

The Mechanism of H₂ and H₂O Desorption from Bridging Hydroxyls of TiO₂(110) surface

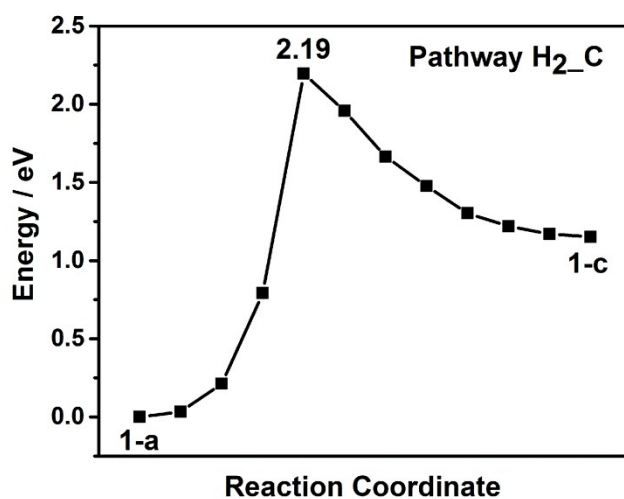
Ruimin Wang^{a,b}, Hongjun Fan^{*,a,b}

a, State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 457 Zhongshan Road, Dalian 116023, Liaoning Province, P. R. China

b, University of Chinese Academy of Sciences, 19 A Yuquan Road, Shijingshan District, Beijing 100049, P.R.China

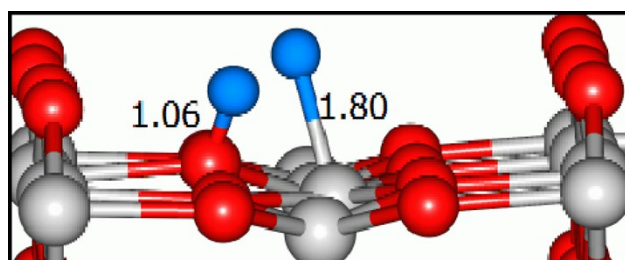
* Correspondence and requests for materials should be addressed to Hongjun Fan (email:fanhj@dicp.ac.cn)

Pathway H₂_C: We calculated the Pathway H₂_C where the proton of BBOH can also transfer to Ti_{5c} directly in the case of 1/4 ML H adatoms on stoichiometric TiO₂(110) surface. We calculated the barrier using CI-NEB method, and the barrier we got is 2.19eV, shown in Supplementary Fig. 1.



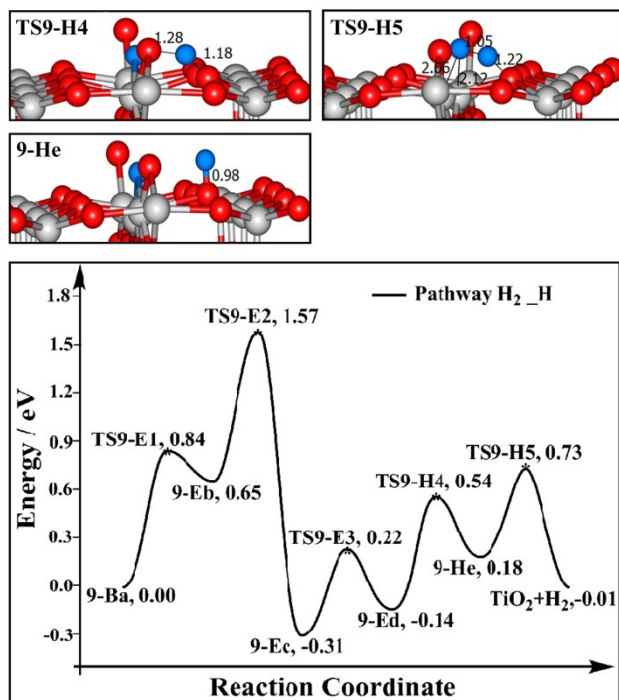
Supplementary Fig. 1. Calculated energy pathway for H transferred from BBO site to Ti_{5c} site by CI-NEB method.

Pathway H₂_D: We calculated the Pathway H₂_D where H₂ has been formed by the coupling of O_s-H and Ti_{5c}-H in the case of 1/4 ML H adatoms on stoichiometric TiO₂(110) surface. However, the intermediate ready for dehydrogenation (one O_s-H, another Ti_{5c}-H) is higher in energy than TS1-3 by 0.45 eV. The side views of structures shown in Supplementary Fig. 2 are expressed by simplified schematic diagrams.



Supplementary Fig. 2. The side view of optimized structure for one H adsorbed on O_s site, another one adsorbed on Ti_{5c} site on stoichiometric TiO₂(110) surface.

Pathway H₂_H: We calculated the Pathway H₂_H where H₂ has been formed by the coupling of O_s-H and Ti_{5c-Ov}-H in the case of two adjacent O_vs are near the H adatoms. The barrier for O_s-H and Ti_{5c-Ov}-H to produce H₂ (TS9-H5) is 073 eV, shown in Supplementary Fig. 3.



Supplementary Fig. 3. Reaction profiles for H₂ desorption of the model where two BBOHs are on the different sides of two adjacent O_vs. The side views of selected intermediates and transition states are shown in the figure with simplified schematic diagrams.

The optimized each structure of Cartesian coordinates from theory.

