Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Unraveling the structural transition mechanism of room-temperature compressed graphite carbon

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1. SSW crystal/surface pathway sampling method

In this work, we employed two levels of pseudopotentials based on the density functional theory (DFT): the traditional first-principles method and a highly optimized neural-network (NN) potential[1]. Both of them are integrated with the stochastic surface walking (SSW) algorithm for free energy surface optimization[2–4]. This SSW algorithm was implemented in LASP (Large-scale Atomic Simulation with neural network Potential) software[5], to sample the low energy barrier to leave graphite under 15 GPa. We would like to note that the NN potential is of high precision and predictable similar to the first-principles method. During the pathway sampling, the one-to-one correspondence for both lattice ($L(e_1,e_2,e_3)$, e_i being the lattice vector) and atom (q_i, i=1,..3N, N is the number of atom in cell) from one crystal phase (the initial state, IS) to another (the final state, FS) are obtained, which constitutes the reaction coordinates of the reaction, i.e. $Q_{IS}(L,q)\rightarrow Q_{FS}(L,q)$. In one SSW pathway sampling simulation, we need to collect as many as possible IS/FS pairs (typically a few thousands) to ensure the best reaction coordinate were contained. Then, we utilize the DESW method to identify the TSs explicitly for all the IS/FS pairs. After the fast DESW pathway screen, the lowest energy pathway were obtained. Then, using the information, enlarged supercell were built to re-searched the lowest energy pathway, which via interface intermediate phase transition pathway, namely in the heterogenous mechanism. It should be mentioned that due to the large number of possible reaction pathways for the bulk /surface structure transition/reconstruction and the large system size of bulk (48 atoms), the NN potential simulation is the practical solution for the initial screening of the pathways, where up to 10^3 pathways are sampled for each surface structure.

In this work, the low energy pathway candidates obtained using DESW method will be further refined by DFT calculations to obtain accurate energetics of the reaction. The DFT calculations were carried out by using the Vienna ab initio simulation package (VASP)[6]. The exchange-correlation

functional is parameterized by the local density approximation (LDA). For all the structures, both lattice and atomic positions were fully optimized in SSW-DFT/DFT until the maximal stress component is less than 0.1 GPa and the maximal force component is less than 0.01 eV/Å.

2. The carbon allotropes parameter

Table S1. The carbon allotropes parameter at 15 GPa from DFT-LDA.

Phase	*IT Number*	*Symmetry group*	*a(Å)*	*b(Å)*	*c(Å)*	*α(°)*	*β(°)*	*γ(°)*
graphite	194	P63/MMC	2.423	2.423	5.613	90	90	120
CD	227	FD-3M	3.500	3.500	3.500	90	90	90
HD	194	P63/MMC	2.461	2.461	4.099	90	90	120
M	12	C2/M	8.988	2.472	4.069	90	96.896	90
BCT	139	I4/MMM	4.284	4.284	2.462	90	90	90

3. The Validation of NN potential

In this work, we developed the carbon NN potential based on the neural networks methods (*Huang, S.-D.; Shang, C.; Zhang, X.-J.; Liu, Z.-P. Material Discovery by Combining Stochastic Surface Walking Global Optimization wit*h a Neural Network. Chem. Sci. 2017, 8 (9), 6327–6337.). In order to build the NN potential for carbon, more than 10^7 structures on high-pressure C PES were visited from 0 GPa to 30 GPa by SSW-NN during NN potential generation and the final training data set of C consists of 51971 structures to represent the global PES. The G-NN follows the feed-forward NN architecture with five-layers (210-90-80-80-1), reaching to 33390 fitting parameters in total, including 97 two-body, 97 three-body, 12 four-body descriptors. For the final G-NN potential, the root-mean-square (RMS) errors for the energy and the force reaches 8.119 meV/atom and 0.237 eV/Å, respectively.

We also compared the accuracy of NN with DFT approach for the equations of states (EOS). The EOS results are summarized in Table S2, as shown below. In general, our NN results agree with the DFT results very well. This indicates that NN can yield reliable geometry comparable to DFT.

Table S2. The energy from NN and DFT, pressure from 0 to 30 GPa, GR: graphite; CD: cubic diamond. Energy unit: eV/atom.

Pressure GPa	GR ΔE(NN-DFT)	HD ΔE(NN-DFT)	ΔE(HD-GR) DFT	ΔE(HD-GR） NN
0	-0.004475	-0.0035785	0.1576415	0.158538
2	0.00023875	-0.003939	0.104765	0.10058725
4	-0.0036283	-0.0042655	0.0635875	0.06295025
6	-0.0055312	-0.0045475	0.02724125	0.028225
8	-0.0061765	-0.0047847	-0.0055863	-0.0041945
10	-0.0072833	-0.0049768	-0.0359278	-0.0336213
12	-0.0081827	-0.0051335	-0.0642892	-0.06124
14	-0.008911	-0.0052408	-0.0910033	-0.087333

16	-0.0094282	-0.0053037	-0.116321	-0.1121965
18	-0.010057	-0.005326	-0.1409613	-0.1362302
20	-0.009404	-0.0053102	-0.1634633	-0.1593695
22	-0.0091043	-0.005263	-0.185508	-0.1816668
24	-0.0086015	-0.0051768	-0.2066078	-0.203183
26	-0.008138	-0.0050633	-0.226948	-0.2238733
28	-0.007799	-0.0049285	-0.246539	-0.2436685
30	-0.007752	-0.0047653	-0.2655622	-0.2625755

4. The transition energy barrier vs pressure

In order to consider the pressure influence, we calculate the energy barrier at different pressure. Here, the DFT calculation are done at 0, 15, and 30 GPa.

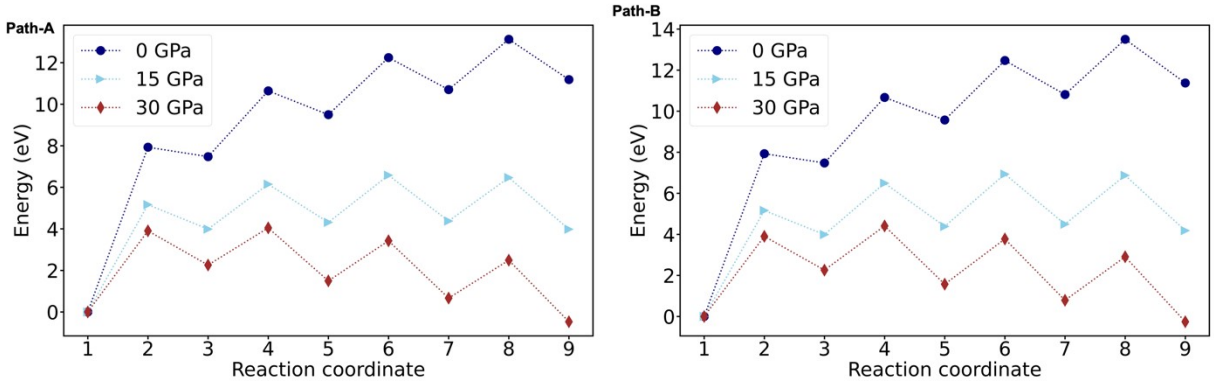

Fig S1. Energy profiles from graphite to x-phase via step-by-step movement at different pressure.

The pressure-induced phase transitions mechanism also can be confirmed by the energy profiles from different pressure in Figure S1 in SI. We can find that the higher pressure will reduce the energy barrier both in Path-A and Path-B, as expected. For example, in the first step of Path-A, the energy barrier drops from 7.93 eV at 0 GPa, and 5.16 eV at 15 GPa to 3.90 eV at 30 GPa.

