

Supplementary Information

Fine-tuned Global Neural Network Potentials for Global Potential Energy Surface Exploration at High Accuracy

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1. MB function parameters for Ti-O and C-H-O-N MBNN basis potentials

The same 45 MBNN function forms are utilized for both MBNN potentials, and their MB function hyperparameters are listed in **Table S1**.

Table S1 MB function hyperparameters used for Ti-O and C-H-O-N MBNN potentials

MB type	r_{MB}	m_d/m_t	l_d/l_t	λ	Counts
one-body				1.00	1
two-body	3.50	6		0.10	2
two-body	4.50	6		0.10	1
two-body	4.50	3		0.10	6
two-body	6.00	6		0.10	3
two-body	6.00	3		0.10	3
two-body	8.00	3		-0.10	2
two-body	8.00	3		0.10	1
two-body	10.00	3		-0.10	1
two-body	10.00	3		0.10	1
NN two-body	4.50			0.10	16
three-body	2.00	1	1	0.10	2
three-body	2.00	2	1	0.10	1
three-body	3.50	1	1	0.10	2
three-body	3.50	2	1	0.10	1
three-body	4.50	1	1	0.10	1
three-body	4.50	2	1	0.10	1

2. More information on the training of the MBNN basis potentials

The global datasets for MBNN are generated by a global-to-global iterative learning procedure, as implemented in LASP. This involves the SSW global optimization based on the G-NN potential to explore PES and DFT calculations using the global PES data to build the global dataset. More details on the training procedure can be found in our recent software review of LASP 3.7 (Figure 1b).¹

Ti-O potential

The Ti-O global database contains 27,279 structures, which is a sub-database of the Ti-O-H global PES data set utilized previously for identifying new TiO₂ crystal phases.² The structure information of the Ti-O dataset for MBNN training is listed in **Table S2**. Training of the Ti-O basis MBNN potential is conducted parallelly on 1536 CPU cores, taking 20,000 epochs with each epoch 1.15 seconds. The final RMSE is 5.01 eV/atom for energy and 0.122 eV/Å for force, respectively.

Table S2 Structure information of the Ti-O dataset for MBNN training. Listed data include the number of the structures in the global dataset, as distinguished by the chemical formula, the number of atoms (Natom), the type of structures (cluster, bulk, layer), and its total number (Ntotal)

chemical formula	Natom	cluster	layer	bulk	Ntotal
Ti8	8	0	11	95	106
Ti13	13	0	7	5	12
Ti16	16	1011	2	3468	4481
Ti21	21	0	3	1276	1279
Ti32	32	0	5	304	309
O1-Ti12	13	0	1437	0	1437
O2-Ti8	10	0	92	294	386
O2-Ti10	12	0	784	0	784
O3-Ti18	21	0	133	0	133
O4	4	0	84	0	84
O4-Ti4	8	0	163	551	714
O4-Ti8	12	0	88	326	414
O4-Ti22	26	0	8	26	34
O5-Ti27	32	0	0	29	29
O6-Ti4	10	0	0	38	38
O6-Ti8	14	0	95	388	483
O6-Ti15	21	0	111	0	111
O6-Ti18	24	0	7	50	57
O8-Ti4	12	1892	173	10320	12385
O8-Ti8	16	0	87	327	414
O8-Ti15	23	0	21	39	60
O10-Ti8	18	0	119	399	518
O10-Ti22	32	0	0	29	29
O11	11	0	442	138	580
O12-Ti8	20	0	0	338	338
O13-Ti6	19	0	133	433	566
O13-Ti7	20	0	39	19	58
O14-Ti7	21	0	0	1	1

O14-Ti8	22	0	0	179	179
O15-Ti9	24	0	2	263	265
O16-Ti8	24	0	116	497	613
O18-Ti8	26	0	0	2	2
O18-Ti12	30	0	310	16	326
O120-Ti59	179	0	1	8	9
O120-Ti60	180	0	1	0	1
O126-Ti63	189	0	0	15	15
O126-Ti64	190	0	0	12	12
O127-Ti63	190	0	0	1	1
O127-Ti64	191	0	0	1	1
O128-Ti63	191	0	0	3	3
O128-Ti64	192	0	0	9	9
O239-Ti119	358	0	1	0	1
O240-Ti120	360	0	2	0	2
total	--	2903	4477	19899	27279

C-H-O-N potential

A global PES dataset for organic molecules containing 126,191 structures is used for training C-H-O-N MBNN, where structures are collected from the SSW optimization trajectories of QM9 molecules³ and glucose global PES exploration⁴. Training of the C-H-O-N basis MBNN potential is conducted parallelly on 3072 CPU cores, taking 30,000 epochs with each epoch 5.65 seconds. The final RMSE is 5.406 meV/atom for energy and 0.167 eV/Å for force, respectively.

3. Accuracy of AtomFT with different NI

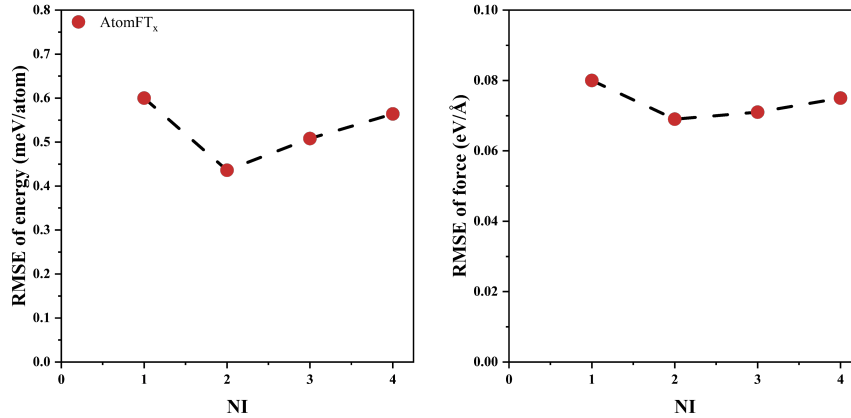
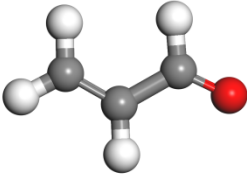
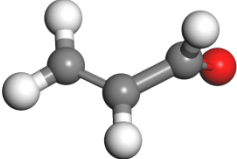
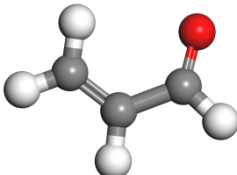
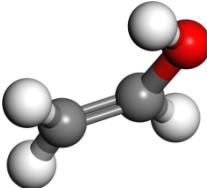
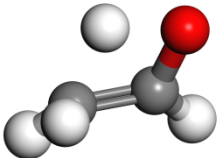
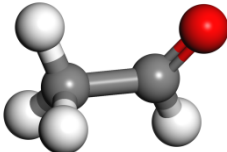

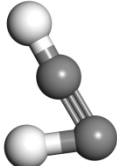
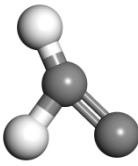
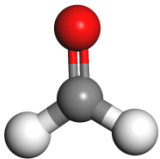
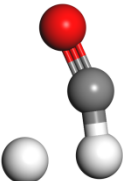
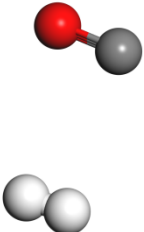