1-a:

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| Ti | 0.000000000 | 3.247194072 | 0.000000000 |

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| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
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1-b:

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| Ti | 3.247200000 | 3.247194072 | 10.350900000 |
| Ti | 0.000000000 | 3.247194072 | 8.872200000 |
| Ti | 0.000000000 | 3.247194072 | 5.914800000 |
| Ti | 9.741600000 | 3.247194072 | 1.478700000 |
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| O | 0.007280093 | 18.539708099 | 0.001998019 |
| O | 6.482588894 | 18.500235775 | 2.969779676 |
| O | 0.039278911 | 18.495806980 | 5.897623303 |
| O | 6.502748032 | 18.500258993 | 8.874993087 |
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| O | 2.026239162 | 19.919059148 | 7.381755810 |

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| O | 4.492430021 | 19.910776989 | 7.428296059 |
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| O | 2.032121789 | 19.938987478 | 1.506577399 |
| O | 6.480695907 | 21.104345796 | 2.962090910 |
| O | 6.483767888 | 21.104682626 | 5.923966166 |
| O | 0.001360837 | 21.075087670 | 3.027414197 |
| O | 0.049860886 | 21.137516935 | 5.908701723 |
| O | 0.003359683 | 21.099826988 | 8.861403361 |
| O | 0.006890688 | 21.146112349 | 0.030173051 |
| O | 6.496424694 | 21.110229425 | 8.879770589 |
| O | 6.498281573 | 21.109963319 | 0.003332872 |
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| H | 0.816399334 | 0.932897449 | 8.400899272 |

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| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
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| H | -0.549962937 | 21.905161980 | 5.911972962 |

TS1-2:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |

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|----|-------------|-------------|--------------|
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |

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|----|--------------|--------------|--------------|
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
| Ti | 6.494400000 | 6.494389931 | 10.350900000 |
| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
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| Ti | 3.238211361 | 9.731449101 | 4.438622780 |
| Ti | -0.014150778 | 9.831671185 | 2.966282373 |
| Ti | -0.005319433 | 9.801119317 | 0.009024802 |
| Ti | 3.236894167 | 9.734685597 | 7.393900787 |
| Ti | 3.242830178 | 9.726341288 | 10.346913070 |
| Ti | -0.013909966 | 9.820972995 | 8.880520349 |
| Ti | -0.013452500 | 9.798086776 | 5.922543183 |
| Ti | 9.730919310 | 9.726146619 | 1.480761190 |
| Ti | 9.723570636 | 9.725723707 | 4.438557245 |
| Ti | 6.483939989 | 9.835329879 | 2.963126946 |
| Ti | 6.486237578 | 9.835587770 | 0.005790234 |
| Ti | 9.724530898 | 9.726018746 | 7.396025265 |
| Ti | 9.731430939 | 9.726333430 | 10.353489973 |
| Ti | 6.484554619 | 9.836252500 | 8.878725444 |
| Ti | 6.477235820 | 9.834905895 | 5.921752966 |
| Ti | -0.024756523 | 13.160551693 | 1.510684991 |

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| Ti | -0.026512609 | 13.154216933 | 4.475409997 |
| Ti | 3.220778573 | 12.985349054 | 2.970150061 |
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| Ti | 6.467067278 | 13.168900289 | 1.505059070 |
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| Ti | 9.714728771 | 12.974079717 | 2.964508643 |
| Ti | 9.711673155 | 12.974447266 | 5.922446772 |
| Ti | -0.028768244 | 13.126025733 | 7.412270145 |
| Ti | -0.027479495 | 13.134916185 | 10.406041906 |
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| Ti | 6.468408502 | 13.170673021 | 7.418430645 |
| Ti | 6.466547597 | 13.168780987 | 10.375760851 |
| Ti | 9.712720442 | 12.974896610 | 8.880679102 |
| Ti | 9.712024243 | 12.975159145 | 0.007915659 |
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| Ti | 6.429378067 | 16.630166031 | 2.975140969 |
| Ti | -0.063843069 | 16.578270291 | 5.926461028 |
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| Ti | 3.186522561 | 16.342740090 | 7.368567344 |
| Ti | 3.207002911 | 16.260316414 | 10.349560180 |
| Ti | -0.058290227 | 16.443274357 | 8.892102356 |
| Ti | 6.435497091 | 16.624469926 | 0.022050138 |
| Ti | 9.673855355 | 16.293149295 | 7.411567821 |
| Ti | 9.667076111 | 16.291771972 | 10.369387772 |
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| Ti | 3.182035710 | 19.501083572 | 0.036819039 |
| Ti | 3.152005474 | 19.524205535 | 8.931420870 |
| Ti | 3.194901636 | 19.516507739 | 2.953103726 |
| Ti | 6.420078606 | 19.996043181 | 1.492294931 |
| Ti | 6.461379613 | 20.011670589 | 7.424477582 |
| Ti | 6.391659761 | 20.011491637 | 4.449249902 |
| Ti | 6.409240102 | 19.995254863 | 10.369900822 |
| Ti | 3.303345257 | 19.633530599 | 6.041909170 |
| Ti | -0.069443580 | 19.982368886 | 1.473056453 |
| Ti | -0.089329693 | 19.846553560 | 4.358387809 |
| Ti | 9.654663104 | 19.535747764 | 2.974422321 |
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| Ti | -0.072854569 | 19.968974628 | 10.384017912 |
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| O | 7.769315794 | 9.780651631 | 1.482512207 |
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| O | 3.237344748 | 11.059634148 | 2.960386146 |
| O | 3.236925859 | 11.056383722 | 0.002329721 |
| O | 3.237170049 | 11.061533683 | 8.874955942 |
| O | 3.237900279 | 11.061916948 | 5.918192374 |
| O | 9.737530869 | 11.059703086 | 8.874922937 |
| O | 9.737096263 | 11.060157431 | 5.918332910 |
| O | 6.469238097 | 11.786921752 | 8.877873949 |
| O | -0.028839812 | 11.790858340 | 2.963173555 |
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| O | 6.468942342 | 11.786688865 | 5.920194652 |
| O | -0.029655509 | 11.790541870 | 0.002481377 |
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| O | -0.029553417 | 11.791436988 | 8.875365838 |
| O | 8.453262230 | 13.080815156 | 1.486775122 |
| O | 8.453443164 | 13.081307006 | 4.444616957 |
| O | 10.976675248 | 13.105351233 | 1.486599334 |
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| O | 6.470032232 | 14.396254244 | 8.884337051 |
| O | 6.470908976 | 14.395307334 | 0.012933538 |
| O | 9.675770164 | 15.102942359 | 8.887538614 |
| O | 3.191154627 | 15.102413361 | 8.869758725 |
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| O | 9.674608835 | 15.100667417 | 0.013809757 |
| O | 3.190731322 | 15.083431941 | 0.008759937 |
| O | 3.200050786 | 15.101376439 | 5.930037589 |
| O | 1.226731113 | 16.440980842 | 10.363428138 |
| O | 5.160684428 | 16.438688755 | 4.454589665 |
| O | 5.158152002 | 16.449596973 | 7.408689443 |
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| O | 9.689847685 | 17.711514751 | 5.931432181 |
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| O | 9.696395989 | 17.712045892 | 0.021087918 |
| O | 6.426435974 | 18.486864735 | 0.024196974 |
| O | 6.420248499 | 18.496497785 | 5.939586088 |
| O | -0.075160341 | 18.485679222 | 0.023344059 |
| O | 6.421189798 | 18.491309961 | 2.986985238 |
| O | -0.124450369 | 18.448096074 | 5.938071544 |
| O | 6.419202122 | 18.490651303 | 8.894050809 |
| O | -0.092959802 | 18.451296852 | 8.892700933 |
| O | -0.092153977 | 18.451289708 | 2.981257109 |
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| O | 4.399356307 | 19.949211677 | 4.433415509 |
| O | 1.917731506 | 19.807602733 | 7.451375135 |
| O | 1.950385349 | 19.873108831 | 10.373302896 |
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| O | 4.403500903 | 19.897849935 | 10.378819276 |
| O | 8.448117886 | 19.891779496 | 1.504515381 |
| O | 8.452257546 | 19.909877228 | 4.457815952 |
| O | 10.899697644 | 19.914584632 | 1.502190510 |
| O | 10.903962257 | 19.916424159 | 4.472991791 |
| O | 8.450682134 | 19.906300330 | 7.420733040 |