5. The surface phase transition energy profiles

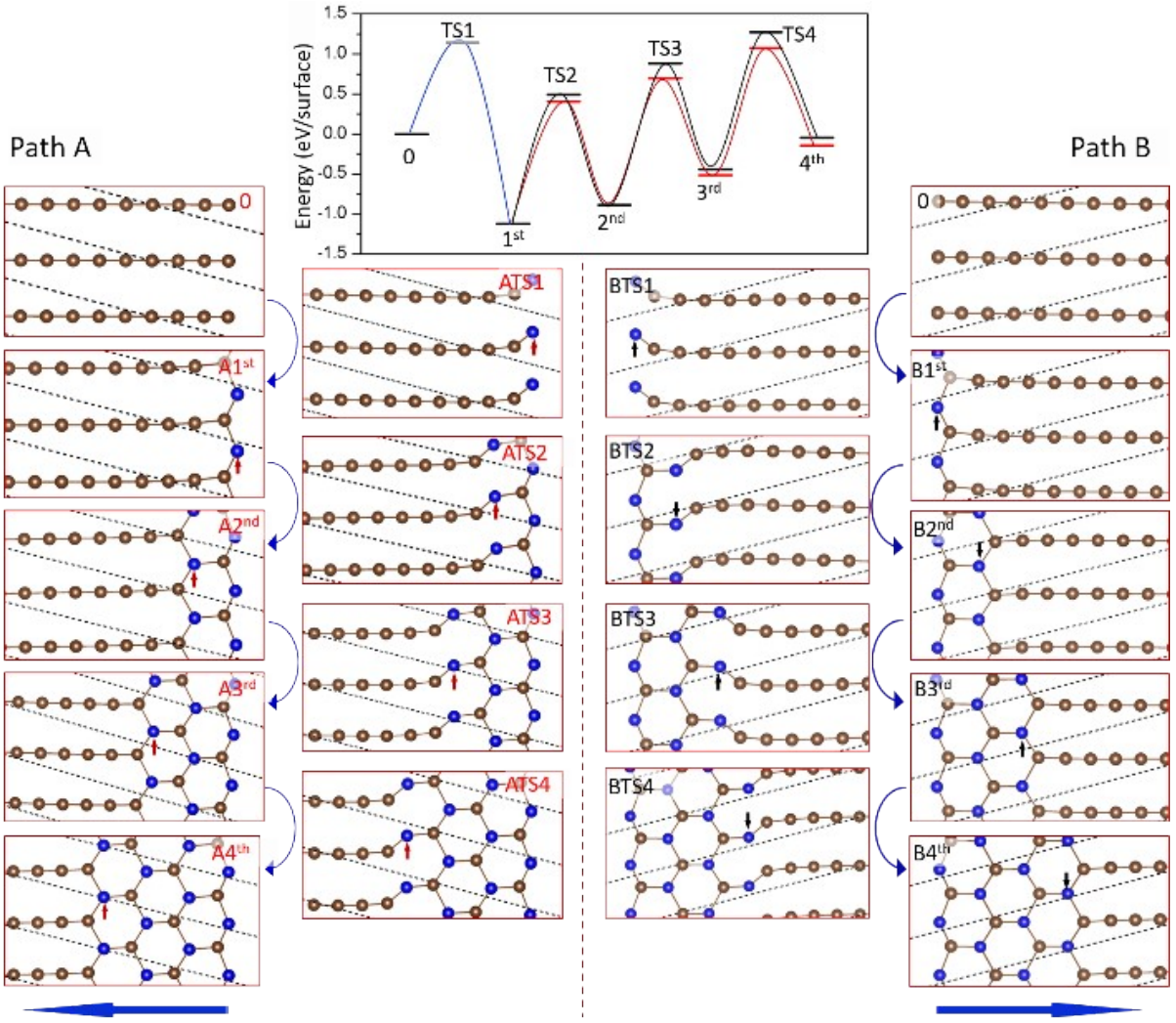

Fig S2. Energy profiles and key structures for the graphite to X structure via step-by-step movement in surface mode. Left is the Path-A (the red line) which the atoms shearing in one direction; Right is for Path-B (the black line) which the every other of atoms shearing to different directions. The moved atom and direction are depicted as the arrow.

6. Structure information of transition pathway

Graphite to BCT-diamond

graphite

PBC 3.96395546 6.27600350 3.95925578 108.55697457 75.41894805 142.31675269

C 3.800272011 -0.432403592 3.699926509 CORE 1 C C 0.0000 1
C -0.661733215 1.484025728 0.576033243 CORE 2 C C 0.0000 2
C 1.319923486 -0.046992136 1.823224418 CORE 3 C C 0.0000 3
C 1.818617081 1.098611594 2.452736999 CORE 4 C C 0.0000 4
C 1.316849887 1.485844732 3.699925959 CORE 5 C C 0.0000 5
C -3.145155135 3.402272011 0.576033405 CORE 6 C C 0.0000 6
C -1.163498156 1.871256494 1.823223544 CORE 7 C C 0.0000 7
C -0.664807713 3.016860202 2.452735649 CORE 8 C C 0.0000 8

end

end

BCT

PBC 3.26980489 6.53947914 3.26960491 98.14869820 98.14690907 135.76635204

C 2.256708107 0.411712001 0.000000028 CORE 1 C C 0.0000 1
C -1.329687108 1.869213681 0.000002411 CORE 2 C C 0.0000 2
C 0.000050752 0.000066158 1.093513247 CORE 3 C C 0.0000 3
C 0.463632539 1.140607773 1.935587549 CORE 4 C C 0.0000 4
C -0.086060434 2.692634229 0.000000029 CORE 5 C C 0.0000 5
C -3.672455838 4.150136172 0.000002312 CORE 6 C C 0.0000 6
C -2.342719248 2.280988899 1.093513616 CORE 7 C C 0.0000 7
C -1.879138468 3.421532717 1.935587657 CORE 8 C C 0.0000 8

end

graphite to HD

graphite

PBC 5.79372439 2.42246555 4.19694698 89.99446828 75.77071901 89.97295256

C 4.176513280 1.513920218 2.204808150 CORE 1 C C 0.0000 1
C 1.279052501 0.302617946 2.204710920 CORE 2 C C 0.0000 2
C 3.660129355 0.302696600 0.170712779 CORE 3 C C 0.0000 3
C 0.763811762 1.513871038 0.170616708 CORE 4 C C 0.0000 4
C 3.840813623 1.514170442 0.846401336 CORE 5 C C 0.0000 5
C 4.356052239 0.302865884 2.880494467 CORE 6 C C 0.0000 6
C 1.459732818 1.514038306 2.880378349 CORE 7 C C 0.0000 7

```
C          0.943352436     0.302865835     0.846288698 CORE     8 C    C       0.0000     8
end
end

HD
PBC     4.26143831      2.46178268      4.09913569      89.99994556     90.00524867
89.99999953
C          3.018345426     1.538581275     2.303868818 CORE     1 C    C       0.0000     1
C          0.887626829     0.307689813     2.303869677 CORE     2 C    C       0.0000     2
C          2.308208168     0.307687850     0.254301418 CORE     3 C    C       0.0000     3
C          0.177488725     1.538579367     0.254301272 CORE     4 C    C       0.0000     4
C          3.018506059     1.538579306     0.770480457 CORE     5 C    C       0.0000     5
C          2.307993655     0.307689967     2.820048632 CORE     6 C    C       0.0000     6
C          0.177274990     1.538581255     2.820048316 CORE     7 C    C       0.0000     7
C          0.887787087     0.307688079     0.770481112 CORE     8 C    C       0.0000     8
end
end
```

graphite to M-damond

```
graphite
PBC     4.84699105      2.42286730      6.08472598    113.04871820     78.17871602
120.03259874
C          1.855162770    -0.902768112     4.199327879 CORE     1 C    C       0.0000     1
C          0.602389735     0.969086709     1.399404326 CORE     2 C    C       0.0000     2
C         -0.609648146     1.668332062     1.399648532 CORE     3 C    C       0.0000     3
C          5.490685136    -1.602010657     4.199105926 CORE     4 C    C       0.0000     4
C          4.278658441    -0.902767761     4.199342801 CORE     5 C    C       0.0000     5
C          3.025885248     0.969086670     1.399403293 CORE     6 C    C       0.0000     6
C          1.813847576     1.668332160     1.399646010 CORE     7 C    C       0.0000     7
C          3.067189794    -1.602011045     4.199092770 CORE     8 C    C       0.0000     8
end
end

PBC     4.76183375      2.47156593      4.66121104    105.39560158     87.76585273
121.29573999
C          0.889563632    -0.184867418     3.862871169 CORE     1 C    C       0.0000     1
C          0.314074495     0.913087404     0.923317742 CORE     2 C    C       0.0000     2
C         -0.958509563     1.585893780     1.307417766 CORE     3 C    C       0.0000     3
C          4.693412831    -0.765812023     2.829295238 CORE     4 C    C       0.0000     4
C          3.264710264    -0.187715354     2.838697905 CORE     5 C    C       0.0000     5
C          2.619513140     0.867343074     0.793711066 CORE     6 C    C       0.0000     6
```

C 1.497884845 1.631638090 1.437026146 CORE 7 C C 0.0000 7
C 2.318266209 -0.762964671 3.853469761 CORE 8 C C 0.0000 8
end
end

graphite to X-phase

graphite
PBC 4.19692540 5.77653880 3.13589308 122.97917031 116.37437884
76.04366799
C 8.301638511 24.107176352 1.256565445 CORE 1 C C 0.0000 1
C 6.203152354 23.058850766 0.649448792 CORE 2 C C 0.0000 2
C 10.400111033 25.155449481 1.863648052 CORE 3 C C 0.0000 3
C 7.602170481 25.159646489 1.856689233 CORE 4 C C 0.0000 4
C 7.602089134 23.062954811 0.642433216 CORE 5 C C 0.0000 5
C 9.700615520 24.111349866 1.249592239 CORE 6 C C 0.0000 6
C 8.301597652 22.010520976 0.042330757 CORE 7 C C 0.0000 7
C 5.503570872 22.014660744 0.035336122 CORE 8 C C 0.0000 8
end
end

x-phase
PBC 4.20899660 5.21551837 3.27764094 115.52958214 129.88934607
66.20669916
C 11.029942715 21.151054565 0.737641407 CORE 1 C C 0.0000 1
C 9.003907317 19.892517487 0.348268480 CORE 2 C C 0.0000 2
C 13.135746194 21.644738172 2.060230483 CORE 3 C C 0.0000 3
C 10.455297742 21.644591292 2.060388030 CORE 4 C C 0.0000 4
C 10.374805286 19.893187933 0.346300925 CORE 5 C C 0.0000 5
C 12.558489178 21.150904808 0.737795962 CORE 6 C C 0.0000 6
C 11.108267087 18.747214030 0.013741652 CORE 7 C C 0.0000 7
C 8.270167601 18.747878636 0.011768742 CORE 8 C C 0.0000 8
end
end

7. Interface structure

Graphite/BCT

PBC 8.41242152 22.29846625 4.87534257 77.34991332 89.99393336
101.29168520
C 2.452542569 1.853309649 1.617703142 CORE 1 C C 0.0000 1
C 0.335336211 4.808135049 4.690789015 CORE 2 C C 0.0000 2