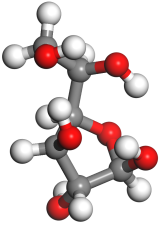
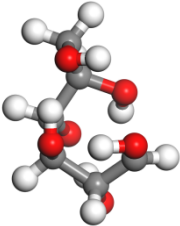
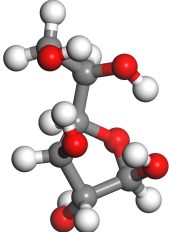
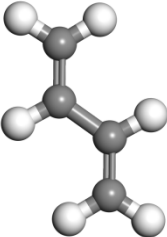
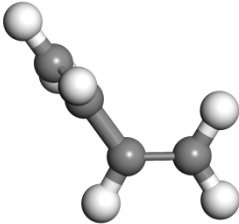
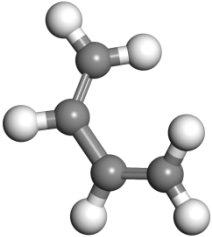
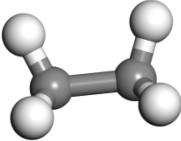
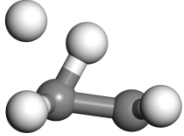
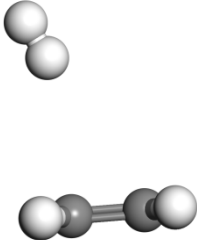
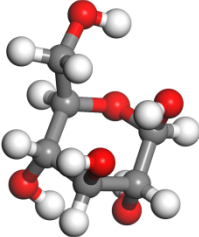
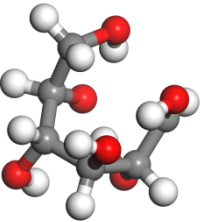
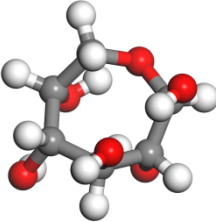
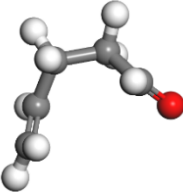
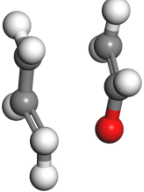
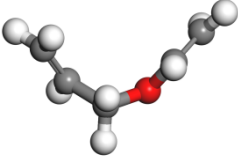
Figure S1 The RMSE of energy (a) and force (b) of the AtomFT potential trained on Example 1's dataset with NI ranging from 1 to 4.

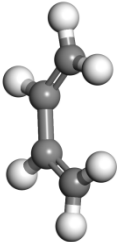
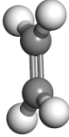
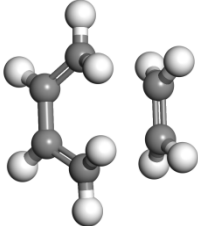
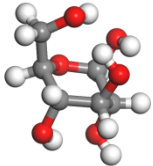
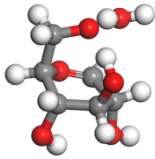
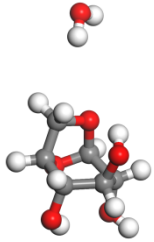
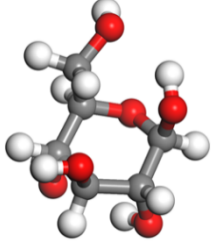
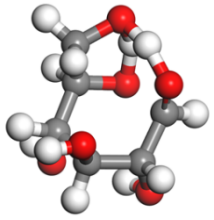
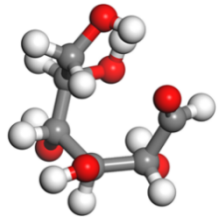
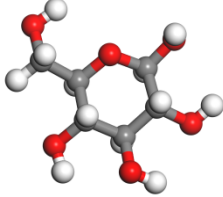
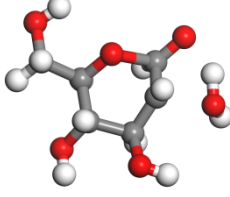
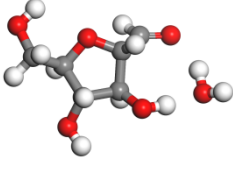
To reveal the relationship between accuracy and NI, we further test the accuracy of the AtomFT potential in Example 1 with NI increasing from 1 to 4, denoted as AtomFT₁, AtomFT₂, AtomFT₃, and AtomFT₄, respectively. The performances for different AtomFT_x are shown in **Figure S2**. It shows a noticeable improvement in energy accuracy when increasing NI from 1 to 2, with the error decreasing from 0.600 meV/atom to 0.436 meV/atom. However, the further increase of NI beyond 2 does not improve accuracy, which may be because the accuracy (<0.6 meV/atom) is already approaching the DFT calculation numerical error. This trend in force prediction is similar (**Figure S2b**), reaching ~0.07 eV/Å. We therefore select NI = 1 or 2 for AtomFT in practice.

4. Reaction-specific benchmark results for molecular reactions

Table S3 The atomic structure snapshots and benchmark results of the initial state (IS), transition state (TS), and final state (FS) of 13 distinct reactions. The energy is in the unit of meV.

	IS	TS	FS
Acrolein rotation			
Molecular structure			
E(AtomFT)-E(DFT)	-0.23	-0.38	-2.92
E(MBNN)-E(DFT)	-93.87	68.86	42.68
H₂CCHOH→H₃CCHO			
Molecular structure			
E(AtomFT)-E(DFT)	-0.32	-2.81	0.41
E(MBNN)-E(DFT)	-3.24	0.95	-7.51
HCCH→CCH₂			
Molecular structure			
E(AtomFT)-E(DFT)	0.57	2.20	-0.94
E(MBNN)-E(DFT)	10.70	-5.74	-39.16
H₂CO→H₂+CO			
Molecular structure			
E(AtomFT)-E(DFT)	-1.45	-0.16	-2.12
E(MBNN)-E(DFT)	-0.51	10.87	43.59
Glucopyranose → Glucofuranose			

Molecular structure			
E(AtomFT)-E(DFT)	2.60	-0.65	-1.22
E(MBNN)-E(DFT)	47.32	93.77	-5.03
Butadiene rotation			
Molecular structure			
E(AtomFT)-E(DFT)	2.20	-0.12	-3.63
E(MBNN)-E(DFT)	-37.85	326.84	-1.39
$\text{H}_3\text{CCH}_3 \rightarrow \text{H}_2\text{CCH}_2 + \text{H}_2$			
Molecular structure			
E(AtomFT)-E(DFT)	-1.20	2.07	-2.86
E(MBNN)-E(DFT)	7.94	661.92	-5.27
Glucopyranose \rightarrow Glucoseptanose			
Molecular structure			
E(AtomFT)-E(DFT)	0.98	-1.13	5.41
E(MBNN)-E(DFT)	50.67	31.44	47.74
Claisen rearrangement			
Molecular structure			
E(AtomFT)-E(DFT)	1.79	-4.81	-1.79
E(MBNN)-E(DFT)	45.56	63.31	47.80

Parent Diels-Alder			
Molecular structure			
E(AtomFT)-E(DFT)	2.85	2.55	3.79
E(MBNN)-E(DFT)	42.45	12.29	30.17
Glucopyranose → Levoglucosan			
Molecular structure			
E(AtomFT)-E(DFT)	3.31	3.86	3.55
E(MBNN)-E(DFT)	38.77	20.88	-24.54
Glucopyranose → D-glucose			
Molecular structure			
E(AtomFT)-E(DFT)	5.74	5.62	-1.34
E(MBNN)-E(DFT)	-2.49	30.91	30.12
Glucopyranose → 2,5-Anhydro-D-mannose			
Molecular structure			
E(AtomFT)-E(DFT)	5.87	-2.11	6.65
E(MBNN)-E(DFT)	44.55	122.90	-1.42

5. XYZ coordinates of A and B phases for the molecular crystal XXIX

Both structures are optimized using DFT (PBE+D3 functional) until the maximum atomic force component is below 0.05 eV/Å