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| O | 10.902757805 | 19.918442638 | 7.407061335 |
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| O | 1.950840087 | 19.877142575 | 1.502900641 |
| O | 6.441156441 | 21.104279358 | 2.972121937 |
| O | 6.435699586 | 21.102496267 | 5.934454407 |
| O | -0.060972025 | 21.048306655 | 2.997255933 |
| O | 0.016047013 | 21.087113891 | 5.938118153 |
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| O | 6.440778077 | 21.104501531 | 8.895771306 |
| O | 6.433721652 | 21.101780816 | 0.019377595 |
| H | 0.000000000 | 0.932897449 | 9.814799089 |
| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |

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| H | -0.036701153 | 0.932897449 | 6.856699960 |
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| H | 2.840144257 | 21.634298927 | 5.940151661 |
| H | 0.829531790 | 21.643138659 | 5.937906639 |

TS1-3:

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| Ti | 3.247200000 | 3.247194072 | 1.478700000 |
| Ti | 3.247200000 | 3.247194072 | 4.436100000 |
| Ti | 0.000000000 | 3.247194072 | 2.957400000 |
| Ti | 0.000000000 | 3.247194072 | 0.000000000 |
| Ti | 3.247200000 | 3.247194072 | 7.393500000 |
| Ti | 3.247200000 | 3.247194072 | 10.350900000 |
| Ti | 0.000000000 | 3.247194072 | 8.872200000 |
| Ti | 0.000000000 | 3.247194072 | 5.914800000 |
| Ti | 9.741600000 | 3.247194072 | 1.478700000 |
| Ti | 9.741600000 | 3.247194072 | 4.436100000 |
| Ti | 6.494400000 | 3.247194072 | 2.957400000 |
| Ti | 6.494400000 | 3.247194072 | 0.000000000 |
| Ti | 9.741600000 | 3.247194072 | 7.393500000 |

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|----|--------------|-------------|--------------|
| Ti | 9.741600000 | 3.247194072 | 10.350900000 |
| Ti | 6.494400000 | 3.247194072 | 8.872200000 |
| Ti | 6.494400000 | 3.247194072 | 5.914800000 |
| Ti | 0.000000000 | 6.494391717 | 4.436100000 |
| Ti | 0.000000000 | 6.494391717 | 1.478700000 |
| Ti | 3.247200000 | 6.494391717 | 2.957400000 |
| Ti | 3.247200000 | 6.494391717 | 0.000000000 |
| Ti | 0.000000000 | 6.494391717 | 10.350900000 |
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| Ti | 3.247200000 | 6.494391717 | 5.914800000 |
| Ti | 6.494400000 | 6.494391717 | 4.436100000 |
| Ti | 6.494400000 | 6.494391717 | 1.478700000 |
| Ti | 9.741600000 | 6.494391717 | 2.957400000 |
| Ti | 9.741600000 | 6.494391717 | 0.000000000 |
| Ti | 6.494400000 | 6.494391717 | 10.350900000 |
| Ti | 6.494400000 | 6.494391717 | 7.393500000 |
| Ti | 9.741600000 | 6.494391717 | 8.872200000 |
| Ti | 9.741600000 | 6.494391717 | 5.914800000 |
| Ti | 3.232018561 | 9.723915612 | 1.484886881 |
| Ti | 3.232429916 | 9.730141430 | 4.438785319 |
| Ti | -0.017752053 | 9.828515056 | 2.967561626 |