C	0.936516221	3.440847495	1.252963933	CORE	3 C	C	0.0000	3
C	3.131150123	1.198632397	0.517228139	CORE	4 C	C	0.0000	4
C	2.440529093	3.440297674	1.253099018	CORE	5 C	C	0.0000	5
C	0.261797892	1.195902725	0.517838952	CORE	6 C	C	0.0000	6
C	0.938702620	1.851707746	1.618053531	CORE	7 C	C	0.0000	7
C	3.039404997	4.808339091	4.690744676	CORE	8 C	C	0.0000	8
C	6.658752926	1.853271447	1.617711939	CORE	9 C	C	0.0000	9
C	4.541548798	4.808111882	4.690794573	CORE	10 C	C	0.0000	10
C	5.142726088	3.440818311	1.252970934	CORE	11 C	C	0.0000	11
C	7.337362393	1.198609247	0.517233569	CORE	12 C	C	0.0000	12
C	6.646740811	3.440273984	1.253104876	CORE	13 C	C	0.0000	13
C	4.468000297	1.195871022	0.517846171	CORE	14 C	C	0.0000	14
C	5.144916397	1.851665062	1.618063347	CORE	15 C	C	0.0000	15
C	7.245612928	4.808324344	4.690748362	CORE	16 C	C	0.0000	16
C	2.346754929	5.952426612	0.675905249	CORE	17 C	C	0.0000	17
C	0.231772890	9.450153150	3.628874099	CORE	18 C	C	0.0000	18
C	0.932396587	9.733569383	4.814372843	CORE	19 C	C	0.0000	19
C	3.027367548	6.398153928	4.325081288	CORE	20 C	C	0.0000	20
C	2.334151107	9.735752957	4.813879282	CORE	21 C	C	0.0000	21
C	0.333048526	6.400712455	4.324499308	CORE	22 C	C	0.0000	22
C	1.011810130	5.955557506	0.675185563	CORE	23 C	C	0.0000	23
C	3.034346405	9.451616572	3.628533262	CORE	24 C	C	0.0000	24
C	6.552968274	5.952428858	0.675905531	CORE	25 C	C	0.0000	25
C	4.437981898	9.450235917	3.628852479	CORE	26 C	C	0.0000	26
C	5.138606367	9.733730407	4.814337761	CORE	27 C	C	0.0000	27
C	7.233573667	6.398154916	4.325081620	CORE	28 C	C	0.0000	28
C	6.540364693	9.735924661	4.813841629	CORE	29 C	C	0.0000	29
C	4.539262891	6.400702976	4.324501984	CORE	30 C	C	0.0000	30
C	5.218016370	5.955552274	0.675187636	CORE	31 C	C	0.0000	31
C	-1.171867604	9.451720123	3.628507012	CORE	32 C	C	0.0000	32
C	0.169009368	11.933433799	1.820675584	CORE	33 C	C	0.0000	33
C	5.062024355	15.493674675	4.743243818	CORE	34 C	C	0.0000	34
C	-2.651403362	14.682753032	1.177836817	CORE	35 C	C	0.0000	35
C	0.869094752	11.666349332	0.631467967	CORE	36 C	C	0.0000	36
C	-1.247695049	14.676595138	1.179194931	CORE	37 C	C	0.0000	37
C	6.477686207	11.664489559	0.631862878	CORE	38 C	C	0.0000	38
C	-1.234446510	11.936310741	1.820047059	CORE	39 C	C	0.0000	39
C	-0.547928626	15.498631215	4.742158366	CORE	40 C	C	0.0000	40
C	4.375223496	11.933618827	1.820632688	CORE	41 C	C	0.0000	41
C	0.855811212	15.493234033	4.743345926	CORE	42 C	C	0.0000	42
C	1.554805164	14.682240868	1.177955594	CORE	43 C	C	0.0000	43
C	5.075307207	11.666690774	0.631388986	CORE	44 C	C	0.0000	44
C	2.958514738	14.676333634	1.179255532	CORE	45 C	C	0.0000	45
C	2.271475101	11.664149260	0.631941451	CORE	46 C	C	0.0000	46

C	2.971765369	11.936123178	1.820090525	CORE	47 C	C	0.0000	47
C	3.658282417	15.498641601	4.742156169	CORE	48 C	C	0.0000	48
C	-0.479240372	17.695266146	1.693617605	CORE	49 C	C	0.0000	49
C	-4.017053956	21.278108820	4.645265778	CORE	50 C	C	0.0000	50
C	-3.317082556	20.481160208	1.076490311	CORE	51 C	C	0.0000	51
C	0.219856561	17.428794427	0.504314834	CORE	52 C	C	0.0000	52
C	-1.910794161	20.476189524	1.077600584	CORE	53 C	C	0.0000	53
C	-2.582479744	17.425629130	0.504975841	CORE	54 C	C	0.0000	54
C	-1.882986180	17.702652350	1.691983189	CORE	55 C	C	0.0000	55
C	-1.210474921	21.278424721	4.645237571	CORE	56 C	C	0.0000	56
C	3.726970344	17.695295408	1.693610189	CORE	57 C	C	0.0000	57
C	0.189155650	21.278043923	4.645280273	CORE	58 C	C	0.0000	58
C	0.889126821	20.481060702	1.076513020	CORE	59 C	C	0.0000	59
C	4.426067160	17.429003491	0.504265877	CORE	60 C	C	0.0000	60
C	2.295416299	20.476106419	1.077619658	CORE	61 C	C	0.0000	61
C	1.623730215	17.425282299	0.505056641	CORE	62 C	C	0.0000	62
C	2.323222368	17.702372772	1.692048615	CORE	63 C	C	0.0000	63
C	2.995736707	21.278391039	4.645245292	CORE	64 C	C	0.0000	64
C	2.452800685	2.397739559	3.993800258	CORE	65 C	C	0.0000	65
C	0.335078140	4.263705100	2.314691979	CORE	66 C	C	0.0000	66
C	0.936774420	3.985277437	3.629061005	CORE	67 C	C	0.0000	67
C	3.131408279	1.743062375	2.893325128	CORE	68 C	C	0.0000	68
C	2.440787268	3.984727626	3.629196110	CORE	69 C	C	0.0000	69
C	0.262055925	1.740332723	2.893935998	CORE	70 C	C	0.0000	70
C	0.938960823	2.396137723	3.994150612	CORE	71 C	C	0.0000	71
C	3.039146856	4.263909105	2.314647606	CORE	72 C	C	0.0000	72
C	6.659010973	2.397701504	3.993809007	CORE	73 C	C	0.0000	73
C	4.541290671	4.263681898	2.314697466	CORE	74 C	C	0.0000	74
C	5.142984126	3.985248325	3.629067973	CORE	75 C	C	0.0000	75
C	7.337620555	1.743039218	2.893330675	CORE	76 C	C	0.0000	76
C	6.646998832	3.984703976	3.629201893	CORE	77 C	C	0.0000	77
C	4.468258377	1.740300963	2.893943191	CORE	78 C	C	0.0000	78
C	5.145174469	2.396095041	3.994160410	CORE	79 C	C	0.0000	79
C	7.245354840	4.263894406	2.314651301	CORE	80 C	C	0.0000	80
C	2.347012996	6.496856631	3.052002291	CORE	81 C	C	0.0000	81
C	0.231514792	8.905723216	1.252777061	CORE	82 C	C	0.0000	82
C	0.932138467	9.189139420	2.438275774	CORE	83 C	C	0.0000	83
C	3.027109370	5.853723902	1.948984224	CORE	84 C	C	0.0000	84
C	2.333893033	9.191322914	2.437782212	CORE	85 C	C	0.0000	85
C	0.332790462	5.856282516	1.948402280	CORE	86 C	C	0.0000	86
C	1.012068298	6.499987489	3.051282625	CORE	87 C	C	0.0000	87
C	3.034088247	8.907186618	1.252436194	CORE	88 C	C	0.0000	88
C	6.553226355	6.496858794	3.052002574	CORE	89 C	C	0.0000	89
C	4.437723796	8.905805922	1.252755410	CORE	90 C	C	0.0000	90

C	5.138348250	9.189300410	2.438240714	CORE	91	C	C	0.0000	91
C	7.233315569	5.853725007	1.948984541	CORE	92	C	C	0.0000	92
C	6.540106572	9.191494738	2.437744559	CORE	93	C	C	0.0000	93
C	4.539004806	5.856272998	1.948404918	CORE	94	C	C	0.0000	94
C	5.218274480	6.499982245	3.051284642	CORE	95	C	C	0.0000	95
C	-1.172125687	8.907290140	1.252409964	CORE	96	C	C	0.0000	96
C	0.169267471	12.477863751	4.196772619	CORE	97	C	C	0.0000	97
C	5.061766257	14.949244701	2.367146771	CORE	98	C	C	0.0000	98
C	-2.651145267	15.227183002	3.553933874	CORE	99	C	C	0.0000	99
C	0.869352845	12.210779298	3.007565020	CORE	100	C	C	0.0000	100
C	-1.247436935	15.221025113	3.555291985	CORE	101	C	C	0.0000	101
C	6.477944315	12.208919524	3.007959937	CORE	102	C	C	0.0000	102
C	-1.234188394	12.480740696	4.196144146	CORE	103	C	C	0.0000	103
C	-0.548186725	14.954201242	2.366061304	CORE	104	C	C	0.0000	104
C	4.375481597	12.478048800	4.196729713	CORE	105	C	C	0.0000	105
C	0.855553087	14.948804062	2.367248875	CORE	106	C	C	0.0000	106
C	1.555063267	15.226670841	3.554052655	CORE	107	C	C	0.0000	107
C	5.075565298	12.211120738	3.007486049	CORE	108	C	C	0.0000	108
C	2.958772850	15.220763601	3.555352598	CORE	109	C	C	0.0000	109
C	2.271733211	12.208579224	3.008038512	CORE	110	C	C	0.0000	110
C	2.972023476	12.480553173	4.196187603	CORE	111	C	C	0.0000	111
C	3.658024310	14.954211618	2.366059107	CORE	112	C	C	0.0000	112
C	-0.478982272	18.239696126	4.069714685	CORE	113	C	C	0.0000	113
C	-4.017312049	20.733678863	2.269168688	CORE	114	C	C	0.0000	114
C	-3.316824469	21.025590200	3.452587334	CORE	115	C	C	0.0000	115
C	0.220114695	17.973224402	2.880411919	CORE	116	C	C	0.0000	116
C	-1.910536022	21.020619499	3.453697627	CORE	117	C	C	0.0000	117
C	-2.582221665	17.970059087	2.881072851	CORE	118	C	C	0.0000	118
C	-1.882728048	18.247082331	4.068080257	CORE	119	C	C	0.0000	119
C	-1.210733044	20.733994748	2.269140552	CORE	120	C	C	0.0000	120
C	3.727228419	18.239725393	4.069707262	CORE	121	C	C	0.0000	121
C	0.188897565	20.733613922	2.269183221	CORE	122	C	C	0.0000	122
C	0.889384925	21.025490675	3.452610068	CORE	123	C	C	0.0000	123
C	4.426325302	17.973433464	2.880362966	CORE	124	C	C	0.0000	124
C	2.295674422	21.020536405	3.453716730	CORE	125	C	C	0.0000	125
C	1.623988293	17.969712253	2.881153644	CORE	126	C	C	0.0000	126
C	2.323480537	18.246802757	4.068145687	CORE	127	C	C	0.0000	127
C	2.995478588	20.733961075	2.269148248	CORE	128	C	C	0.0000	128