A phase structure (a crystal structure observed in the experiment)⁵

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PBC	24.75858429	9.77298583	8.89729653	89.99652706	93.69621226	90.00443971		
O	7.181266341	4.015777860	7.574428443	CORE	1 O O	0.0000	1	
O	9.626246844	2.349461324	8.549904849	CORE	2 O O	0.0000	2	
O	11.619163268	1.665663033	1.301514891	CORE	3 O O	0.0000	3	
O	5.814685588	5.730043566	7.014172154	CORE	4 O O	0.0000	4	
N	7.441655285	2.882523854	1.103344961	CORE	5 N N	0.0000	5	
N	11.704978789	8.833235856	1.875059371	CORE	6 N N	0.0000	6	
C	10.277036113	0.041012699	0.156308360	CORE	7 C C	0.0000	7	
C	6.255082113	4.792496627	7.881530723	CORE	8 C C	0.0000	8	
C	6.485221310	3.822377218	1.286677894	CORE	9 C C	0.0000	9	
C	10.765526183	1.385140662	0.440008146	CORE	10 C C	0.0000	10	
C	6.145474199	4.795083259	0.288876883	CORE	11 C C	0.0000	11	
C	10.778241839	8.697727705	0.901937730	CORE	12 C C	0.0000	12	
C	5.782152579	3.873979748	2.517939870	CORE	13 C C	0.0000	13	
H	6.017158146	3.137143791	3.286621802	CORE	14 H H	0.0000	14	
C	8.747263340	9.597705106	8.018336473	CORE	15 C C	0.0000	15	
H	8.387135081	0.684425427	7.456541066	CORE	16 H H	0.0000	16	
C	5.150769150	5.759704133	0.562860255	CORE	17 C C	0.0000	17	
H	4.329800819	6.477198431	8.659228183	CORE	18 H H	0.0000	18	
C	10.265615107	7.411712869	0.589622206	CORE	19 C C	0.0000	19	
H	10.620629594	6.563211104	1.175373383	CORE	20 H H	0.0000	20	
C	4.504094167	5.802742981	1.784335915	CORE	21 C C	0.0000	21	
H	3.747242729	6.559816814	1.979630495	CORE	22 H H	0.0000	22	
C	8.270339186	8.332136670	7.728494571	CORE	23 C C	0.0000	23	
H	7.522017309	8.192246230	6.950031914	CORE	24 H H	0.0000	24	
C	4.829202457	4.842059648	2.757459857	CORE	25 C C	0.0000	25	
H	4.315866966	4.847276918	3.716602345	CORE	26 H H	0.0000	26	
C	10.089429800	3.695091691	8.783050601	CORE	27 C C	0.0000	27	
H	9.627314382	4.297728570	7.999960583	CORE	28 H H	0.0000	28	
H	11.182360810	3.742013041	8.710138620	CORE	29 H H	0.0000	29	
H	10.336002864	4.039587504	0.895998206	CORE	30 H H	0.0000	30	
C	8.756814611	7.237771416	8.468054642	CORE	31 C C	0.0000	31	
H	8.391983670	6.232144323	8.260137961	CORE	32 H H	0.0000	32	
C	6.505430403	5.756988342	5.743273624	CORE	33 C C	0.0000	33	
H	6.080978812	6.603712138	5.200603625	CORE	34 H H	0.0000	34	
H	6.333605954	4.825173724	5.193661638	CORE	35 H H	0.0000	35	
H	7.581229373	5.896691033	5.894148406	CORE	36 H H	0.0000	36	
H	12.092919734	9.762032565	2.014546878	CORE	37 H H	0.0000	37	
H	12.093485684	8.018803369	2.356014375	CORE	38 H H	0.0000	38	

H	7.575590650	2.146259757	1.798047223	CORE	39	H	H	0.0000	39
H	7.953566675	2.868517507	0.226136761	CORE	40	H	H	0.0000	40
O	16.716581264	8.901843105	5.743411098	CORE	41	O	O	0.0000	41
O	14.271136646	7.235104121	4.768305877	CORE	42	O	O	0.0000	42
O	12.851249480	6.551789604	3.138383201	CORE	43	O	O	0.0000	43
O	18.083709379	0.843314053	6.303432835	CORE	44	O	O	0.0000	44
N	17.029860429	7.768774133	3.335838762	CORE	45	N	N	0.0000	45
N	12.765566788	3.946398104	2.564525226	CORE	46	N	N	0.0000	46
C	14.194125605	4.927199480	4.283156628	CORE	47	C	C	0.0000	47
C	17.642612288	9.678570394	5.436221232	CORE	48	C	C	0.0000	48
C	17.986184106	8.708743316	3.152390407	CORE	49	C	C	0.0000	49
C	13.705325227	6.271242559	3.999633170	CORE	50	C	C	0.0000	50
C	18.325803082	9.681627083	4.150063208	CORE	51	C	C	0.0000	51
C	13.692297102	3.810877441	3.537568790	CORE	52	C	C	0.0000	52
C	18.689238283	8.760260244	1.921155409	CORE	53	C	C	0.0000	53
H	18.454387876	8.023276281	1.152542953	CORE	54	H	H	0.0000	54
C	15.149757798	4.710514775	5.299803750	CORE	55	C	C	0.0000	55
H	15.510576393	5.570224446	5.861623120	CORE	56	H	H	0.0000	56
C	19.321074483	0.873376972	3.875951504	CORE	57	C	C	0.0000	57
H	19.568395715	1.590510333	4.658285094	CORE	58	H	H	0.0000	58
C	14.205144462	2.524875808	3.849821406	CORE	59	C	C	0.0000	59
H	13.850139664	1.676314970	3.264156765	CORE	60	H	H	0.0000	60
C	19.967751121	0.916381056	2.654468792	CORE	61	C	C	0.0000	61
H	20.724465430	1.673523166	2.459063309	CORE	62	H	H	0.0000	62
C	15.626935779	3.444989149	5.589503584	CORE	63	C	C	0.0000	63
H	16.375428013	3.305203667	6.367855461	CORE	64	H	H	0.0000	64
C	19.642046966	9.728437942	1.681481524	CORE	65	C	C	0.0000	65
H	20.155395656	9.733555887	0.722394563	CORE	66	H	H	0.0000	66
C	13.807710287	8.580634655	4.535118944	CORE	67	C	C	0.0000	67
H	14.269706553	9.183449963	5.318128766	CORE	68	H	H	0.0000	68
H	12.714767870	8.627282791	4.608058444	CORE	69	H	H	0.0000	69
H	14.134631847	8.925502617	3.543293554	CORE	70	H	H	0.0000	70
C	15.140528091	2.350568669	4.850033573	CORE	71	C	C	0.0000	71
H	15.505562347	1.344959579	5.057857014	CORE	72	H	H	0.0000	72
C	17.392915187	0.870423170	7.574294284	CORE	73	C	C	0.0000	73
H	17.817217588	1.717305931	8.116839021	CORE	74	H	H	0.0000	74
H	17.564062600	9.711709778	8.124082147	CORE	75	H	H	0.0000	75
H	16.317115758	1.009937120	7.423284449	CORE	76	H	H	0.0000	76
H	12.377085128	4.875052431	2.425621121	CORE	77	H	H	0.0000	77
H	12.376670021	3.131888891	2.083910304	CORE	78	H	H	0.0000	78
H	16.896034716	7.032432050	2.641189391	CORE	79	H	H	0.0000	79
H	16.517871654	7.754842884	4.213004465	CORE	80	H	H	0.0000	80
O	17.003176591	5.757910175	1.304234568	CORE	81	O	O	0.0000	81
O	14.558010506	7.424305473	0.328772097	CORE	82	O	O	0.0000	82