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| Ti | -0.016349003 | 9.820303264 | 0.009877716 |
| Ti | 3.232602407 | 9.729330609 | 7.395735794 |
| Ti | 3.233268343 | 9.724747864 | 10.350426816 |
| Ti | -0.015934530 | 9.827918549 | 8.882882129 |
| Ti | -0.016552018 | 9.815895542 | 5.925127241 |
| Ti | 9.721854426 | 9.724944319 | 1.479492583 |
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| Ti | 6.475356861 | 9.834815883 | 2.967857366 |
| Ti | 6.475310101 | 9.834801595 | 0.009972353 |
| Ti | 9.723322291 | 9.724447825 | 7.394529175 |
| Ti | 9.722802739 | 9.724026341 | 10.351988323 |
| Ti | 6.476314135 | 9.836398234 | 8.881746487 |
| Ti | 6.476221135 | 9.835326664 | 5.924902478 |
| Ti | -0.033008048 | 13.159713011 | 1.508640718 |
| Ti | -0.035666595 | 13.149665264 | 4.474179482 |
| Ti | 3.215678131 | 12.984000662 | 2.987825731 |
| Ti | 3.210758493 | 12.977974871 | 5.941061712 |
| Ti | 6.459439086 | 13.167689058 | 1.510308691 |
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| Ti | 9.707447899 | 12.972988503 | 2.978716939 |
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| Ti | -0.034262246 | 13.155633905 | 10.389287052 |
| Ti | 3.209962409 | 12.981857524 | 8.893635235 |
| Ti | 3.211211542 | 12.963555122 | 0.026935999 |
| Ti | 6.458413620 | 13.170003648 | 7.424410745 |
| Ti | 6.454969250 | 13.169060667 | 10.382082826 |
| Ti | 9.703697123 | 12.972452718 | 8.896722761 |
| Ti | 9.703890786 | 12.972809908 | 0.022180500 |
| Ti | 9.683356662 | 16.298017791 | 1.501318195 |
| Ti | 9.681437697 | 16.295278146 | 4.458801002 |
| Ti | 6.435638669 | 16.623267625 | 2.990901427 |
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| Ti | 3.179642913 | 16.336397829 | 7.386236626 |
| Ti | 3.195086986 | 16.248868483 | 10.363936219 |
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| Ti | 3.176485726 | 19.496666206 | 0.022559047 |
| Ti | 6.400875574 | 19.999896544 | 7.407328802 |
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| Ti | 6.410170100 | 19.996856859 | 10.365710659 |
| Ti | 3.117085086 | 19.687734142 | 5.939062510 |
| Ti | -0.058501685 | 19.966274274 | 1.493096623 |
| Ti | -0.087291101 | 19.875844547 | 4.410512575 |
| Ti | 9.680692270 | 19.551894884 | 2.979686966 |
| Ti | 9.647246629 | 19.548137248 | 5.938991532 |
| Ti | -0.094246083 | 19.877241159 | 7.472013055 |
| Ti | -0.065589284 | 19.963209586 | 10.386045742 |
| Ti | 9.670730769 | 19.550937615 | 8.900389937 |
| Ti | 9.669178088 | 19.547244273 | 0.026439156 |
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| O | 1.266698949 | 3.247194072 | 4.436100000 |
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| O | 1.266698949 | 3.247194072 | 7.393500000 |
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| O | 6.494400000 | 5.227596870 | 0.000000000 |
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| O | 11.008298949 | 6.494391717 | 7.393500000 |
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| O | 6.494400000 | 7.761086550 | 5.914800000 |
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| O | 9.741600000 | 8.474887384 | 2.957400000 |
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| O | 1.266099776 | 9.778787100 | 4.447480075 |
| O | 5.202526808 | 9.770814625 | 1.488341124 |
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| O | 1.266181865 | 9.779483620 | 7.403223931 |
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| O | 5.202190009 | 9.772486273 | 7.403425034 |
| O | 5.202442251 | 9.771904054 | 10.360541124 |
| O | 7.764443175 | 9.778779957 | 1.488778819 |
| O | 7.764468893 | 9.778429911 | 4.446107842 |
| O | 11.695628707 | 9.771253969 | 1.488672353 |
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| O | 9.728226472 | 11.061255433 | 2.967727241 |
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| O | 3.230554333 | 11.059165873 | 2.968235914 |
| O | 3.230328198 | 11.054600988 | 0.010622981 |
| O | 3.229371443 | 11.059022997 | 8.882077716 |
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| O | 6.463198564 | 11.787632917 | 0.016738884 |
| O | 6.465644875 | 11.787775793 | 5.931420588 |
| O | -0.036340324 | 11.789783199 | 0.016667906 |
| O | -0.038983675 | 11.789786771 | 5.932083046 |
| O | 6.465209490 | 11.787457894 | 2.974056077 |
| O | -0.036792724 | 11.789986798 | 8.887803242 |
| O | 8.446503378 | 13.087474958 | 1.500064258 |
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| O | 10.967653487 | 13.110349389 | 1.498254329 |

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| O | 1.949187652 | 13.081109837 | 1.501933334 |
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| O | -0.034743481 | 14.398939954 | 2.980384913 |
| O | -0.033331859 | 14.394278628 | 5.937702106 |
| O | -0.037798187 | 14.399772206 | 8.895717245 |
| O | -0.030233900 | 14.394792981 | 0.022783810 |
| O | 6.462873715 | 14.396614649 | 2.980810778 |
| O | 6.463714869 | 14.396864681 | 5.937749424 |
| O | 6.460395971 | 14.397186152 | 8.895279550 |
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| O | 9.672514521 | 15.114741050 | 8.899881264 |

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| O | 9.669355905 | 15.112765791 | 5.939239954 |
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| O | 1.222269330 | 16.453016707 | 4.455181145 |
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| O | 5.162480130 | 16.419444444 | 1.502158097 |
| O | 7.723317907 | 16.465346897 | 7.424268790 |
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| O | 9.692113711 | 17.722451186 | 5.941085371 |
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| O | 3.181093373 | 17.716600418 | 5.941511237 |
| O | 9.699835942 | 17.725962361 | 8.895255890 |
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| O | 6.430283127 | 18.488844637 | 0.027267228 |
| O | 6.414150518 | 18.497727946 | 5.943344825 |
| O | -0.076091897 | 18.477975353 | 0.023990429 |
| O | 6.406971478 | 18.491327106 | 2.990854109 |
| O | -0.155792083 | 18.442913609 | 5.938636644 |
| O | 6.399196123 | 18.493913160 | 8.894262204 |
| O | -0.128067750 | 18.456518966 | 8.903524781 |
| O | -0.120506320 | 18.455490259 | 2.974813171 |
| O | 1.906113674 | 19.689495088 | 4.376904682 |
| O | 4.407611079 | 19.898097468 | 1.480557247 |
| O | 4.374615501 | 19.951708076 | 4.463402717 |
| O | 1.903958832 | 19.684644451 | 7.498937225 |
| O | 1.949637584 | 19.860131770 | 10.370004804 |

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| O | 4.372707446 | 19.953515456 | 7.409517278 |
| O | 4.404761466 | 19.904884073 | 10.394243654 |
| O | 8.448018002 | 19.901305032 | 1.512426190 |
| O | 8.441422679 | 19.907305819 | 4.452673270 |
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| O | 8.439114049 | 19.906059227 | 7.422967534 |
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| O | 1.952314965 | 19.864443051 | 1.504062662 |
| O | 6.418912471 | 21.102530558 | 2.973369960 |
| O | 6.423245665 | 21.105016598 | 5.932023898 |
| O | -0.051452144 | 21.053202654 | 2.996603294 |
| O | 0.228840055 | 21.045644519 | 5.940470232 |
| O | -0.050675284 | 21.053581275 | 8.882633707 |
| O | -0.053909625 | 21.085592620 | 0.022831128 |
| O | 6.421130439 | 21.105130899 | 8.891375782 |
| O | 6.439220850 | 21.103916454 | 0.018832723 |
| H | 0.000000000 | 0.932897449 | 9.814799089 |
| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |