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PBC 4.88556465 23.43005161 8.31193114 90.00753928 90.00474474 64.99433197

C	1.494523951	0.251129293	0.560900187	CORE	1 C	C	0.0000	1
C	3.937306264	0.251129307	0.560900191	CORE	2 C	C	0.0000	2
C	1.494179773	0.250686461	4.716866049	CORE	3 C	C	0.0000	3
C	3.936962092	0.250686461	4.716866044	CORE	4 C	C	0.0000	4
C	2.715437132	0.738328811	4.076766182	CORE	5 C	C	0.0000	5
C	5.158219459	0.738328803	4.076766179	CORE	6 C	C	0.0000	6
C	2.715092986	0.737886125	8.232731645	CORE	7 C	C	0.0000	7
C	5.157875314	0.737886118	8.232731649	CORE	8 C	C	0.0000	8
C	1.494401837	0.250675814	1.906688764	CORE	9 C	C	0.0000	9
C	3.937184150	0.250675830	1.906688767	CORE	10 C	C	0.0000	10
C	1.494057688	0.250232867	6.062654625	CORE	11 C	C	0.0000	11
C	3.936840010	0.250232878	6.062654626	CORE	12 C	C	0.0000	12
C	2.715547442	0.738356624	2.547069765	CORE	13 C	C	0.0000	13
C	5.158329768	0.738356613	2.547069765	CORE	14 C	C	0.0000	14
C	2.715203299	0.737913938	6.703035363	CORE	15 C	C	0.0000	15
C	5.157985629	0.737913935	6.703035366	CORE	16 C	C	0.0000	16
C	2.710873966	2.246640764	0.464585185	CORE	17 C	C	0.0000	17
C	5.153656291	2.246640761	0.464585190	CORE	18 C	C	0.0000	18
C	2.710529779	2.246197926	4.620550747	CORE	19 C	C	0.0000	19
C	5.153312104	2.246197924	4.620550749	CORE	20 C	C	0.0000	20
C	1.488151309	2.925484226	4.081844375	CORE	21 C	C	0.0000	21
C	3.930933639	2.925484227	4.081844371	CORE	22 C	C	0.0000	22
C	1.487807180	2.925041260	8.237809968	CORE	23 C	C	0.0000	23
C	3.930589511	2.925041259	8.237809963	CORE	24 C	C	0.0000	24
C	2.710757589	2.246270996	2.003749350	CORE	25 C	C	0.0000	25
C	5.153539914	2.246270992	2.003749347	CORE	26 C	C	0.0000	26
C	2.710413447	2.245828022	6.159714916	CORE	27 C	C	0.0000	27
C	5.153195773	2.245828022	6.159714916	CORE	28 C	C	0.0000	28
C	1.488283062	2.925444296	2.542672754	CORE	29 C	C	0.0000	29
C	3.931065394	2.925444299	2.542672752	CORE	30 C	C	0.0000	30
C	1.487938930	2.925001323	6.698638206	CORE	31 C	C	0.0000	31
C	3.930721260	2.925001322	6.698638202	CORE	32 C	C	0.0000	32
C	3.926384840	4.433682571	0.469642726	CORE	33 C	C	0.0000	33
C	6.369167161	4.433682572	0.469642729	CORE	34 C	C	0.0000	34
C	3.926040639	4.433240143	4.625608231	CORE	35 C	C	0.0000	35
C	6.368822965	4.433240133	4.625608235	CORE	36 C	C	0.0000	36
C	2.704523121	4.921065097	3.985397512	CORE	37 C	C	0.0000	37
C	5.147305456	4.921065112	3.985397519	CORE	38 C	C	0.0000	38
C	2.704179010	4.920621476	8.141362980	CORE	39 C	C	0.0000	39
C	5.146961336	4.920621464	8.141362979	CORE	40 C	C	0.0000	40
C	3.926255083	4.433434385	1.999341174	CORE	41 C	C	0.0000	41

C	6.369037402	4.433434384	1.999341174	CORE	42 C	C	0.0000	42
C	3.925910949	4.432991072	6.155306673	CORE	43 C	C	0.0000	43
C	6.368693276	4.432991063	6.155306679	CORE	44 C	C	0.0000	44
C	2.704608178	4.920937037	2.639605903	CORE	45 C	C	0.0000	45
C	5.147390508	4.920937045	2.639605903	CORE	46 C	C	0.0000	46
C	2.704264060	4.920493411	6.795571486	CORE	47 C	C	0.0000	47
C	5.147046388	4.920493406	6.795571478	CORE	48 C	C	0.0000	48
C	5.183299832	7.537992601	0.539032847	CORE	49 C	C	0.0000	49
C	7.626082155	7.537992586	0.539032841	CORE	50 C	C	0.0000	50
C	5.182955606	7.537554925	4.694998251	CORE	51 C	C	0.0000	51
C	7.625737928	7.537554909	4.694998245	CORE	52 C	C	0.0000	52
C	3.961465155	7.565647789	4.006869021	CORE	53 C	C	0.0000	53
C	6.404247481	7.565647751	4.006869012	CORE	54 C	C	0.0000	54
C	3.961121086	7.565196790	8.162834567	CORE	55 C	C	0.0000	55
C	6.403903410	7.565196745	8.162834560	CORE	56 C	C	0.0000	56
C	5.183202864	7.539922221	1.932986632	CORE	57 C	C	0.0000	57
C	7.625985186	7.539922212	1.932986631	CORE	58 C	C	0.0000	58
C	5.182858753	7.539476135	6.088952046	CORE	59 C	C	0.0000	59
C	7.625641075	7.539476111	6.088952045	CORE	60 C	C	0.0000	60
C	3.961562506	7.563283002	2.620888795	CORE	61 C	C	0.0000	61
C	6.404344828	7.563282952	2.620888795	CORE	62 C	C	0.0000	62
C	3.961218415	7.562833060	6.776854362	CORE	63 C	C	0.0000	63
C	6.404000737	7.562833021	6.776854359	CORE	64 C	C	0.0000	64
C	6.425799707	10.379181632	4.031636551	CORE	65 C	C	0.0000	65
C	8.868582035	10.379181637	4.031636557	CORE	66 C	C	0.0000	66
C	6.425455650	10.378729222	8.187602076	CORE	67 C	C	0.0000	67
C	8.868237976	10.378729217	8.187602075	CORE	68 C	C	0.0000	68
C	5.204456954	10.380552707	3.344080578	CORE	69 C	C	0.0000	69
C	7.647239276	10.380552722	3.344080577	CORE	70 C	C	0.0000	70
C	5.204112896	10.380099444	7.500046110	CORE	71 C	C	0.0000	71
C	7.646895225	10.380099455	7.500046113	CORE	72 C	C	0.0000	72
C	6.426050420	10.375475613	1.266125556	CORE	73 C	C	0.0000	73
C	8.868832747	10.375475604	1.266125556	CORE	74 C	C	0.0000	74
C	6.425706278	10.375033959	5.422091045	CORE	75 C	C	0.0000	75
C	8.868488606	10.375033953	5.422091045	CORE	76 C	C	0.0000	76
C	5.204574640	10.376645812	1.953840112	CORE	77 C	C	0.0000	77
C	7.647356969	10.376645828	1.953840111	CORE	78 C	C	0.0000	78
C	5.204230522	10.376198413	6.109805628	CORE	79 C	C	0.0000	79
C	7.647012851	10.376198430	6.109805625	CORE	80 C	C	0.0000	80
C	7.664985081	13.201802167	0.543420704	CORE	81 C	C	0.0000	81
C	10.107767402	13.201802164	0.543420709	CORE	82 C	C	0.0000	82
C	7.664640839	13.201365950	4.699386231	CORE	83 C	C	0.0000	83
C	10.107423155	13.201365945	4.699386233	CORE	84 C	C	0.0000	84
C	6.443333208	13.201601572	4.011613783	CORE	85 C	C	0.0000	85

C	8.886115540	13.201601558	4.011613777	CORE	86	C	0.0000	86
C	6.442989149	13.201148608	8.167579311	CORE	87	C	0.0000	87
C	8.885771473	13.201148587	8.167579299	CORE	88	C	0.0000	88
C	7.664876739	13.201754047	1.933629326	CORE	89	C	0.0000	89
C	10.107659069	13.201754033	1.933629331	CORE	90	C	0.0000	90
C	7.664532609	13.201307738	6.089594855	CORE	91	C	0.0000	91
C	10.107314934	13.201307715	6.089594862	CORE	92	C	0.0000	92
C	6.443428930	13.201840096	2.621405248	CORE	93	C	0.0000	93
C	8.886211252	13.201840073	2.621405252	CORE	94	C	0.0000	94
C	6.443084815	13.201388998	6.777370787	CORE	95	C	0.0000	95
C	8.885867133	13.201388974	6.777370788	CORE	96	C	0.0000	96
C	8.902132122	16.027649948	-0.127388242	CORE	97	C	0.0000	97
C	11.344914450	16.027649943	-0.127388241	CORE	98	C	0.0000	98
C	8.901787846	16.027216930	4.028577277	CORE	99	C	0.0000	99
C	11.344570171	16.027216936	4.028577279	CORE	100	C	0.0000	100
C	7.680444857	16.028551346	3.340868263	CORE	101	C	0.0000	101
C	10.123227178	16.028551355	3.340868264	CORE	102	C	0.0000	102
C	7.680100818	16.028097567	7.496833791	CORE	103	C	0.0000	103
C	10.122883138	16.028097574	7.496833788	CORE	104	C	0.0000	104
C	8.902040716	16.023474271	1.262854050	CORE	105	C	0.0000	105
C	11.344823042	16.023474269	1.262854052	CORE	106	C	0.0000	106
C	8.901696573	16.023032506	5.418819569	CORE	107	C	0.0000	107
C	11.344478897	16.023032505	5.418819569	CORE	108	C	0.0000	108
C	7.680560159	16.024702572	1.950408476	CORE	109	C	0.0000	109
C	10.123342480	16.024702583	1.950408475	CORE	110	C	0.0000	110
C	7.680216038	16.024254813	6.106373994	CORE	111	C	0.0000	111
C	10.122998359	16.024254833	6.106373991	CORE	112	C	0.0000	112
C	10.142080345	18.841828481	0.538481811	CORE	113	C	0.0000	113
C	12.584862677	18.841828478	0.538481815	CORE	114	C	0.0000	114
C	10.141736109	18.841390156	4.694447249	CORE	115	C	0.0000	115
C	12.584518438	18.841390144	4.694447250	CORE	116	C	0.0000	116
C	8.920230879	18.864801447	4.006536033	CORE	117	C	0.0000	117
C	11.363013204	18.864801383	4.006536039	CORE	118	C	0.0000	118
C	8.919886824	18.864350501	8.162501553	CORE	119	C	0.0000	119
C	11.362669154	18.864350441	8.162501562	CORE	120	C	0.0000	120
C	10.141975925	18.838987521	1.924463347	CORE	121	C	0.0000	121
C	12.584758259	18.838987510	1.924463357	CORE	122	C	0.0000	122
C	10.141631857	18.838541078	6.080428739	CORE	123	C	0.0000	123
C	12.584414189	18.838541078	6.080428745	CORE	124	C	0.0000	124
C	8.920352427	18.866865176	2.612603402	CORE	125	C	0.0000	125
C	11.363134754	18.866865121	2.612603407	CORE	126	C	0.0000	126
C	8.920008368	18.866414876	6.768568909	CORE	127	C	0.0000	127
C	11.362790692	18.866414816	6.768568914	CORE	128	C	0.0000	128