O	12.564261206	8.108039629	7.577882139	CORE	83	O	O	0.0000	83
O	18.369981855	4.043875883	1.864725652	CORE	84	O	O	0.0000	84
N	16.742840556	6.891017641	7.775290128	CORE	85	N	N	0.0000	85
N	12.478871414	0.940403640	7.003999761	CORE	86	N	N	0.0000	86
C	13.906982081	9.732757361	8.722514857	CORE	87	C	C	0.0000	87
C	17.929481289	4.981212410	0.997226719	CORE	88	C	C	0.0000	88
C	17.699268407	5.951172017	7.591991261	CORE	89	C	C	0.0000	89
C	13.418368309	8.388630972	8.439010167	CORE	90	C	C	0.0000	90
C	18.039044045	4.978516746	8.589888103	CORE	91	C	C	0.0000	91
C	13.405692807	1.076018295	7.976945981	CORE	92	C	C	0.0000	92
C	18.402373724	5.899497725	6.360771638	CORE	93	C	C	0.0000	93
H	18.167428591	6.636374298	5.592058077	CORE	94	H	H	0.0000	94
C	15.436947592	0.176103544	0.860339744	CORE	95	C	C	0.0000	95
H	15.797123931	9.089434091	1.422159502	CORE	96	H	H	0.0000	96
C	19.033733900	4.013909808	8.315953460	CORE	97	C	C	0.0000	97
H	19.854765279	3.296489966	0.219640614	CORE	98	H	H	0.0000	98
C	13.918392216	2.362071429	8.289099986	CORE	99	C	C	0.0000	99
H	13.563311634	3.210566691	7.703446059	CORE	100	H	H	0.0000	100
C	19.680399338	3.970773572	7.094457690	CORE	101	C	C	0.0000	101
H	20.437256025	3.213721967	6.899231507	CORE	102	H	H	0.0000	102
C	15.913958169	1.441704911	1.150012609	CORE	103	C	C	0.0000	103
H	16.662402568	1.581637919	1.928381227	CORE	104	H	H	0.0000	104
C	19.355285233	4.931440799	6.121296049	CORE	105	C	C	0.0000	105
H	19.868705699	4.926206713	5.162201866	CORE	106	H	H	0.0000	106
C	14.094788707	6.078688724	0.095617724	CORE	107	C	C	0.0000	107
H	14.556898695	5.475965111	0.878648497	CORE	108	H	H	0.0000	108
H	13.001876026	6.031825741	0.168577051	CORE	109	H	H	0.0000	109
H	13.848194435	5.734284509	7.982617595	CORE	110	H	H	0.0000	110
C	15.427417573	2.536031000	0.410513319	CORE	111	C	C	0.0000	111
H	15.792324908	3.541679247	0.618281383	CORE	112	H	H	0.0000	112
C	17.679088499	4.016762111	3.135530988	CORE	113	C	C	0.0000	113
H	18.103464413	3.169953197	3.678120702	CORE	114	H	H	0.0000	114
H	17.850802212	4.948489312	3.685329532	CORE	115	H	H	0.0000	115
H	16.603303381	3.877083884	2.984470036	CORE	116	H	H	0.0000	116
H	12.090594538	0.011697843	6.864920065	CORE	117	H	H	0.0000	117
H	12.090053031	1.754885427	6.523230805	CORE	118	H	H	0.0000	118
H	16.608890168	7.627210935	7.080502654	CORE	119	H	H	0.0000	119
H	16.230831814	6.905021505	8.652442819	CORE	120	H	H	0.0000	120
O	7.468115410	0.871528426	3.135362087	CORE	121	O	O	0.0000	121
O	9.913147492	2.538036358	4.110537463	CORE	122	O	O	0.0000	122
O	11.332442974	3.221441638	5.740941656	CORE	123	O	O	0.0000	123
O	6.101140924	8.929855705	2.575413101	CORE	124	O	O	0.0000	124
N	7.154713067	2.004541743	5.542996857	CORE	125	N	N	0.0000	125
N	11.418469941	5.826863934	6.314642762	CORE	126	N	N	0.0000	126

C	9.990019024	4.845954189	4.595823901	CORE	127	C	C	0.0000	127
C	6.542062624	0.094683635	3.442585032	CORE	128	C	C	0.0000	128
C	6.198378939	1.064588796	5.726391739	CORE	129	C	C	0.0000	129
C	10.478737473	3.501909944	4.879469822	CORE	130	C	C	0.0000	130
C	5.858808729	0.091733951	4.728690548	CORE	131	C	C	0.0000	131
C	10.491789066	5.962297917	5.341503328	CORE	132	C	C	0.0000	132
C	5.495286252	1.013013331	6.957643510	CORE	133	C	C	0.0000	133
H	5.730192210	1.749963031	7.726297911	CORE	134	H	H	0.0000	134
C	9.034619422	5.062625534	3.579032472	CORE	135	C	C	0.0000	135
H	8.673866782	4.202881922	3.017188273	CORE	136	H	H	0.0000	136
C	4.863469238	8.899989628	5.002734769	CORE	137	C	C	0.0000	137
H	4.616192440	8.182887796	4.220401234	CORE	138	H	H	0.0000	138
C	9.979012252	7.248253211	5.029190313	CORE	139	C	C	0.0000	139
H	10.333876675	8.096806539	5.614975864	CORE	140	H	H	0.0000	140
C	4.216776217	8.856989721	6.224224833	CORE	141	C	C	0.0000	141
H	3.460025377	8.099866468	6.419555227	CORE	142	H	H	0.0000	142
C	8.557527521	6.328150486	3.289162388	CORE	143	C	C	0.0000	143
H	7.809238972	6.467916142	2.510701628	CORE	144	H	H	0.0000	144
C	4.542505905	0.044852980	7.197249405	CORE	145	C	C	0.0000	145
H	4.029141241	0.039644357	8.156375018	CORE	146	H	H	0.0000	146
C	10.376486450	1.192441966	4.343630715	CORE	147	C	C	0.0000	147
H	9.914385311	0.589802108	3.560546089	CORE	148	H	H	0.0000	148
H	11.469395321	1.145598919	4.270720124	CORE	149	H	H	0.0000	149
H	10.049507420	0.847414556	5.335383670	CORE	150	H	H	0.0000	150
C	9.043828948	7.422593662	4.028764732	CORE	151	C	C	0.0000	151
H	8.678877890	8.428156230	3.820827128	CORE	152	H	H	0.0000	152
C	6.791789076	8.902875052	1.304454424	CORE	153	C	C	0.0000	153
H	6.367412595	8.056031244	0.761902310	CORE	154	H	H	0.0000	154
H	6.620482850	0.061628144	0.754782296	CORE	155	H	H	0.0000	155
H	7.867600599	8.763378583	1.455214542	CORE	156	H	H	0.0000	156
H	11.806671629	4.898127650	6.453920708	CORE	157	H	H	0.0000	157
H	11.807031235	6.641319549	6.795524837	CORE	158	H	H	0.0000	158
H	7.288485483	2.740907037	6.237630449	CORE	159	H	H	0.0000	159
H	7.666668576	2.018528798	4.665816318	CORE	160	H	H	0.0000	160
O	2.058472658	7.300891402	0.302440786	CORE	161	O	O	0.0000	161
O	0.141869149	8.125611616	7.551527216	CORE	162	O	O	0.0000	162
N	0.213973973	0.977282293	7.089460594	CORE	163	N	N	0.0000	163
C	1.490514808	9.635345338	8.842907530	CORE	164	C	C	0.0000	164
C	0.969850562	8.328305819	8.459325981	CORE	165	C	C	0.0000	165
C	1.096399480	1.029185822	8.111087843	CORE	166	C	C	0.0000	166
C	2.976219677	9.767982651	1.036839914	CORE	167	C	C	0.0000	167
H	3.279111782	8.871964354	1.577278533	CORE	168	H	H	0.0000	168
C	1.673099382	2.271095124	8.480813120	CORE	169	C	C	0.0000	169
H	1.399447111	3.153446782	7.901611084	CORE	170	H	H	0.0000	170