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| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 1.399021050 | 21.354460053 | 5.940553039 |

TS2-1:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |

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|----|-------------|-------------|--------------|
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
| Ti | 6.494400000 | 6.494389931 | 4.436100000 |
| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |

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|----|--------------|--------------|--------------|
| Ti | 6.494400000 | 6.494389931 | 10.350900000 |
| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
| Ti | 9.741600000 | 6.494389931 | 5.914800000 |
| Ti | 3.245550163 | 9.734522719 | 1.482679714 |
| Ti | 3.237275518 | 9.736326884 | 4.439428021 |
| Ti | -0.015647867 | 9.769797706 | 2.965147442 |
| Ti | -0.008170475 | 9.769948797 | 0.011065171 |
| Ti | 3.241392708 | 9.734507360 | 7.397128257 |
| Ti | 3.246851900 | 9.735866110 | 10.354651639 |
| Ti | -0.013610964 | 9.780378738 | 8.888187350 |
| Ti | -0.013777740 | 9.742100499 | 5.928112440 |
| Ti | 9.720340452 | 9.735273532 | 1.478707808 |
| Ti | 9.720149257 | 9.734668095 | 4.436586670 |
| Ti | 6.478003978 | 9.833002788 | 2.967503425 |
| Ti | 6.483956096 | 9.834477982 | 0.008427407 |
| Ti | 9.720535414 | 9.734950632 | 7.393878074 |
| Ti | 9.721170176 | 9.735738593 | 10.351076853 |
| Ti | 6.481388340 | 9.834143295 | 8.879284747 |
| Ti | 6.478305188 | 9.833806465 | 5.923038488 |
| Ti | -0.028493531 | 13.127413772 | 1.442120747 |
| Ti | -0.027429878 | 13.029925976 | 4.428586666 |

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| Ti | 3.220054187 | 12.988030834 | 2.966161830 |
| Ti | 3.221780399 | 12.988612339 | 5.924254335 |
| Ti | 6.468835314 | 13.167487961 | 1.508210948 |
| Ti | 6.467797898 | 13.167820147 | 4.465490168 |
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| Ti | 9.710276729 | 12.987974041 | 5.922524019 |
| Ti | -0.026342196 | 13.040012300 | 7.430210088 |
| Ti | -0.026322193 | 13.152397408 | 10.407388469 |
| Ti | 3.219382666 | 12.988160137 | 8.882265215 |
| Ti | 3.222096546 | 12.988221931 | 0.009539153 |
| Ti | 6.467926228 | 13.167607262 | 7.422857518 |
| Ti | 6.466348348 | 13.169057095 | 10.379449675 |
| Ti | 9.716266515 | 12.987895817 | 8.880697911 |
| Ti | 9.708594550 | 12.988533400 | 0.004893432 |
| Ti | 9.673521673 | 16.297650958 | 1.485886127 |
| Ti | 9.685218607 | 16.291186895 | 4.443704540 |
| Ti | 6.439116940 | 16.620996256 | 2.970695051 |
| Ti | -0.051969618 | 16.308505239 | 5.932493769 |
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| Ti | 3.207135787 | 16.296407937 | 7.404376016 |
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| Ti | 9.685261729 | 16.314546389 | 10.363053968 |
| Ti | 6.440717030 | 16.623050454 | 8.883061702 |
| Ti | -0.053638029 | 16.758425366 | 0.013203726 |
| Ti | 6.422329565 | 19.988362173 | 7.403986586 |
| Ti | 6.438768060 | 19.983764069 | 10.358888174 |
| Ti | 3.183797251 | 19.554083742 | 8.893812088 |
| Ti | 3.177709790 | 19.550427905 | 0.022166896 |
| Ti | 6.420141732 | 19.987145585 | 1.484563223 |
| Ti | 6.416693595 | 19.995229146 | 4.442310777 |
| Ti | 3.170666613 | 19.537301897 | 2.977731060 |
| Ti | 3.167113008 | 19.536214254 | 5.933184855 |
| Ti | -0.067914668 | 20.105994399 | 1.564059200 |
| Ti | -0.087800002 | 19.474744757 | 4.431906998 |
| Ti | 9.672982378 | 19.535358785 | 2.967310129 |
| Ti | 9.656042385 | 19.521915592 | 5.932047557 |
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| O | 3.247200000 | 1.980499953 | 2.957400000 |
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| O | 1.266699988 | 3.247190143 | 7.393500000 |
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| O | 0.000000000 | 5.227600085 | 8.872200000 |
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| O | 9.741600000 | 8.474889884 | 2.957400000 |
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| O | 1.264374863 | 9.779768301 | 4.443278320 |
| O | 5.206759858 | 9.774586192 | 1.481734884 |
| O | 5.205572552 | 9.774696206 | 4.440496826 |
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| O | 7.764414470 | 9.782768337 | 1.483329277 |
| O | 7.763525517 | 9.782886924 | 4.439743044 |
| O | 11.706463835 | 9.773346386 | 1.483332471 |
| O | 11.705738540 | 9.771517932 | 4.443732221 |
| O | 7.763907777 | 9.782473298 | 7.396835947 |
| O | 7.765007799 | 9.783584873 | 10.354212525 |
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| O | 11.706512802 | 9.774394738 | 10.356943979 |
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| O | 3.234431620 | 11.065315251 | 2.961371315 |
| O | 3.232585002 | 11.066185723 | 0.003803216 |
| O | 3.233304971 | 11.065872467 | 8.873869748 |
| O | 3.231606946 | 11.066502907 | 5.918845487 |
| O | 9.739000941 | 11.065654224 | 8.873577084 |
| O | 9.738739606 | 11.065703516 | 5.918211302 |
| O | 6.466566430 | 11.789467086 | 8.875044782 |
| O | -0.027952677 | 11.794538466 | 2.970200100 |
| O | 6.467301596 | 11.789458871 | 0.004496904 |
| O | 6.466677614 | 11.790017516 | 5.919094027 |