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PBC 21.45537189 4.86173049 8.36820481 89.98617831 87.53392909 89.54580206

C	2.842052775	0.011198218	3.170444199	CORE	1 C	C	0.0000	1
C	5.635876904	4.859356338	1.750363868	CORE	2 C	C	0.0000	2
C	8.497963488	1.199121345	3.811677801	CORE	3 C	C	0.0000	3
C	-0.037280049	1.243327126	1.106049480	CORE	4 C	C	0.0000	4
C	2.729908436	0.011477884	0.384884468	CORE	5 C	C	0.0000	5
C	-0.045466074	0.027827694	1.800776972	CORE	6 C	C	0.0000	6
C	18.702228036	1.196869638	0.311035024	CORE	7 C	C	0.0000	7
C	5.630482875	1.213077372	2.445672721	CORE	8 C	C	0.0000	8
C	5.696956771	1.212962853	3.840493784	CORE	9 C	C	0.0000	9
C	0.015253114	0.027511058	3.198186718	CORE	10 C	C	0.0000	10
C	-0.116275926	1.243168050	-0.287928724	CORE	11 C	C	0.0000	11
C	5.569400633	4.859470242	0.355541770	CORE	12 C	C	0.0000	12
C	2.761567978	1.226784412	1.080042055	CORE	13 C	C	0.0000	13
C	18.783529868	4.846447639	0.999628238	CORE	14 C	C	0.0000	14
C	2.826565366	1.226659282	2.475384141	CORE	15 C	C	0.0000	15
C	8.504832883	4.845393480	3.116561085	CORE	16 C	C	0.0000	16
C	14.019667837	4.884258233	3.885196275	CORE	17 C	C	0.0000	17
C	16.647445481	-0.000753177	1.806168702	CORE	18 C	C	0.0000	18
C	18.135672883	1.203802766	3.224397874	CORE	19 C	C	0.0000	19
C	11.273291332	1.181979577	2.395703502	CORE	20 C	C	0.0000	20
C	14.586347285	4.876698778	0.971748757	CORE	21 C	C	0.0000	21
C	11.303723516	4.828014294	3.090484624	CORE	22 C	C	0.0000	22
C	8.385817006	1.199421875	1.026148959	CORE	23 C	C	0.0000	23
C	16.035966764	1.219717478	2.390232991	CORE	24 C	C	0.0000	24
C	16.587566760	1.215744393	3.791780509	CORE	25 C	C	0.0000	25
C	11.382711987	4.828227065	4.484454041	CORE	26 C	C	0.0000	26
C	11.212607974	1.182372204	0.998398747	CORE	27 C	C	0.0000	27
C	16.095823419	0.002994322	0.404631827	CORE	28 C	C	0.0000	28
C	14.578668303	1.230080599	1.846992139	CORE	29 C	C	0.0000	29
C	8.439828660	4.845493665	1.721177254	CORE	30 C	C	0.0000	30
C	13.938407161	1.233535246	3.196788724	CORE	31 C	C	0.0000	31
C	18.143332701	4.850296860	2.349490670	CORE	32 C	C	0.0000	32
C	2.861322650	2.441987132	3.170444129	CORE	33 C	C	0.0000	33
C	5.616607012	2.428567410	1.750363781	CORE	34 C	C	0.0000	34
C	8.517233419	3.629910172	3.811677953	CORE	35 C	C	0.0000	35
C	-0.018010260	3.674115938	1.106049478	CORE	36 C	C	0.0000	36
C	2.749178330	2.442266723	0.384884481	CORE	37 C	C	0.0000	37

C	-0.026196251	2.458616318	1.800776842	CORE	38 C	C	0.0000	38
C	18.721497716	3.627658652	0.311034940	CORE	39 C	C	0.0000	39
C	5.649752765	3.643866196	2.445672766	CORE	40 C	C	0.0000	40
C	5.716226674	3.643751789	3.840493803	CORE	41 C	C	0.0000	41
C	0.034522951	2.458299959	3.198186798	CORE	42 C	C	0.0000	42
C	-0.097006108	3.673956779	-0.287928886	CORE	43 C	C	0.0000	43
C	5.550130768	2.428681484	0.355541891	CORE	44 C	C	0.0000	44
C	2.780837849	3.657573331	1.080042057	CORE	45 C	C	0.0000	45
C	18.764260079	2.415658701	0.999628210	CORE	46 C	C	0.0000	46
C	2.845835233	3.657448103	2.475384162	CORE	47 C	C	0.0000	47
C	8.485562999	2.414604538	3.116561104	CORE	48 C	C	0.0000	48
C	14.000397982	2.453469224	3.885196197	CORE	49 C	C	0.0000	49
C	16.666715416	2.430035457	1.806168766	CORE	50 C	C	0.0000	50
C	18.154942535	3.634591669	3.224397937	CORE	51 C	C	0.0000	51
C	11.292561183	3.612768552	2.395703385	CORE	52 C	C	0.0000	52
C	14.567077648	2.445909965	0.971748741	CORE	53 C	C	0.0000	53
C	11.284453716	2.397225544	3.090484677	CORE	54 C	C	0.0000	54
C	8.405086896	3.630210908	1.026148854	CORE	55 C	C	0.0000	55
C	16.055236684	3.650506401	2.390233005	CORE	56 C	C	0.0000	56
C	16.606836773	3.646533429	3.791780461	CORE	57 C	C	0.0000	57
C	11.363442037	2.397438263	4.484453928	CORE	58 C	C	0.0000	58
C	11.231877827	3.613161347	0.998398927	CORE	59 C	C	0.0000	59
C	16.115093152	2.433782980	0.404631848	CORE	60 C	C	0.0000	60
C	14.597938223	3.660869638	1.846991978	CORE	61 C	C	0.0000	61
C	8.420558775	2.414704738	1.721177290	CORE	62 C	C	0.0000	62
C	13.957676919	3.664324178	3.196788741	CORE	63 C	C	0.0000	63
C	18.124062811	2.419507963	2.349490746	CORE	64 C	C	0.0000	64
C	3.022078970	0.010780666	7.350671685	CORE	65 C	C	0.0000	65
C	5.815915756	4.858938458	5.930590919	CORE	66 C	C	0.0000	66
C	8.677987067	1.198703774	7.991905494	CORE	67 C	C	0.0000	67
C	0.142759106	1.242909273	5.286276220	CORE	68 C	C	0.0000	68
C	2.909952417	0.011060071	4.565111201	CORE	69 C	C	0.0000	69
C	0.134569508	0.027409725	5.981004276	CORE	70 C	C	0.0000	70
C	18.882261759	1.196452030	4.491262096	CORE	71 C	C	0.0000	71
C	5.810515064	1.212659480	6.625899957	CORE	72 C	C	0.0000	72
C	5.876978795	1.212545166	8.020721891	CORE	73 C	C	0.0000	73
C	0.195280521	0.027093462	7.378414393	CORE	74 C	C	0.0000	74
C	0.063764773	1.242750384	3.892298752	CORE	75 C	C	0.0000	75
C	5.749445570	4.859052171	4.535768737	CORE	76 C	C	0.0000	76
C	2.941610010	1.226366460	5.260268967	CORE	77 C	C	0.0000	77
C	18.963563816	4.846029788	5.179855438	CORE	78 C	C	0.0000	78
C	3.006597650	1.226241292	6.655611757	CORE	79 C	C	0.0000	79
C	8.684860743	4.844975431	7.296788836	CORE	80 C	C	0.0000	80
C	14.199699574	4.883840336	8.065423810	CORE	81 C	C	0.0000	81