C	3.514141720	1.222476784	1.383064836	CORE	171	C	C	0.0000	171
H	4.214924390	1.308186819	2.212198346	CORE	172	H	H	0.0000	172
C	3.143715020	2.363979021	0.645800113	CORE	173	C	C	0.0000	173
H	3.568369151	3.334356549	0.903895963	CORE	174	H	H	0.0000	174
C	0.978878165	5.992092421	8.858945027	CORE	175	C	C	0.0000	175
H	1.300397810	5.696264135	7.850179361	CORE	176	H	H	0.0000	176
H	0.457232792	5.983090088	0.038137443	CORE	177	H	H	0.0000	177
H	1.977542430	5.317488861	0.727113152	CORE	178	H	H	0.0000	178
H	-0.126307873	1.822586355	6.627785989	CORE	179	H	H	0.0000	179
H	-0.226849261	0.078854702	6.910331087	CORE	180	H	H	0.0000	180
O	22.412331036	2.414642880	4.136536688	CORE	181	O	O	0.0000	181
O	23.754596599	3.238937251	5.766814625	CORE	182	O	O	0.0000	182
N	23.683244910	5.863587654	6.228824192	CORE	183	N	N	0.0000	183
C	22.406052900	4.748627185	4.475281935	CORE	184	C	C	0.0000	184
C	22.926838955	3.441607092	4.858774714	CORE	185	C	C	0.0000	185
C	22.800819216	5.915415390	5.207212619	CORE	186	C	C	0.0000	186
C	21.494056255	4.881867828	3.402455629	CORE	187	C	C	0.0000	187
H	21.191320028	3.985925726	2.861775576	CORE	188	H	H	0.0000	188
C	22.224087993	7.157347758	4.837538929	CORE	189	C	C	0.0000	189
H	22.497765826	8.039677752	5.416757127	CORE	190	H	H	0.0000	190
C	20.956857507	6.109350916	3.056302048	CORE	191	C	C	0.0000	191
H	20.256236340	6.195148677	2.227053256	CORE	192	H	H	0.0000	192
C	21.327160133	7.250798514	3.793705895	CORE	193	C	C	0.0000	193
H	20.902574395	8.221220535	3.535624738	CORE	194	H	H	0.0000	194
C	22.918801672	1.105508340	4.458830659	CORE	195	C	C	0.0000	195
H	22.597382230	0.809656355	5.467617947	CORE	196	H	H	0.0000	196
H	24.014007623	1.097450715	4.400835528	CORE	197	H	H	0.0000	197
H	22.493974728	0.431126722	3.711944864	CORE	198	H	H	0.0000	198
H	24.023362325	6.708954413	6.690508017	CORE	199	H	H	0.0000	199
H	24.124112995	4.965194989	6.407986034	CORE	200	H	H	0.0000	200
O	22.125450912	2.472694511	8.575669235	CORE	201	O	O	0.0000	201
O	24.041674738	1.648079561	1.326931674	CORE	202	O	O	0.0000	202
N	23.969672417	8.796346554	1.789096926	CORE	203	N	N	0.0000	203
C	22.693263913	0.138219549	0.035408558	CORE	204	C	C	0.0000	204
C	23.213888241	1.445301356	0.418980566	CORE	205	C	C	0.0000	205
C	23.087318017	8.744445781	0.767317409	CORE	206	C	C	0.0000	206
C	21.207685996	0.005430944	7.841362728	CORE	207	C	C	0.0000	207
H	20.904817331	0.901365509	7.300758043	CORE	208	H	H	0.0000	208
C	22.510748394	7.502496283	0.397601706	CORE	209	C	C	0.0000	209
H	22.784481250	6.620152895	0.976769361	CORE	210	H	H	0.0000	210
C	20.669831999	8.550902948	7.495170793	CORE	211	C	C	0.0000	211
H	19.969153618	8.465042292	6.665936793	CORE	212	H	H	0.0000	212
C	21.040226198	7.409467772	8.232511004	CORE	213	C	C	0.0000	213
H	20.615752626	6.439035236	7.974409106	CORE	214	H	H	0.0000	214

C	23.205190275	3.781428337	0.019319889	CORE	215	C	C	0.0000	215
H	22.883642166	4.077106057	1.028115485	CORE	216	H	H	0.0000	216
H	23.726796967	3.790225951	8.840152798	CORE	217	H	H	0.0000	217
H	22.206673631	4.456246132	8.151235959	CORE	218	H	H	0.0000	218
H	24.309886263	7.950988362	2.250682891	CORE	219	H	H	0.0000	219
H	24.410644265	9.694677799	1.968152453	CORE	220	H	H	0.0000	220
O	1.771884712	7.358868795	4.742756395	CORE	221	O	O	0.0000	221
O	0.429504927	6.534615632	3.112552337	CORE	222	O	O	0.0000	222
N	0.500613623	3.909916590	2.650654598	CORE	223	N	N	0.0000	223
C	1.778044695	5.024879143	4.404071791	CORE	224	C	C	0.0000	224
C	1.257246262	6.331914292	4.020563703	CORE	225	C	C	0.0000	225
C	1.383236719	3.858091332	3.672205395	CORE	226	C	C	0.0000	226
C	2.690344472	4.891700853	5.476690217	CORE	227	C	C	0.0000	227
H	2.993310947	5.787638495	6.017189928	CORE	228	H	H	0.0000	228
C	1.960105161	2.616196514	4.041728694	CORE	229	C	C	0.0000	229
H	1.686500982	1.733876659	3.462454326	CORE	230	H	H	0.0000	230
C	3.227624681	3.664212212	5.822750693	CORE	231	C	C	0.0000	231
H	3.928466995	3.578433853	6.651833013	CORE	232	H	H	0.0000	232
C	2.857212830	2.522780176	5.085408084	CORE	233	C	C	0.0000	233
H	3.281933115	1.552381223	5.343350766	CORE	234	H	H	0.0000	234
C	1.265565442	8.668004831	4.420269773	CORE	235	C	C	0.0000	235
H	1.587015840	8.963636161	3.411445426	CORE	236	H	H	0.0000	236
H	0.170333458	8.676113320	4.478228254	CORE	237	H	H	0.0000	237
H	1.690369002	9.342467878	5.167062045	CORE	238	H	H	0.0000	238
H	0.160874380	3.064608298	2.188634116	CORE	239	H	H	0.0000	239
H	0.060075590	4.808362984	2.471218261	CORE	240	H	H	0.0000	240

end

end

B phase structure:

PBC	10.1717	15.2593	15.1585	90.3980	76.6383	100.7602				
H	5.729057307	15.302481246	9.187630591	CORE	1	H	H	0.0000	1	
H	5.456986014	6.131686708	10.573683469	CORE	2	H	H	0.0000	2	
H	1.847490877	0.954258396	5.662631633	CORE	3	H	H	0.0000	3	
H	12.188140324	5.495098747	14.100409657	CORE	4	H	H	0.0000	4	
H	10.926707368	2.940061962	6.704867384	CORE	5	H	H	0.0000	5	
H	4.367547198	8.119493957	11.615467815	CORE	6	H	H	0.0000	6	
H	9.235040239	2.591851267	8.499666859	CORE	7	H	H	0.0000	7	
H	7.267221668	2.332464452	10.106461136	CORE	8	H	H	0.0000	8	
H	6.992250149	3.222118916	8.564307204	CORE	9	H	H	0.0000	9	
H	5.785810922	2.015058738	9.135785065	CORE	10	H	H	0.0000	10	
H	2.676200740	7.774217555	13.411196450	CORE	11	H	H	0.0000	11	
H	-0.671031044	11.829994793	4.219501117	CORE	12	H	H	0.0000	12	
H	0.809955993	12.146951797	5.191187064	CORE	13	H	H	0.0000	13	