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| O | -0.026678086 | 11.797706025 | 0.007268225 |
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| O | 10.988885629 | 13.103071648 | 4.444648069 |
| O | 1.947339865 | 13.083788046 | 1.490942926 |
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| O | 8.455012470 | 13.087682128 | 7.401097206 |
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| O | 10.989249575 | 13.109255317 | 7.400357619 |
| O | 10.986339305 | 13.101824342 | 10.354628217 |
| O | -0.029597449 | 14.413710821 | 2.972919371 |
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| O | -0.028570814 | 14.420999635 | 8.881747788 |
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| O | 6.468821935 | 14.396536067 | 5.926978573 |
| O | 6.467500845 | 14.396917188 | 8.885880932 |
| O | 6.469184713 | 14.397538698 | 0.010305119 |
| O | 9.694780831 | 15.103059160 | 8.893252193 |
| O | 3.186939761 | 15.102199047 | 8.891540923 |
| O | 9.695185173 | 15.094704134 | 5.925713279 |
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| O | 3.184129245 | 15.097505216 | 2.967343015 |
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| O | 3.186346433 | 15.099800518 | 0.003865677 |
| O | 3.185566455 | 15.097997424 | 5.923533557 |
| O | 1.225809298 | 16.481586529 | 10.373137755 |
| O | 5.157831958 | 16.434202452 | 4.448119938 |
| O | 5.159005106 | 16.434236742 | 7.405371713 |
| O | 7.729312628 | 16.454620132 | 1.488414822 |
| O | 7.729074413 | 16.449442310 | 4.445562970 |
| O | 5.156147440 | 16.445191395 | 10.363471434 |
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| O | 1.227630977 | 16.469687467 | 4.441258652 |
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| O | 9.684908434 | 17.701716322 | 5.933126061 |
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| O | 3.202876369 | 17.711682630 | 5.935149278 |
| O | 9.719504233 | 17.735994035 | 8.874648964 |
| O | 9.707361134 | 17.728922393 | 0.016381039 |
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| O | 6.428680699 | 18.491181373 | 5.924208317 |
| O | -0.066085845 | 18.601946625 | 0.028685360 |
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| O | 6.435359150 | 21.098334650 | 5.927555266 |
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| H | 0.834099951 | 0.932899949 | -0.439200043 |
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| H | 6.457700016 | 0.932899949 | 0.941899960 |
| H | 0.834099951 | 0.932899949 | 5.475599957 |
| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
| H | -0.036699984 | 0.932899949 | 6.856699960 |
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TS2-2:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
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| Ti | 3.240933553 | 9.734741319 | 4.438797031 |
| Ti | -0.007992139 | 9.808682096 | 2.957646292 |
| Ti | -0.010306743 | 9.761425179 | -0.001275467 |
| Ti | 3.244841104 | 9.730823305 | 7.397623325 |
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| Ti | -0.004060429 | 9.830840718 | 8.873296367 |
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| Ti | 6.483055972 | 9.836726491 | 2.958181937 |

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| Ti | -0.025352969 | 13.102673739 | 1.445927749 |
| Ti | -0.024476614 | 13.085987977 | 4.470273348 |
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| Ti | 3.237253307 | 12.983979588 | 5.916039151 |
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| Ti | -0.032200144 | 16.519352200 | 5.915252955 |
| Ti | 3.219873253 | 16.318486192 | 1.481921318 |
| Ti | 3.221507634 | 16.301585403 | 4.436629138 |
| Ti | -0.030693314 | 16.330727442 | 2.940283752 |
| Ti | 6.459131252 | 16.630591801 | 5.917242458 |
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| Ti | -0.033192619 | 16.700200580 | 0.000669910 |
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| Ti | 3.198307689 | 19.534946588 | 8.904733411 |
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| O | 6.494400000 | 1.266689833 | 2.957400000 |
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| O | 5.208256298 | 9.776896495 | 7.393625512 |
| O | 5.209029001 | 9.777061874 | 10.350706468 |
| O | 7.766574508 | 9.782011452 | 1.479023185 |
| O | 7.765651264 | 9.782061459 | 4.436045584 |
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| O | -0.019959110 | 11.795048533 | 2.965475358 |
| O | 6.474467388 | 11.791970272 | -0.001678384 |
| O | 6.473501151 | 11.791945983 | 5.912698235 |
| O | -0.020148746 | 11.796086884 | -0.001735284 |
| O | -0.020446320 | 11.804509418 | 5.921023316 |
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| O | -0.017392523 | 11.803760034 | 8.863042943 |
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| O | 10.988154879 | 13.098866096 | 1.481843953 |
| O | 10.989329716 | 13.101094960 | 4.436387459 |
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| O | 6.471316435 | 14.402017501 | 5.920926668 |
| O | 6.474015897 | 14.401441353 | 8.879297169 |
| O | 6.470557239 | 14.403158007 | 0.006383252 |
| O | 9.709293088 | 15.103475286 | 8.879989437 |
| O | 3.209556639 | 15.097519504 | 8.881777126 |
| O | 9.709878233 | 15.098750380 | 5.915471448 |
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| O | 3.213317286 | 15.112347164 | 2.954839246 |
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| O | 3.200298612 | 17.731751335 | 0.006097804 |
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| O | -0.051612945 | 18.490611298 | 0.012696946 |
| O | 6.468614894 | 18.533068656 | 2.974906152 |
| O | -0.051306020 | 18.491229593 | 5.927703609 |
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| O | -0.051360183 | 18.491455694 | 2.970218318 |
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| O | 1.985421598 | 19.938179872 | 7.407338621 |
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| O | 10.899185366 | 19.929305136 | 4.448945644 |
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| O | 8.427620650 | 20.011174096 | 10.364909795 |
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| O | 10.898734914 | 19.928615402 | 10.364263189 |
| O | 1.986118707 | 19.938162727 | 1.492585584 |
| O | 6.430565503 | 21.185566099 | 2.973881472 |
| O | 6.430597326 | 21.185392148 | 5.931534980 |
| O | -0.056364508 | 21.094758109 | 2.968579090 |
| O | -0.056704295 | 21.094768467 | 5.927138864 |
| O | -0.056659224 | 21.095747167 | 8.885045289 |