C	16.827478551	-0.001171004	5.986396025	CORE	82 C	C	0.0000	82
C	18.315705400	1.203384988	7.404625238	CORE	83 C	C	0.0000	83
C	11.453324540	1.181561622	6.575930529	CORE	84 C	C	0.0000	84
C	14.766380154	4.876280978	5.151976514	CORE	85 C	C	0.0000	85
C	11.483753162	4.827596693	7.270712929	CORE	86 C	C	0.0000	86
C	8.565859101	1.199004058	5.206375882	CORE	87 C	C	0.0000	87
C	16.215999700	1.219299692	6.570460394	CORE	88 C	C	0.0000	88
C	16.767599158	1.215326566	7.972007833	CORE	89 C	C	0.0000	89
C	11.562737543	4.827809367	8.664680783	CORE	90 C	C	0.0000	90
C	11.392646630	1.181954240	5.178625713	CORE	91 C	C	0.0000	91
C	16.275856390	0.002576510	4.584859322	CORE	92 C	C	0.0000	92
C	14.758700907	1.229662771	6.027219773	CORE	93 C	C	0.0000	93
C	8.619866772	4.845075801	5.901404389	CORE	94 C	C	0.0000	94
C	14.118438921	1.233117494	7.377016031	CORE	95 C	C	0.0000	95
C	18.323365737	4.849879045	6.529718021	CORE	96 C	C	0.0000	96
C	3.041348846	2.441569581	7.350671639	CORE	97 C	C	0.0000	97
C	5.796645863	2.428149517	5.930590813	CORE	98 C	C	0.0000	98
C	8.697256989	3.629492573	7.991905604	CORE	99 C	C	0.0000	99
C	0.162028865	3.673698008	5.286276072	CORE	100 C	C	0.0000	100
C	2.929222306	2.441848919	4.565111219	CORE	101 C	C	0.0000	101
C	0.153839323	2.458198307	5.981003902	CORE	102 C	C	0.0000	102
C	18.901531494	3.627240793	4.491262142	CORE	103 C	C	0.0000	103
C	5.829784966	3.643448310	6.625900051	CORE	104 C	C	0.0000	104
C	5.896248701	3.643334089	8.020721844	CORE	105 C	C	0.0000	105
C	0.214550400	2.457882568	7.378414761	CORE	106 C	C	0.0000	106
C	0.083034598	3.673539266	3.892298835	CORE	107 C	C	0.0000	107
C	5.730175711	2.428263456	4.535768879	CORE	108 C	C	0.0000	108
C	2.960879883	3.657155381	5.260268957	CORE	109 C	C	0.0000	109
C	18.944294030	2.415240907	5.179855432	CORE	110 C	C	0.0000	110
C	3.025867519	3.657030143	6.655611783	CORE	111 C	C	0.0000	111
C	8.665590867	2.414186508	7.296788897	CORE	112 C	C	0.0000	112
C	14.180429706	2.453051410	8.065423588	CORE	113 C	C	0.0000	113
C	16.846748417	2.429617629	5.986396037	CORE	114 C	C	0.0000	114
C	18.334975035	3.634173758	7.404625425	CORE	115 C	C	0.0000	115
C	11.472594395	3.612350584	6.575930731	CORE	116 C	C	0.0000	116
C	14.747110500	2.445492247	5.151976415	CORE	117 C	C	0.0000	117
C	11.464483305	2.396808046	7.270712940	CORE	118 C	C	0.0000	118
C	8.585128991	3.629793099	5.206375724	CORE	119 C	C	0.0000	119
C	16.235269568	3.650088565	6.570460394	CORE	120 C	C	0.0000	120
C	16.786869195	3.646115615	7.972007728	CORE	121 C	C	0.0000	121
C	11.543467654	2.397020359	8.664680709	CORE	122 C	C	0.0000	122
C	11.411916470	3.612743392	5.178625505	CORE	123 C	C	0.0000	123
C	16.295126086	2.433365227	4.584859388	CORE	124 C	C	0.0000	124
C	14.777970826	3.660451856	6.027219669	CORE	125 C	C	0.0000	125

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C          8.600596894     2.414286843     5.901404405 CORE  126 C    C       0.0000   126
C         14.137708679     3.663906225     7.377016001 CORE  127 C    C       0.0000   127
C         18.304095895     2.419090065     6.529718022 CORE  128 C    C       0.0000   128
end
end

graphite-to-64

PBC      5.77629324      4.19680352     15.69407946     84.84295247    112.11972548
104.14683629
C         -2.813378964     2.613062841     8.743176524 CORE    1 C    C       0.0000     1
C          0.062048488     2.609837744     9.954869732 CORE    2 C    C       0.0000     2
C          0.040028175     2.604293177    12.378113638 CORE    3 C    C       0.0000     3
C          0.563295562     0.572146929    11.166532923 CORE    4 C    C       0.0000     4
C          0.088144462     2.616440606     7.531536877 CORE    5 C    C       0.0000     5
C          0.587624277     0.578333204     8.743203936 CORE    6 C    C       0.0000     6
C         -2.313232279     0.575068897     9.954941246 CORE    7 C    C       0.0000     7
C         -2.335267052     0.569570853    12.378282425 CORE    8 C    C       0.0000     8
C         -2.837719986     2.606909646    11.166670013 CORE    9 C    C       0.0000     9
C         -2.287150416     0.581738581     7.531518009 CORE   10 C    C       0.0000    10
C          0.639054255     0.591794295     3.897119140 CORE   11 C    C       0.0000    11
C          0.114391329     2.623367292     5.108532833 CORE   12 C    C       0.0000    12
C          3.034381001     2.632055556     1.474129278 CORE   13 C    C       0.0000    13
C          3.537748256     0.594753031     2.685664018 CORE   14 C    C       0.0000    14
C         -2.857482634     2.601942013    13.589859479 CORE   15 C    C       0.0000    15
C          3.556085501     0.599613026     0.262534530 CORE   16 C    C       0.0000    16
C         -2.786591620     2.619970603     6.319968183 CORE   17 C    C       0.0000    17
C          3.014327040     2.626591221     3.897113031 CORE   18 C    C       0.0000    18
C          3.515397775     0.588626222     5.108556954 CORE   19 C    C       0.0000    19
C          0.659110029     0.597251950     1.474147799 CORE   20 C    C       0.0000    20
C          0.136754009     2.629434692     2.685731338 CORE   21 C    C       0.0000    21
C         -5.232768069     0.567209316    13.589791355 CORE   22 C    C       0.0000    22
C          0.155065392     2.634415070     0.262509186 CORE   23 C    C       0.0000    23
C          0.614428545     0.585181505     6.319911148 CORE   24 C    C       0.0000    24
C         -0.054099207     3.302761216     3.897063599 CORE   25 C    C       0.0000    25
C          0.446905630     1.265023334     5.108871829 CORE   26 C    C       0.0000    26
C          3.367083606     1.273010726     1.473749082 CORE   27 C    C       0.0000    27
C          2.844686609     3.305354795     2.685389961 CORE   28 C    C       0.0000    28
C         -2.524774597     1.242878296    13.589451877 CORE   29 C    C       0.0000    29
C          2.863064819     3.310054452     0.262135492 CORE   30 C    C       0.0000    30
C         -2.454105637     1.261734469     6.320507958 CORE   31 C    C       0.0000    31
C          3.346918125     1.267978905     3.897068077 CORE   32 C    C       0.0000    32
C          2.822191556     3.299772447     5.108829424 CORE   33 C    C       0.0000    33
C         -0.033937940     3.307820942     1.473674077 CORE   34 C    C       0.0000    34
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C          0.469388933     1.270664315     2.685363797 CORE    35 C    C       0.0000     35
C         -5.925788036     3.277635242    13.589584779 CORE    36 C    C       0.0000     36
C          0.487789473     1.275271575     0.262132094 CORE    37 C    C       0.0000     37
C         -0.078833693     3.296532640     6.320511026 CORE    38 C    C       0.0000     38
C         -2.480864926     1.254737724     8.743504171 CORE    39 C    C       0.0000     39
C          0.394613799     1.251312671     9.954916169 CORE    40 C    C       0.0000     40
C          0.372688881     1.245386079    12.378008066 CORE    41 C    C       0.0000     41
C         -0.129814286     3.282937793    11.166459618 CORE    42 C    C       0.0000     42
C          0.420601881     1.258306188     7.532112467 CORE    43 C    C       0.0000     43
C         -0.105576001     3.289463382     8.743517938 CORE    44 C    C       0.0000     44
C         -3.006405125     3.286110457     9.954880089 CORE    45 C    C       0.0000     45
C         -3.028309823     3.280106708    12.377861232 CORE    46 C    C       0.0000     46
C         -2.505094784     1.248189715    11.166326896 CORE    47 C    C       0.0000     47
C         -2.980393727     3.293002327     7.532098944 CORE    48 C    C       0.0000     48
end
end

PBC       5.30838219      4.19334579     15.84801197     90.00207769    115.45150848
90.00053249
C         -3.359392921     2.777073087     8.400548786 CORE     1 C    C       0.0000      1
C         -0.767270620     2.697171159     9.715390376 CORE     2 C    C       0.0000      2
C         -0.818852746     2.712058350    12.127191082 CORE     3 C    C       0.0000      3
C         -0.797448389     0.616791339    10.914629245 CORE     4 C    C       0.0000      4
C          0.524233025     2.777102872     7.618276576 CORE     5 C    C       0.0000      5
C         -0.705182525     0.680400460     8.400548960 CORE     6 C    C       0.0000      6
C         -3.421442099     0.600497709     9.715389792 CORE     7 C    C       0.0000      7
C         -3.473024322     0.615384628    12.127190294 CORE     8 C    C       0.0000      8
C         -3.451658979     2.713463570    10.914628421 CORE     9 C    C       0.0000      9
C         -2.129938587     0.680429757     7.618276404 CORE    10 C    C       0.0000     10
C          0.637748941     0.615721944     3.891638188 CORE    11 C    C       0.0000     11
C          0.616418091     2.713692161     5.104213331 CORE    12 C    C       0.0000     12
C          3.311968451     2.712936099     1.461401324 CORE    13 C    C       0.0000     13
C          3.304815889     0.614815252     2.675038830 CORE    14 C    C       0.0000     14
C         -3.485967239     2.711047518    13.343796573 CORE    15 C    C       0.0000     15
C          3.317504391     0.616340243     0.247466140 CORE    16 C    C       0.0000     16
C         -2.067914290     2.697313068     6.303445218 CORE    17 C    C       0.0000     17
C          3.291920507     2.712393950     3.891637348 CORE    18 C    C       0.0000     18
C         -2.037753430     0.617018657     5.104212513 CORE    19 C    C       0.0000     19
C          0.657796840     0.616264349     1.461401830 CORE    20 C    C       0.0000     20
C          0.650605262     2.711489220     2.675039520 CORE    21 C    C       0.0000     21
C         -6.140138834     0.614375599    13.343797205 CORE    22 C    C       0.0000     22
C          0.663293800     2.713014245     0.247466632 CORE    23 C    C       0.0000     23
C          0.586296088     0.600640500     6.303445751 CORE    24 C    C       0.0000     24
C          0.637723716     3.413770170     3.891619507 CORE    25 C    C       0.0000     25
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C          0.616432148     1.315676865     5.104194016 CORE   26 C    C      0.0000     26
C          3.311981640     1.316779124     1.461382435 CORE   27 C    C      0.0000     27
C          3.304789820     3.414790862     2.675020713 CORE   28 C    C      0.0000     28
C         -3.485953021     1.317605136    13.343777112 CORE   29 C    C      0.0000     29
C          3.317478775     3.413479890     0.247446513 CORE   30 C    C      0.0000     30
C         -2.067902089     1.331937495     6.303430825 CORE   31 C    C      0.0000     31
C          3.291934321     1.317096412     3.891619830 CORE   32 C    C      0.0000     32
C         -2.037778455     3.412349125     5.104194416 CORE   33 C    C      0.0000     33
C          0.657771036     3.413453140     1.461382458 CORE   34 C    C      0.0000     34
C          0.650618206     1.318119009     2.675020625 CORE   35 C    C      0.0000     35
C         -6.140163653     3.414279002    13.343777043 CORE   36 C    C      0.0000     36
C          0.663307160     1.316808063     0.247446590 CORE   37 C    C      0.0000     37
C          0.586269455     3.428610728     6.303430632 CORE   38 C    C      0.0000     38
C         -3.359376669     1.251988596     8.400543605 CORE   39 C    C      0.0000     39
C         -0.767258189     1.331784494     9.715371924 CORE   40 C    C      0.0000     40
C         -0.818839674     1.316698921    12.127168744 CORE   41 C    C      0.0000     41
C         -0.797472906     3.412059985    10.914606449 CORE   42 C    C      0.0000     42
C          0.524248362     1.252021931     7.618274329 CORE   43 C    C      0.0000     43
C         -0.705205003     3.348661721     8.400543737 CORE   44 C    C      0.0000     44
C         -3.421468573     3.428456878     9.715372049 CORE   45 C    C      0.0000     45
C         -3.473050268     3.413371045    12.127169043 CORE   46 C    C      0.0000     46
C         -3.451644550     1.315386468    10.914606735 CORE   47 C    C      0.0000     47
C         -2.129962066     3.348694594     7.618274246 CORE   48 C    C      0.0000     48
end
end