H	0.534806847	13.038661433	3.650063495 CORE	14	H	H	0.0000	14
H	3.547561369	2.470646923	12.808425989 CORE	15	H	H	0.0000	15
H	12.452358824	3.108768165	13.869197257 CORE	16	H	H	0.0000	16
H	5.997825698	12.917276092	8.956626539 CORE	17	H	H	0.0000	17
H	7.265813854	12.281127491	7.895818476 CORE	18	H	H	0.0000	18
H	3.815590258	12.808776081	5.915142938 CORE	19	H	H	0.0000	19
H	2.609829896	10.163428879	12.436953964 CORE	20	H	H	0.0000	20
H	0.370163919	12.167964745	9.436501201 CORE	21	H	H	0.0000	21
H	1.287946458	14.900897235	13.140478449 CORE	22	H	H	0.0000	22
H	1.460731827	10.181403466	8.393480245 CORE	23	H	H	0.0000	23
H	11.094296213	10.729863156	14.184826589 CORE	24	H	H	0.0000	24
H	3.154817323	10.528685353	6.601007616 CORE	25	H	H	0.0000	25
H	4.749762881	9.010118892	9.415029701 CORE	26	H	H	0.0000	26
H	5.957005721	10.260994662	9.899108496 CORE	27	H	H	0.0000	27
H	4.739501411	10.626733605	8.626384913 CORE	28	H	H	0.0000	28
H	10.459366048	13.118625255	14.524693807 CORE	29	H	H	0.0000	29
H	11.582764659	0.977442131	9.907804831 CORE	30	H	H	0.0000	30
H	2.892277023	1.293288226	10.879427362 CORE	31	H	H	0.0000	31
H	9.008092905	15.077072274	11.449353080 CORE	32	H	H	0.0000	32
H	3.753191386	14.310148332	10.540869849 CORE	33	H	H	0.0000	33
H	5.610285820	0.545198696	11.351083800 CORE	34	H	H	0.0000	34
H	3.548972732	15.194296768	6.146439687 CORE	35	H	H	0.0000	35
H	5.130410978	0.840169707	7.207255519 CORE	36	H	H	0.0000	36
H	4.542233799	3.402388166	6.875736769 CORE	37	H	H	0.0000	37
H	6.934022501	6.989965438	4.524545207 CORE	38	H	H	0.0000	38
H	3.220328092	8.140390430	7.574635435 CORE	39	H	H	0.0000	39
H	0.207912921	7.628705290	1.003102865 CORE	40	H	H	0.0000	40
H	4.907162624	7.571973558	5.826995826 CORE	41	H	H	0.0000	41
H	8.025919585	5.002968226	3.484025521 CORE	42	H	H	0.0000	42
H	5.542601487	5.182859959	5.490136541 CORE	43	H	H	0.0000	43
H	5.397421700	9.900242658	6.534009225 CORE	44	H	H	0.0000	44
H	6.605835446	11.106255043	5.964698403 CORE	45	H	H	0.0000	45
H	5.125218702	10.790703683	4.991760116 CORE	46	H	H	0.0000	46
H	-0.451329375	5.349358251	1.691283078 CORE	47	H	H	0.0000	47
H	1.075502106	9.295822216	10.594867897 CORE	48	H	H	0.0000	48
H	10.044825404	8.039969758	10.112216383 CORE	49	H	H	0.0000	49
H	11.261260424	7.681227516	11.387842280 CORE	50	H	H	0.0000	50
H	-1.326630084	10.652267446	2.292413383 CORE	51	H	H	0.0000	51
H	-0.058893405	10.014406174	1.232608257 CORE	52	H	H	0.0000	52
H	3.065880444	2.768624882	8.664024398 CORE	53	H	H	0.0000	53
H	2.073173021	3.995280170	9.471746599 CORE	54	H	H	0.0000	54
H	7.846811068	9.717877072	8.228242107 CORE	55	H	H	0.0000	55
H	9.784882948	2.955268339	2.658438616 CORE	56	H	H	0.0000	56
H	9.169432955	4.979954608	7.529783807 CORE	57	H	H	0.0000	57

H	-1.917422520	13.207030751	1.961492152 CORE	58	H	H	0.0000	58
H	7.484347936	5.548363682	9.278526399 CORE	59	H	H	0.0000	59
H	1.297663022	2.384898750	0.909645326 CORE	60	H	H	0.0000	60
H	6.848321740	7.937400516	9.615749839 CORE	61	H	H	0.0000	61
H	7.648238884	4.113981069	5.680844798 CORE	62	H	H	0.0000	62
H	6.439940529	2.863726856	5.198439324 CORE	63	H	H	0.0000	63
H	7.656337657	2.498363985	6.472053714 CORE	64	H	H	0.0000	64
H	-0.916992875	14.986513228	0.573657289 CORE	65	H	H	0.0000	65
H	2.344000747	5.077554904	4.994618459 CORE	66	H	H	0.0000	66
H	1.139045911	3.827171010	4.504514565 CORE	67	H	H	0.0000	67
H	1.132505454	5.444440180	3.716600522 CORE	68	H	H	0.0000	68
H	5.790184564	13.802872231	4.560410997 CORE	69	H	H	0.0000	69
H	6.780850166	12.575250079	3.750968927 CORE	70	H	H	0.0000	70
H	9.323085007	10.351908332	6.440326842 CORE	71	H	H	0.0000	71
H	0.143476969	9.125179971	5.632123604 CORE	72	H	H	0.0000	72
H	6.828563143	2.357195210	14.349021083 CORE	73	H	H	0.0000	73
H	10.272879753	3.003799390	10.827722695 CORE	74	H	H	0.0000	74
H	5.073570443	15.363278846	13.306193770 CORE	75	H	H	0.0000	75
H	9.616265515	0.722754740	11.513777058 CORE	76	H	H	0.0000	76
H	1.515128336	5.598065112	0.087193526 CORE	77	H	H	0.0000	77
H	2.996952339	5.914258959	1.057823774 CORE	78	H	H	0.0000	78
H	1.790826077	4.706269085	1.628090679 CORE	79	H	H	0.0000	79
H	10.002451989	5.388742135	11.058943387 CORE	80	H	H	0.0000	80
H	8.734234729	6.023804199	12.120314235 CORE	81	H	H	0.0000	81
H	6.834459308	13.323154287	12.485542756 CORE	82	H	H	0.0000	82
H	8.146473941	8.582496355	11.786011839 CORE	83	H	H	0.0000	83
H	8.519137432	12.751761829	10.737288278 CORE	84	H	H	0.0000	84
H	9.148934811	10.361248783	10.399171151 CORE	85	H	H	0.0000	85
H	1.198960560	12.307865198	1.558265054 CORE	86	H	H	0.0000	86
H	-0.017870211	12.673153528	0.284926997 CORE	87	H	H	0.0000	87
H	1.190230232	13.923719794	0.767829057 CORE	88	H	H	0.0000	88
H	6.673826464	7.951726898	13.577469699 CORE	89	H	H	0.0000	89
H	5.684477383	9.179999198	14.386912692 CORE	90	H	H	0.0000	90
H	2.715298723	14.788110314	2.620985993 CORE	91	H	H	0.0000	91
H	4.245667229	4.536534780	3.315714606 CORE	92	H	H	0.0000	92
H	3.878814221	0.368012397	4.368563774 CORE	93	H	H	0.0000	93
H	3.246242534	2.757821056	4.705274392 CORE	94	H	H	0.0000	94
H	6.060654690	14.884590268	0.077798068 CORE	95	H	H	0.0000	95
H	8.358643310	14.189087211	14.335263485 CORE	96	H	H	0.0000	96
H	11.194128014	0.812921069	13.542682707 CORE	97	H	H	0.0000	97
H	5.718508860	5.168025704	1.526688002 CORE	98	H	H	0.0000	98
H	6.707377318	3.940425084	0.715217892 CORE	99	H	H	0.0000	99
H	5.565002465	10.757695904	0.754409790 CORE	100	H	H	0.0000	100
H	2.115952098	10.119301099	4.272646335 CORE	101	H	H	0.0000	101