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| H | 0.000000000 | 0.932897449 | 9.814799089 |
| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 7.226519167 | 21.747458066 | 8.890136631 |
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TS3-1:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |

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|----|--------------|-------------|--------------|
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |
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| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 3.226517284 | 9.737743142 | 1.478796056 |
| Ti | 3.225740424 | 9.735501419 | 4.436386986 |
| Ti | -0.013076085 | 9.836817932 | 2.959219747 |
| Ti | -0.012392224 | 9.837029745 | -0.000052997 |
| Ti | 3.226212048 | 9.737784933 | 7.393786868 |
| Ti | 3.226191006 | 9.736162934 | 10.351136355 |
| Ti | -0.014762161 | 9.836597188 | 8.871376068 |
| Ti | -0.017794786 | 9.835803155 | 5.916328029 |
| Ti | 9.739555433 | 9.735431052 | 1.482379715 |
| Ti | 9.733608771 | 9.739790553 | 4.439105665 |

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| Ti | 6.482643707 | 9.757920790 | 2.960488945 |
| Ti | 6.481486665 | 9.759350263 | 0.006963376 |
| Ti | 9.730157257 | 9.739332636 | 7.393842704 |
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| Ti | 6.480387683 | 9.755208291 | 8.880462857 |
| Ti | 6.476456882 | 9.748534558 | 5.919475649 |
| Ti | -0.034105082 | 13.174932866 | 1.503768460 |
| Ti | -0.033856087 | 13.174161336 | 4.461712740 |
| Ti | 3.212241554 | 12.989855002 | 2.958748220 |
| Ti | 3.212097898 | 12.989827856 | 5.915794751 |
| Ti | 6.459701330 | 13.104500050 | 1.473564061 |
| Ti | 6.461405461 | 13.056152633 | 4.425859588 |
| Ti | 9.709168525 | 12.994580265 | 2.960497699 |
| Ti | 9.709128390 | 12.998592578 | 5.918053140 |
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| Ti | -0.035507872 | 13.176600942 | 10.376682731 |
| Ti | 3.211724080 | 12.990429721 | 8.873638124 |
| Ti | 3.210704200 | 12.991245185 | 0.000552561 |
| Ti | 6.459865898 | 13.045106183 | 7.401491250 |
| Ti | 6.460147106 | 13.084626370 | 10.372758262 |
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| Ti | 9.706027573 | 16.297841697 | 1.479143965 |
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| Ti | 6.443461433 | 16.367249736 | 2.962179158 |
| Ti | -0.040266969 | 16.634729130 | 5.918482081 |
| Ti | 3.178096077 | 16.305736662 | 1.486041568 |
| Ti | 3.187846769 | 16.305476985 | 4.444930915 |
| Ti | -0.050936618 | 16.632368106 | 2.960958580 |
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| Ti | 3.192848496 | 16.303909993 | 7.402540062 |
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| Ti | 9.704072889 | 16.326929086 | 7.393836789 |
| Ti | 9.705319944 | 16.306103853 | 10.348467243 |
| Ti | 6.447952831 | 16.334197540 | 8.881112657 |
| Ti | -0.049393289 | 16.643679233 | 0.000314431 |
| Ti | 6.437727787 | 19.768462953 | 7.429186354 |
| Ti | 6.451545013 | 19.708860486 | 10.411848583 |
| Ti | 3.208855634 | 19.550396473 | 8.891431262 |
| Ti | 3.246624856 | 19.560345636 | 0.001979329 |
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| Ti | -0.050073383 | 19.999670800 | 4.437598810 |
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| Ti | 9.677544044 | 19.596513597 | 5.926856492 |
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| O | 0.000000000 | 1.266689833 | 8.872200000 |
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| O | 6.494400000 | 1.266689833 | 2.957400000 |
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| O | 6.494400000 | 7.761090122 | 5.914800000 |
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| O | 9.741600000 | 8.474889884 | 0.000000000 |

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| O | 5.210247351 | 9.776991150 | 1.480940526 |
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| O | 1.267473991 | 9.786213075 | 7.393077802 |
| O | 1.268276829 | 9.786753860 | 10.350696649 |
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| O | 5.210165911 | 9.778375261 | 10.354156334 |
| O | 7.758824610 | 9.782991938 | 1.480663832 |
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| O | 11.698801482 | 9.780329446 | 4.435483914 |
| O | 7.757085800 | 9.782726546 | 7.395380906 |
| O | 7.758194524 | 9.783527365 | 10.353818481 |
| O | 11.698365188 | 9.780406599 | 7.393592034 |
| O | 11.699638090 | 9.780050480 | 10.351415652 |
| O | 9.720948977 | 11.072592992 | 2.958118766 |
| O | 9.720926636 | 11.071205667 | 0.001270972 |
| O | 3.240682999 | 11.069579739 | 2.957961315 |
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| O | 6.466641895 | 11.800800360 | 8.879141136 |
| O | -0.028962686 | 11.797797823 | 2.956183207 |
| O | 6.468236011 | 11.807580178 | 0.008000004 |
| O | 6.466027525 | 11.797009505 | 5.918810826 |
| O | -0.029563808 | 11.797159882 | -0.001426058 |
| O | -0.029406643 | 11.797385269 | 5.912412314 |
| O | 6.467209376 | 11.803667165 | 2.954795714 |
| O | -0.029494967 | 11.797032008 | 8.869710106 |
| O | 8.433460025 | 13.107281129 | 1.482930738 |
| O | 8.432733171 | 13.101069243 | 4.440206172 |
| O | 10.966458907 | 13.110751228 | 1.480899478 |
| O | 10.966634516 | 13.112162127 | 4.439191193 |
| O | 1.956638937 | 13.096402916 | 1.481396912 |
| O | 1.956926898 | 13.096889766 | 4.438191946 |
| O | 4.490955273 | 13.111901022 | 1.481200423 |
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| O | 4.492235189 | 13.106108476 | 7.396214302 |
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| O | -0.035460723 | 14.409015205 | 2.963444334 |
| O | -0.033549031 | 14.408295467 | 5.920597924 |
| O | -0.035201337 | 14.407870054 | 8.877900093 |
| O | -0.033043118 | 14.406895284 | 0.006045517 |
| O | 6.453158871 | 14.429524682 | 2.971798989 |
| O | 6.457510509 | 14.419258335 | 5.919479671 |
| O | 6.453858188 | 14.424051107 | 8.875504599 |
| O | 6.460674191 | 14.439334541 | 0.000216127 |
| O | 9.694196465 | 15.113148698 | 8.865006420 |
| O | 3.213436913 | 15.104121799 | 8.883051055 |
| O | 9.691727035 | 15.120240701 | 5.917800696 |
| O | 9.694186464 | 15.111891748 | 2.966577995 |
| O | 3.210172568 | 15.105193011 | 2.965134666 |
| O | 9.691487002 | 15.105268021 | -0.001504134 |
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| O | 9.682932578 | 17.738875485 | 2.957170387 |
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3-b:

