.69801	8.44693
Pt	11.03622	9.00123	8.21681
Pt	10.75402	6.67654	12.16189
Pt	7.23972	12.70324	11.03978
Pt	6.27106	5.94513	9.64602
Pt	8.50384	6.21996	10.95789
Pt	6.88190	10.30708	12.38189
Pt	6.39554	10.48971	9.72007
Pt	13.94506	13.88240	9.56711
Pt	13.70770	11.68348	8.13394
Pt	12.80290	7.26375	5.57400
Pt	10.93261	9.07594	5.51826
Pt	11.43023	11.27839	9.59205
Pt	8.51401	8.40878	6.55559
Pt	11.70144	11.41705	12.65808
Pt	8.68764	8.30586	12.68255
Pt	11.71415	13.60696	8.25260
Pt	11.14388	8.94919	13.53180
Pt	7.41038	12.56191	13.63471
Pt	11.77396	13.58142	11.02690
Pt	11.52847	11.52074	6.52855
Pt	13.38874	9.40470	12.13444

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Pt	6.16048	6.48199	10.05857
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Pt	8.36056	6.73868	11.48278
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Pt	12.91352	7.45652	11.49227
Pt	10.52932	7.08448	12.82178
Pt	10.90638	9.41794	14.23953
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Pt	12.96855	7.47398	8.92541
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Pt	7.46356	13.19681	6.22049
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Pt	11.70260	11.89738	7.17881
Pt	8.49887	8.83179	13.18780
Pt	8.76579	9.05094	10.13220
Pt	8.62878	8.87023	7.06615
Pt	11.00754	9.40070	11.51954
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Pt	9.12917	11.30850	11.49268
Pt	9.18726	11.32360	8.81595
Pt	11.43511	11.68076	10.20636
Pt	9.50969	14.04282	10.18044
Pt	11.06462	9.41726	8.84387
Pt	6.41715	11.03237	10.09501
Pt	13.76395	9.71819	10.24337

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Pt	7.30083	13.09631	8.29031
Pt	12.71633	7.71915	12.04391
Pt	8.67962	14.44535	10.25663
Pt	7.32353	13.01343	12.19060
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Pt	10.04870	7.34026	12.23986
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Pt	9.99465	10.44395	8.27790
Pt	8.65472	11.73082	10.20351
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Pt	11.33434	11.75516	10.18534
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Pt	14.94043	9.15442	10.31694
Pt	10.49253	10.28655	14.17638
Pt	9.65262	9.89446	6.22101
Pt	13.88359	13.01492	6.94789
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Pt	14.70598	10.16160	12.80554
Pt	11.01843	12.65362	13.09422
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Pt	14.19480	8.47051	7.81309
Pt	12.16729	10.15964	8.52840
Pt	9.93807	9.77799	11.47803
Pt	7.55797	10.89431	11.87317
Pt	13.34646	12.40184	12.05160
Pt	11.67299	5.11885	9.88179
Pt	8.06437	9.47996	14.05893
Pt	7.77875	12.03037	9.49509
Pt	14.14198	10.46489	6.03425
Pt	9.57560	9.81550	8.86686
Pt	14.52614	7.49071	12.33814
Pt	8.95394	13.19376	11.57928
Pt	12.51468	8.76493	13.50317

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Pt	14.61137	9.33013	11.05197
Pt	7.98596	11.96560	12.90886
Pt	12.08110	5.89298	9.92655
Pt	7.06788	13.31817	10.80309
Pt	8.55992	12.94359	6.55384
Pt	10.37465	6.69031	8.12609
Pt	12.16882	9.19713	10.04703
Pt	7.07939	9.13651	8.70504
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Pt	15.12424	9.04643	8.47494
Pt	8.97541	10.05119	14.44892
Pt	13.28729	9.72965	13.32428
Pt	14.46264	6.92219	9.95116
Pt	7.29180	11.83370	8.58909
Pt	12.74803	7.49334	11.95140
Pt	10.43783	12.35741	13.81988
Pt	9.37034	11.42309	10.24020
Pt	11.41648	14.41933	9.78326
Pt	11.87485	11.82790	9.71423
Pt	9.53336	13.72991	11.66293
Pt	10.26971	6.60474	11.85305
Pt	7.88656	6.65104	9.20864
Pt	10.75936	9.00275	6.82792
Pt	6.63233	9.69265	13.34337
Pt	10.95356	8.39384	13.62710
Pt	6.78988	8.12333	11.16244
Pt	12.12705	13.47584	12.08807
Pt	8.42907	10.37339	6.69972
Pt	10.78164	14.27970	7.21691
Pt	6.69528	10.70321	10.84650
Pt	8.34954	7.56273	13.52853
Pt	7.81814	5.73889	11.65272
Pt	14.66844	11.49453	9.28796
Pt	9.69786	4.87144	9.95091
Pt	8.93370	13.92901	9.03041
Pt	13.07193	12.21841	14.19774
Pt	12.93242	10.30066	7.57041
Pt	14.24289	11.78801	11.87951
Pt	12.83181	7.69247	7.98681
Pt	10.80314	11.66408	6.99370
Pt	8.35549	7.76956	6.83660
Pt	13.99121	13.85281	10.20168
Pt	9.06277	9.26546	11.69914
Pt	11.45569	10.39691	15.26190
Pt	11.25150	10.67289	11.95636
Pt	13.06427	13.02158	7.74774