H	4.471188396	12.745036544	1.792986729	CORE	102	H	H	0.0000	102
H	2.776755963	12.398636221	3.585725911	CORE	103	H	H	0.0000	103
H	7.372333262	6.955394257	0.285147595	CORE	104	H	H	0.0000	104
H	9.393190970	7.198131431	14.052667062	CORE	105	H	H	0.0000	105
H	10.600887946	8.403511762	13.480469762	CORE	106	H	H	0.0000	106
H	2.383819180	7.733912685	4.044464873	CORE	107	H	H	0.0000	107
H	3.652931787	7.095818134	2.986278045	CORE	108	H	H	0.0000	108
C	4.383945788	4.690417138	11.754169759	CORE	109	C	C	0.0000	109
C	8.760269319	13.354324762	6.223471866	CORE	110	C	C	0.0000	110
C	7.097822770	14.298066170	7.850009275	CORE	111	C	C	0.0000	111
C	5.045201964	3.541957619	11.136450614	CORE	112	C	C	0.0000	112
C	8.098376171	14.501839130	6.841841614	CORE	113	C	C	0.0000	113
C	3.383441759	4.487792594	12.762938371	CORE	114	C	C	0.0000	114
C	9.334474073	0.456682164	8.415294676	CORE	115	C	C	0.0000	115
C	4.708012356	6.004531015	11.353682003	CORE	116	C	C	0.0000	116
C	11.270030644	0.825564490	6.442210887	CORE	117	C	C	0.0000	117
C	2.772809617	5.638857288	13.327834551	CORE	118	C	C	0.0000	118
C	10.663842793	1.931021845	7.014051344	CORE	119	C	C	0.0000	119
C	4.103417884	7.110655221	11.925346843	CORE	120	C	C	0.0000	120
C	9.696697003	1.730033336	8.014610926	CORE	121	C	C	0.0000	121
C	6.514228395	2.775404683	9.441563903	CORE	122	C	C	0.0000	122
C	3.136518340	6.911730960	12.926091377	CORE	123	C	C	0.0000	123
C	0.056938852	12.590292681	4.526576653	CORE	124	C	C	0.0000	124
C	2.890940387	12.191916994	11.783129384	CORE	125	C	C	0.0000	125
C	0.783875453	14.759068919	8.877373707	CORE	126	C	C	0.0000	126
C	2.446800440	13.814191084	7.251879877	CORE	127	C	C	0.0000	127
C	3.869651077	11.831612020	10.759082067	CORE	128	C	C	0.0000	128
C	1.445167350	13.610677357	8.259284242	CORE	129	C	C	0.0000	129
C	2.525100058	13.567047694	11.973517085	CORE	130	C	C	0.0000	130
C	3.058004523	12.663884802	6.686517035	CORE	131	C	C	0.0000	131
C	2.297071050	11.196059561	12.588690353	CORE	132	C	C	0.0000	132
C	1.120336025	12.296202463	8.657743355	CORE	133	C	C	0.0000	133
C	1.565798295	13.857769585	12.979304429	CORE	134	C	C	0.0000	134
C	1.725506035	11.190433284	8.085635929	CORE	135	C	C	0.0000	135
C	1.364134727	11.506079838	13.563285299	CORE	136	C	C	0.0000	136
C	2.693860000	11.390788203	7.086140663	CORE	137	C	C	0.0000	137
C	4.928425953	10.080680777	9.558739766	CORE	138	C	C	0.0000	138
C	1.005595867	12.853476952	13.748399241	CORE	139	C	C	0.0000	139
C	12.335287073	0.533560633	10.572637270	CORE	140	C	C	0.0000	140
C	8.008914448	8.432141951	3.346539054	CORE	141	C	C	0.0000	141
C	1.959458878	6.473675933	9.253695471	CORE	142	C	C	0.0000	142
C	3.304041329	4.737184989	8.040804112	CORE	143	C	C	0.0000	143
C	7.346694661	9.580130680	3.963609884	CORE	144	C	C	0.0000	144
C	2.938657843	6.112549012	8.230179096	CORE	145	C	C	0.0000	145

C	9.010506424	8.635056464	2.339027979	CORE	146	C	C	0.0000	146
C	4.263785241	4.445445940	7.035727807	CORE	147	C	C	0.0000	147
C	7.684560187	7.117769825	3.746151776	CORE	148	C	C	0.0000	148
C	3.532768861	7.107598036	7.423722423	CORE	149	C	C	0.0000	149
C	-0.549301517	7.484531809	1.774861119	CORE	150	C	C	0.0000	150
C	4.465608680	6.796446086	6.449387998	CORE	151	C	C	0.0000	151
C	8.290369006	6.011747709	3.175124576	CORE	152	C	C	0.0000	152
C	4.824286037	5.449054126	6.265609092	CORE	153	C	C	0.0000	153
C	5.876954650	10.346852215	5.657569746	CORE	154	C	C	0.0000	154
C	9.258757347	6.211523828	2.175728682	CORE	155	C	C	0.0000	155
C	11.072289789	8.224290222	10.453733206	CORE	156	C	C	0.0000	156
C	9.502998420	0.927879764	3.316096483	CORE	157	C	C	0.0000	157
C	0.257076743	6.647613756	5.849549000	CORE	158	C	C	0.0000	158
C	9.084394627	8.383084377	7.063114493	CORE	159	C	C	0.0000	159
C	8.525651838	1.290127489	4.340715326	CORE	160	C	C	0.0000	160
C	9.449999261	7.008091710	6.873333729	CORE	161	C	C	0.0000	161
C	7.018501458	14.543379094	3.126835510	CORE	162	C	C	0.0000	162
C	8.125319962	8.674790994	8.068550824	CORE	163	C	C	0.0000	163
C	10.096693093	1.922229852	2.508235390	CORE	164	C	C	0.0000	164
C	8.856902411	6.012850092	7.680480352	CORE	165	C	C	0.0000	165
C	7.977139574	14.250473905	2.120992772	CORE	166	C	C	0.0000	166
C	7.924953201	6.324054897	8.655509754	CORE	167	C	C	0.0000	167
C	0.856761903	1.609827992	1.533349163	CORE	168	C	C	0.0000	168
C	7.565807985	7.671228930	8.839264307	CORE	169	C	C	0.0000	169
C	7.468565765	3.043435878	5.538851161	CORE	170	C	C	0.0000	170
C	1.214675885	0.262420915	1.350078250	CORE	171	C	C	0.0000	171
C	1.316989939	4.897664741	4.649479735	CORE	172	C	C	0.0000	172
C	7.901650971	3.801691818	13.172445187	CORE	173	C	C	0.0000	173
C	7.238961534	4.948968665	13.791261538	CORE	174	C	C	0.0000	174
C	8.902745525	4.007127844	12.164767917	CORE	175	C	C	0.0000	175
C	7.579035638	2.486605045	13.570686213	CORE	176	C	C	0.0000	176
C	9.515854378	2.857659206	11.599249071	CORE	177	C	C	0.0000	177
C	8.185861041	1.381831604	12.998454981	CORE	178	C	C	0.0000	178
C	9.153720110	1.583951144	11.999079752	CORE	179	C	C	0.0000	179
C	2.268437341	5.154276315	0.751250550	CORE	180	C	C	0.0000	180
C	6.549465904	11.295679875	13.141503743	CORE	181	C	C	0.0000	181
C	5.570750559	11.658378511	14.164809451	CORE	182	C	C	0.0000	182
C	6.913107207	9.919809083	12.952845366	CORE	183	C	C	0.0000	183
C	7.144571482	12.289611381	12.334456754	CORE	184	C	C	0.0000	184
C	7.870830103	9.626310750	11.946476398	CORE	185	C	C	0.0000	185
C	8.076386624	11.976919206	11.359615286	CORE	186	C	C	0.0000	186
C	8.432219192	10.628685122	11.175745375	CORE	187	C	C	0.0000	187
C	1.010752584	12.853144689	0.625315206	CORE	188	C	C	0.0000	188
C	5.844922834	1.824298124	1.961518922	CORE	189	C	C	0.0000	189