PBC       5.16930635      4.19671666     14.96794821     90.00672889    110.31239894
90.00221671
C         -0.660583364     2.765748044     8.722954077 CORE    1 C    C      0.0000      1
C         -3.309717848     2.682920823    10.039011784 CORE    2 C    C      0.0000      2
C         -3.342082808     2.699386361    12.454227797 CORE    3 C    C      0.0000      3
C         -3.332026688     0.600976407    11.241976905 CORE    4 C    C      0.0000      4
C         -2.050420390     2.766255492     7.949847978 CORE    5 C    C      0.0000      5
C          1.924150493     0.667391232     8.722954006 CORE    6 C    C      0.0000      6
C         -0.724983806     0.584559507    10.039011571 CORE    7 C    C      0.0000      7
C         -0.757348475     0.601023297    12.454227830 CORE    8 C    C      0.0000      8
C         -0.747454642     2.699330711    11.241976862 CORE    9 C    C      0.0000      9
C          0.534313592     0.667896625     7.949847824 CORE   10 C    C      0.0000     10
C          1.865896417     0.585331620     4.483364350 CORE   11 C    C      0.0000     11
C          1.925025638     2.766169711     5.799749236 CORE   12 C    C      0.0000     12
C         -0.736674175     2.700818047     2.067932000 CORE   13 C    C      0.0000     13
C         -0.733180609     0.602059575     3.280256295 CORE   14 C    C      0.0000     14
C         -0.761608998     2.697556258    13.671330697 CORE   15 C    C      0.0000     15
C          4.432785885     0.600982064     0.850812964 CORE   16 C    C      0.0000     16
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C	0.534901985	2.766522852	6.572900834	CORE	17	C	C	0.0000	17
C	-0.718838001	2.683687664	4.483364526	CORE	18	C	C	0.0000	18
C	-0.659546055	0.667810284	5.799749162	CORE	19	C	C	0.0000	19
C	1.848060180	0.602463938	2.067931901	CORE	20	C	C	0.0000	20
C	1.851391330	2.700421258	3.280256229	CORE	21	C	C	0.0000	21
C	-3.346180940	0.599202903	13.671330597	CORE	22	C	C	0.0000	22
C	1.848051547	2.699345185	0.850812846	CORE	23	C	C	0.0000	23
C	3.119636474	0.668164973	6.572900638	CORE	24	C	C	0.0000	24
C	1.865789309	3.418498609	4.483298853	CORE	25	C	C	0.0000	25
C	1.925079581	1.237329743	5.799722738	CORE	26	C	C	0.0000	26
C	-0.736619369	1.303628067	2.067849260	CORE	27	C	C	0.0000	27
C	-0.733289342	3.402071983	3.280165402	CORE	28	C	C	0.0000	28
C	-0.761554331	1.303681400	13.671251231	CORE	29	C	C	0.0000	29
C	4.432678374	3.403806206	0.850731986	CORE	30	C	C	0.0000	30
C	0.534957192	1.236788458	6.572890461	CORE	31	C	C	0.0000	31
C	-0.718782487	1.320137966	4.483298750	CORE	32	C	C	0.0000	32
C	-0.659655030	3.335686969	5.799722852	CORE	33	C	C	0.0000	33
C	1.847952625	3.401990587	2.067849257	CORE	34	C	C	0.0000	34
C	1.851445004	1.303716986	3.280165362	CORE	35	C	C	0.0000	35
C	-3.346288667	3.402044670	13.671251208	CORE	36	C	C	0.0000	36
C	1.848106413	1.305452643	0.850731995	CORE	37	C	C	0.0000	37
C	3.119529046	3.335147232	6.572890589	CORE	38	C	C	0.0000	38
C	-0.660520442	1.236968495	8.722932690	CORE	39	C	C	0.0000	39
C	-3.309658202	1.319408936	10.038950486	CORE	40	C	C	0.0000	40
C	-3.342027266	1.302221125	12.454147566	CORE	41	C	C	0.0000	41
C	-3.332133458	3.400986834	11.241894064	CORE	42	C	C	0.0000	42
C	-2.050360584	1.236666020	7.949838400	CORE	43	C	C	0.0000	43
C	1.924052081	3.335328341	8.722932710	CORE	44	C	C	0.0000	44
C	-0.725086006	3.417764292	10.038950774	CORE	45	C	C	0.0000	45
C	-0.757455290	3.400574743	12.454147630	CORE	46	C	C	0.0000	46
C	-0.747399211	1.302624499	11.241894212	CORE	47	C	C	0.0000	47
C	0.534211776	3.335023808	7.949838621	CORE	48	C	C	0.0000	48

end
end

graphite to BCT
PBC 5.77629324 4.19680352 15.69407946 84.84295247 112.11972548
104.14683629

C	-2.813378964	2.613062841	8.743176524	CORE	1	C	C	0.0000	1
C	0.062048488	2.609837744	9.954869732	CORE	2	C	C	0.0000	2
C	0.040028175	2.604293177	12.378113638	CORE	3	C	C	0.0000	3
C	0.563295562	0.572146929	11.166532923	CORE	4	C	C	0.0000	4
C	0.088144462	2.616440606	7.531536877	CORE	5	C	C	0.0000	5
C	0.587624277	0.578333204	8.743203936	CORE	6	C	C	0.0000	6

C	-2.313232279	0.575068897	9.954941246	CORE	7	C	C	0.0000	7
C	-2.335267052	0.569570853	12.378282425	CORE	8	C	C	0.0000	8
C	-2.837719986	2.606909646	11.166670013	CORE	9	C	C	0.0000	9
C	-2.287150416	0.581738581	7.531518009	CORE	10	C	C	0.0000	10
C	0.639054255	0.591794295	3.897119140	CORE	11	C	C	0.0000	11
C	0.114391329	2.623367292	5.108532833	CORE	12	C	C	0.0000	12
C	3.034381001	2.632055556	1.474129278	CORE	13	C	C	0.0000	13
C	3.537748256	0.594753031	2.685664018	CORE	14	C	C	0.0000	14
C	-2.857482634	2.601942013	13.589859479	CORE	15	C	C	0.0000	15
C	3.556085501	0.599613026	0.262534530	CORE	16	C	C	0.0000	16
C	-2.786591620	2.619970603	6.319968183	CORE	17	C	C	0.0000	17
C	3.014327040	2.626591221	3.897113031	CORE	18	C	C	0.0000	18
C	3.515397775	0.588626222	5.108556954	CORE	19	C	C	0.0000	19
C	0.659110029	0.597251950	1.474147799	CORE	20	C	C	0.0000	20
C	0.136754009	2.629434692	2.685731338	CORE	21	C	C	0.0000	21
C	-5.232768069	0.567209316	13.589791355	CORE	22	C	C	0.0000	22
C	0.155065392	2.634415070	0.262509186	CORE	23	C	C	0.0000	23
C	0.614428545	0.585181505	6.319911148	CORE	24	C	C	0.0000	24
C	-0.054099207	3.302761216	3.897063599	CORE	25	C	C	0.0000	25
C	0.446905630	1.265023334	5.108871829	CORE	26	C	C	0.0000	26
C	3.367083606	1.273010726	1.473749082	CORE	27	C	C	0.0000	27
C	2.844686609	3.305354795	2.685389961	CORE	28	C	C	0.0000	28
C	-2.524774597	1.242878296	13.589451877	CORE	29	C	C	0.0000	29
C	2.863064819	3.310054452	0.262135492	CORE	30	C	C	0.0000	30
C	-2.454105637	1.261734469	6.320507958	CORE	31	C	C	0.0000	31
C	3.346918125	1.267978905	3.897068077	CORE	32	C	C	0.0000	32
C	2.822191556	3.299772447	5.108829424	CORE	33	C	C	0.0000	33
C	-0.033937940	3.307820942	1.473674077	CORE	34	C	C	0.0000	34
C	0.469388933	1.270664315	2.685363797	CORE	35	C	C	0.0000	35
C	-5.925788036	3.277635242	13.589584779	CORE	36	C	C	0.0000	36
C	0.487789473	1.275271575	0.262132094	CORE	37	C	C	0.0000	37
C	-0.078833693	3.296532640	6.320511026	CORE	38	C	C	0.0000	38
C	-2.480864926	1.254737724	8.743504171	CORE	39	C	C	0.0000	39
C	0.394613799	1.251312671	9.954916169	CORE	40	C	C	0.0000	40
C	0.372688881	1.245386079	12.378008066	CORE	41	C	C	0.0000	41
C	-0.129814286	3.282937793	11.166459618	CORE	42	C	C	0.0000	42
C	0.420601881	1.258306188	7.532112467	CORE	43	C	C	0.0000	43
C	-0.105576001	3.289463382	8.743517938	CORE	44	C	C	0.0000	44
C	-3.006405125	3.286110457	9.954880089	CORE	45	C	C	0.0000	45
C	-3.028309823	3.280106708	12.377861232	CORE	46	C	C	0.0000	46
C	-2.505094784	1.248189715	11.166326896	CORE	47	C	C	0.0000	47
C	-2.980393727	3.293002327	7.532098944	CORE	48	C	C	0.0000	48