C	6.822423909	1.462472017	0.936974077	CORE	190	C	C	0.0000	190
C	5.480122447	3.199683225	2.150030889	CORE	191	C	C	0.0000	191
C	5.252087742	0.830266718	2.770269647	CORE	192	C	C	0.0000	192
C	4.522600037	3.492938104	3.156583805	CORE	193	C	C	0.0000	193
C	4.320261743	1.142755669	3.745289332	CORE	194	C	C	0.0000	194
C	3.962642447	2.490590540	3.928312285	CORE	195	C	C	0.0000	195
C	8.535291688	15.260287035	14.476216049	CORE	196	C	C	0.0000	196
C	4.489202041	9.315913833	1.931728270	CORE	197	C	C	0.0000	197
C	5.152129348	8.167100500	1.315954112	CORE	198	C	C	0.0000	198
C	3.486403958	9.112701831	2.938198768	CORE	199	C	C	0.0000	199
C	4.813442661	10.630118466	1.532035664	CORE	200	C	C	0.0000	200
C	2.873922556	10.263572777	3.501628179	CORE	201	C	C	0.0000	201
C	4.206850830	11.736132169	2.102020259	CORE	202	C	C	0.0000	202
C	3.237981727	11.536384544	3.100955339	CORE	203	C	C	0.0000	203
C	10.122654868	7.957623088	14.358056817	CORE	204	C	C	0.0000	204
N	6.728723080	13.062451122	8.258766234	CORE	205	N	N	0.0000	205
N	3.013187294	3.253571847	13.172433236	CORE	206	N	N	0.0000	206
N	2.817969054	15.049085673	6.844327044	CORE	207	N	N	0.0000	207
N	3.053795814	14.566053643	11.232405300	CORE	208	N	N	0.0000	208
N	2.774731761	3.739252143	8.782538253	CORE	209	N	N	0.0000	209
N	-0.790962542	9.869870305	1.929654159	CORE	210	N	N	0.0000	210
N	9.613690710	9.381555217	6.321145236	CORE	211	N	N	0.0000	211
N	6.488860341	13.545863572	3.868737710	CORE	212	N	N	0.0000	212
N	9.271500581	5.242420599	11.756823620	CORE	213	N	N	0.0000	213
N	6.383909264	8.922481120	13.696218030	CORE	214	N	N	0.0000	214
N	6.008457419	4.197370650	1.406578880	CORE	215	N	N	0.0000	215
N	3.115716799	7.878468092	3.347134528	CORE	216	N	N	0.0000	216
O	8.618486301	12.167334759	6.577120609	CORE	217	O	O	0.0000	217
O	5.855892984	3.872957091	10.104519940	CORE	218	O	O	0.0000	218
O	4.901668446	2.355843942	11.490137047	CORE	219	O	O	0.0000	219
O	-0.602238525	13.686303084	5.190970311	CORE	220	O	O	0.0000	220
O	3.776462837	0.954363425	8.524594513	CORE	221	O	O	0.0000	221
O	3.992948828	10.492798680	10.573641414	CORE	222	O	O	0.0000	222
O	4.536891257	12.644085941	10.095654383	CORE	223	O	O	0.0000	223
O	-0.027258917	14.427474220	9.908740659	CORE	224	O	O	0.0000	224
O	11.460958430	5.661958169	9.914688234	CORE	225	O	O	0.0000	225
O	6.535510221	9.249185888	4.995121541	CORE	226	O	O	0.0000	226
O	7.490140966	10.766575775	3.609924439	CORE	227	O	O	0.0000	227
O	1.839089539	7.812401305	9.441377028	CORE	228	O	O	0.0000	228
O	0.927337768	7.460097416	5.188962885	CORE	229	O	O	0.0000	229
O	8.403833483	2.629127712	4.524728826	CORE	230	O	O	0.0000	230
O	7.858157004	0.478993773	5.005914583	CORE	231	O	O	0.0000	231
O	0.377495425	5.309230271	5.660937695	CORE	232	O	O	0.0000	232
O	2.926796835	4.057759228	0.086482597	CORE	233	O	O	0.0000	233

O	7.380231555	6.135377970	13.438122141	CORE	234	O	O	0.0000	234
O	5.449100966	12.997550688	14.348497766	CORE	235	O	O	0.0000	235
O	1.399072367	10.289004138	0.090953948	CORE	236	O	O	0.0000	236
O	6.945700423	0.123511730	0.753411146	CORE	237	O	O	0.0000	237
O	7.489089960	2.273960542	0.271549768	CORE	238	O	O	0.0000	238
O	5.962190643	8.497474787	0.283198337	CORE	239	O	O	0.0000	239
O	5.010164437	6.981512868	1.671482224	CORE	240	O	O	0.0000	240

end
end

6. Cross-testing of AtomFT

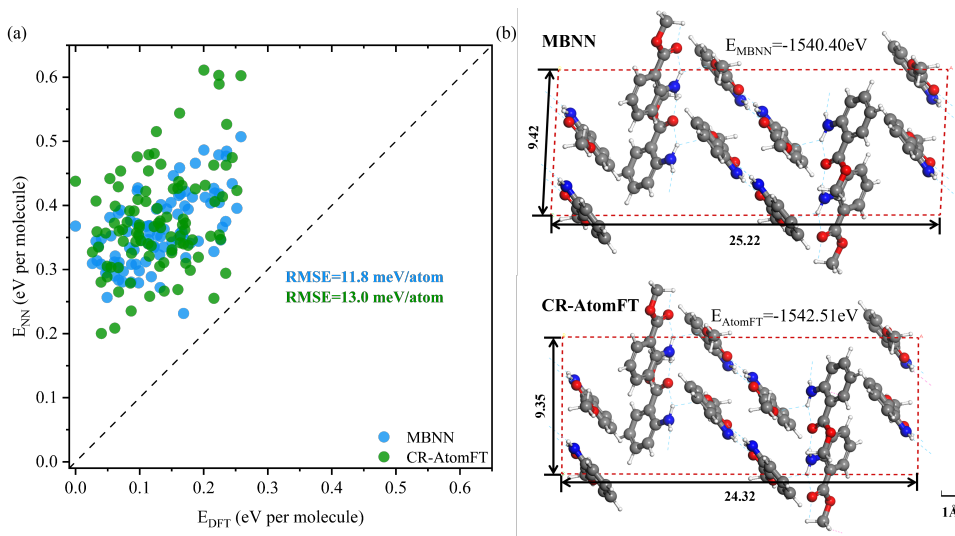


Figure S2 The cross-testing results. (a) Scatter plot illustrating the correlation between energies calculated using NN potentials (MBNN and CR-AtomFT) and DFT for 95 molecular crystal structures; (b) Structures optimized from A phase using MBNN and CR-AtomFT.

Cross-testing is conducted to examine whether the AtomFT potential maintains reasonable accuracy beyond the specific fine-tuning domain. The AtomFT potential fine-tuned for the chemical reaction system (Example 2), CR-AtomFT, is utilized to predict the molecule crystal system (Example 3). The results by benchmarking MBNN and CR-AtomFT with DFT energetics of molecular crystals are presented in **Figure S3**.

Figure S3a illustrates the single-point energies for 95 molecular crystal structures calculated by MBNN and CR-AtomFT, presented in a scatter plot. Both models yield energies within a similar range compared to DFT energies, both exhibiting a systematic overestimation. The RMSE of energy indicates a marginal increase for CR-AtomFT (13.0 meV/atom) compared to the basis MBNN performance (11.8 meV/atom), suggesting that the overall predictive capability remains largely unaffected despite this slight deviation. Further testing of the CR-AtomFT potential for the global PES exploration is also successful. Taking A phase as an example, we show in **Figure S3b** that the optimized structures using MBNN and CR-AtomFT are highly consistent, with the lattice differing by only 3%. In fact, the energy of the corresponding structure calculated by CR-AtomFT (-1542.51 eV) is closer to the standard DFT energy of A phase (-1542.99 eV) compared to the results obtained from MBNN (-1540.40 eV), implying the error origin in two examples (e.g. local interaction) share similarities.

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