end
end

PBC 5.30838219 4.19334579 15.84801197 90.00207769 115.45150848 90.00053249

C	-3.359392921	2.777073087	8.400548786	CORE	1 C	C	0.0000	1
C	-0.767270620	2.697171159	9.715390376	CORE	2 C	C	0.0000	2
C	-0.818852746	2.712058350	12.127191082	CORE	3 C	C	0.0000	3
C	-0.797448389	0.616791339	10.914629245	CORE	4 C	C	0.0000	4
C	0.524233025	2.777102872	7.618276576	CORE	5 C	C	0.0000	5
C	-0.705182525	0.680400460	8.400548960	CORE	6 C	C	0.0000	6
C	-3.421442099	0.600497709	9.715389792	CORE	7 C	C	0.0000	7
C	-3.473024322	0.615384628	12.127190294	CORE	8 C	C	0.0000	8
C	-3.451658979	2.713463570	10.914628421	CORE	9 C	C	0.0000	9
C	-2.129938587	0.680429757	7.618276404	CORE	10 C	C	0.0000	10
C	0.637748941	0.615721944	3.891638188	CORE	11 C	C	0.0000	11
C	0.616418091	2.713692161	5.104213331	CORE	12 C	C	0.0000	12
C	3.311968451	2.712936099	1.461401324	CORE	13 C	C	0.0000	13
C	3.304815889	0.614815252	2.675038830	CORE	14 C	C	0.0000	14
C	-3.485967239	2.711047518	13.343796573	CORE	15 C	C	0.0000	15
C	3.317504391	0.616340243	0.247466140	CORE	16 C	C	0.0000	16
C	-2.067914290	2.697313068	6.303445218	CORE	17 C	C	0.0000	17
C	3.291920507	2.712393950	3.891637348	CORE	18 C	C	0.0000	18
C	-2.037753430	0.617018657	5.104212513	CORE	19 C	C	0.0000	19
C	0.657796840	0.616264349	1.461401830	CORE	20 C	C	0.0000	20
C	0.650605262	2.711489220	2.675039520	CORE	21 C	C	0.0000	21
C	-6.140138834	0.614375599	13.343797205	CORE	22 C	C	0.0000	22
C	0.663293800	2.713014245	0.247466632	CORE	23 C	C	0.0000	23
C	0.586296088	0.600640500	6.303445751	CORE	24 C	C	0.0000	24
C	0.637723716	3.413770170	3.891619507	CORE	25 C	C	0.0000	25
C	0.616432148	1.315676865	5.104194016	CORE	26 C	C	0.0000	26
C	3.311981640	1.316779124	1.461382435	CORE	27 C	C	0.0000	27
C	3.304789820	3.414790862	2.675020713	CORE	28 C	C	0.0000	28
C	-3.485953021	1.317605136	13.343777112	CORE	29 C	C	0.0000	29
C	3.317478775	3.413479890	0.247446513	CORE	30 C	C	0.0000	30
C	-2.067902089	1.331937495	6.303430825	CORE	31 C	C	0.0000	31
C	3.291934321	1.317096412	3.891619830	CORE	32 C	C	0.0000	32
C	-2.037778455	3.412349125	5.104194416	CORE	33 C	C	0.0000	33
C	0.657771036	3.413453140	1.461382458	CORE	34 C	C	0.0000	34
C	0.650618206	1.318119009	2.675020625	CORE	35 C	C	0.0000	35
C	-6.140163653	3.414279002	13.343777043	CORE	36 C	C	0.0000	36
C	0.663307160	1.316808063	0.247446590	CORE	37 C	C	0.0000	37
C	0.586269455	3.428610728	6.303430632	CORE	38 C	C	0.0000	38
C	-3.359376669	1.251988596	8.400543605	CORE	39 C	C	0.0000	39
C	-0.767258189	1.331784494	9.715371924	CORE	40 C	C	0.0000	40
C	-0.818839674	1.316698921	12.127168744	CORE	41 C	C	0.0000	41

```
C          -0.797472906      3.412059985     10.914606449 CORE    42 C    C       0.0000     42
C           0.524248362      1.252021931      7.618274329 CORE    43 C    C       0.0000     43
C          -0.705205003      3.348661721      8.400543737 CORE    44 C    C       0.0000     44
C          -3.421468573      3.428456878      9.715372049 CORE    45 C    C       0.0000     45
C          -3.473050268      3.413371045     12.127169043 CORE    46 C    C       0.0000     46
C          -3.451644550      1.315386468     10.914606735 CORE    47 C    C       0.0000     47
C          -2.129962066      3.348694594      7.618274246 CORE    48 C    C       0.0000     48
end
end

PBC       5.17008246       4.19876017      16.07710898      89.99500949     119.25901954
89.99795541
C          -3.119578193      2.767612221      8.714964681 CORE     1 C    C       0.0000      1
C          -5.771700344      2.687137945     10.029047667 CORE     2 C    C       0.0000      2
C          -5.812062480      2.703775422     12.443597552 CORE     3 C    C       0.0000      3
C          -5.799039640      0.604299957     11.231613531 CORE     4 C    C       0.0000      4
C          -4.515723850      2.769410008      7.941182131 CORE     5 C    C       0.0000      5
C          -0.534615702      0.668232791      8.714999429 CORE     6 C    C       0.0000      6
C          -3.186725689      0.587758153     10.029000962 CORE     7 C    C       0.0000      7
C          -3.227096615      0.604396771     12.443535016 CORE     8 C    C       0.0000      8
C          -3.213922096      2.703681521     11.231557061 CORE     9 C    C       0.0000      9
C          -1.930740483      0.670029947      7.941173284 CORE    10 C    C       0.0000     10
C           1.991073245      0.587095405      4.481744826 CORE    11 C    C       0.0000     11
C           1.924270673      2.767268702      5.795827692 CORE    12 C    C       0.0000     12
C          -0.554338570      2.702516759      2.067111673 CORE    13 C    C       0.0000     13
C          -0.567070532      0.603334001      3.279100351 CORE    14 C    C       0.0000     14
C          -3.232926337      2.701960777     13.660251881 CORE    15 C    C       0.0000     15
C           4.621309066      0.601040991      0.850388890 CORE    16 C    C       0.0000     16
C          -1.849675022      2.769245721      6.569613651 CORE    17 C    C       0.0000     17
C          -0.593885094      2.686477157      4.481698394 CORE    18 C    C       0.0000     18
C          -0.660841152      0.667890485      5.795793052 CORE    19 C    C       0.0000     19
C           2.030628192      0.603135436      2.067173504 CORE    20 C    C       0.0000     20
C           2.018044218      2.702713295      3.279155822 CORE    21 C    C       0.0000     21
C          -5.818042641      0.602579370     13.660316680 CORE    22 C    C       0.0000     22
C           2.036342680      2.700419622      0.850453462 CORE    23 C    C       0.0000     23
C           0.735274824      0.669865035      6.569622793 CORE    24 C    C       0.0000     24
C           1.991173176      3.421105275      4.481785420 CORE    25 C    C       0.0000     25
C           1.924213389      1.241279959      5.795839637 CORE    26 C    C       0.0000     26
C          -0.554389924      1.305053566      2.067166684 CORE    27 C    C       0.0000     27
C          -0.566973059      3.404542230      3.279155807 CORE    28 C    C       0.0000     28
C          -3.232978684      1.308408649     13.660306232 CORE    29 C    C       0.0000     29
C           4.621408505      3.406246031      0.850441217 CORE    30 C    C       0.0000     30
C          -1.849727833      1.239483364      6.569622733 CORE    31 C    C       0.0000     31
C          -0.593934726      1.321725722      4.481739070 CORE    32 C    C       0.0000     32
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C       -0.660749133    3.340659426    5.795804885 CORE  33 C   C    0.0000   33
C        2.030726663    3.404431548    2.067229927 CORE  34 C   C    0.0000   34
C        2.017991889    1.305160170    3.279212092 CORE  35 C   C    0.0000   35
C       -5.817945112    3.407786383   13.660372122 CORE  36 C   C    0.0000   36
C        2.036292242    1.306863805    0.850507590 CORE  37 C   C    0.0000   37
C        0.735371277    3.338863432    6.569631626 CORE  38 C   C    0.0000   38
C       -3.119636270    1.241625970    8.714980420 CORE  39 C   C    0.0000   39
C       -5.771748344    1.322396094   10.029092716 CORE  40 C   C    0.0000   40
C       -5.812113203    1.306320491   12.443655557 CORE  41 C   C    0.0000   41
C       -5.798942579    3.405517173   11.231676395 CORE  42 C   C    0.0000   42
C       -4.515776522    1.239661933    7.941194982 CORE  43 C   C    0.0000   43
C       -0.534524398    3.341004226    8.715014730 CORE  44 C   C    0.0000   44
C       -3.186624161    3.421777819   10.029046888 CORE  45 C   C    0.0000   45
C       -3.226997486    3.405702742   12.443593153 CORE  46 C   C    0.0000   46
C       -3.213974827    1.306138512   11.231621379 CORE  47 C   C    0.0000   47
C       -1.930643908    3.339042601    7.941185794 CORE  48 C   C    0.0000   48
end
end
```

Reference

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