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| Ti | 3.247200000 | 3.247194072 | 10.350900000 |
| Ti | 0.000000000 | 3.247194072 | 8.872200000 |
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| O | 9.667845307 | 17.722515123 | 0.000718648 |
| O | 6.472884572 | 18.525264418 | 0.009574168 |
| O | 6.506531669 | 18.558486993 | 5.901390912 |
| O | -0.030659543 | 18.508863336 | 0.003718753 |
| O | 6.474100844 | 18.540254242 | 2.986120258 |
| O | -0.047790601 | 18.507209905 | 5.921361643 |
| O | 6.486064567 | 18.519349713 | 8.885999347 |
| O | -0.026745888 | 18.512343079 | 8.874203343 |
| O | -0.057518823 | 18.504113070 | 2.964255490 |
| O | 1.970046755 | 19.942439002 | 4.440649073 |
| O | 4.462676058 | 19.916631686 | 1.488454570 |
| O | 4.406371038 | 19.942153965 | 4.449101913 |

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| O | 1.993789762 | 19.976162714 | 7.412785679 |
| O | 1.995776659 | 19.949341694 | 10.358965185 |
| O | 4.473048654 | 19.867652758 | 7.396402747 |
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| O | 10.880289000 | 19.952429242 | 4.440449626 |
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| O | 10.917250708 | 19.926504411 | 10.351946920 |
| O | 1.985166238 | 19.952194569 | 1.471559180 |
| O | 6.458053051 | 21.112188968 | 3.007589799 |
| O | 6.386597246 | 21.168168459 | 5.940887935 |
| O | -0.063467433 | 21.107034720 | 2.959797623 |
| O | -0.066884786 | 21.109875093 | 5.917953653 |
| O | -0.045043860 | 21.120383972 | 8.878082623 |
| O | -0.042356737 | 21.118399426 | 0.002602275 |
| O | 6.430863466 | 21.154007671 | 8.868034206 |
| O | 6.427659909 | 21.182018491 | 0.003969777 |
| H | 0.000000000 | 0.932897449 | 9.814799089 |

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| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
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| H | 0.000000000 | 0.932897449 | 3.899999089 |
| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 7.148767561 | 21.834041573 | -0.025548269 |
| H | 7.233670151 | 21.703145106 | 8.886907387 |
| H | 8.376683512 | 21.159107269 | 4.290105110 |
| H | 6.908519832 | 21.979003815 | 6.038376260 |

TS3-2:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |

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|----|-------------|-------------|--------------|
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |
| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |

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|----|--------------|-------------|--------------|
| Ti | 6.494400000 | 6.494389931 | 4.436100000 |
| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
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| Ti | 3.226213346 | 9.736728723 | 1.478748738 |
| Ti | 3.225438694 | 9.735083864 | 4.436172634 |
| Ti | -0.012487173 | 9.837287993 | 2.960119980 |
| Ti | -0.011633419 | 9.837240487 | 0.000703270 |
| Ti | 3.226241402 | 9.737102343 | 7.393702523 |
| Ti | 3.226809013 | 9.735985054 | 10.350977484 |
| Ti | -0.013403143 | 9.836770782 | 8.872522120 |
| Ti | -0.016781789 | 9.836547539 | 5.917606454 |
| Ti | 9.741712873 | 9.732797850 | 1.483691500 |
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| Ti | 6.485192629 | 9.785256878 | 2.959041712 |
| Ti | 6.482210920 | 9.766171873 | 0.007294486 |
| Ti | 9.732042062 | 9.744293644 | 7.390844728 |
| Ti | 9.739367875 | 9.732708552 | 10.345852901 |

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| Ti | 6.481857365 | 9.755551908 | 8.878474775 |
| Ti | 6.475638198 | 9.756485244 | 5.915385092 |
| Ti | -0.033720743 | 13.173236215 | 1.503346972 |
| Ti | -0.032264179 | 13.173883800 | 4.461169762 |
| Ti | 3.212466260 | 12.988969172 | 2.957935171 |
| Ti | 3.212162582 | 12.989124192 | 5.915822551 |
| Ti | 6.462314287 | 13.161154272 | 1.497760798 |
| Ti | 6.460147755 | 13.112710414 | 4.409027251 |
| Ti | 9.710263481 | 13.003721822 | 2.962161414 |
| Ti | 9.709622354 | 13.005875676 | 5.917827313 |
| Ti | -0.033160926 | 13.173380877 | 7.418235339 |
| Ti | -0.035046640 | 13.173749497 | 10.375019726 |
| Ti | 3.211673424 | 12.989736058 | 8.873659654 |
| Ti | 3.211699921 | 12.989468166 | 0.001262573 |
| Ti | 6.458850564 | 13.033143184 | 7.382856554 |
| Ti | 6.459890837 | 13.056126558 | 10.392294018 |
| Ti | 9.706619603 | 13.003449287 | 8.872763562 |
| Ti | 9.710340634 | 12.978673892 | 0.002670296 |
| Ti | 9.703262258 | 16.279919344 | 1.498740880 |
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| Ti | 3.187126151 | 16.302610537 | 1.487573856 |
| Ti | 3.183583845 | 16.302718051 | 4.445520502 |
| Ti | -0.049165076 | 16.639854088 | 2.957743650 |
| Ti | 6.452392143 | 16.362852730 | 5.912843857 |
| Ti | 3.194349092 | 16.306408178 | 7.400590899 |
| Ti | 3.180308200 | 16.301456100 | 10.359691640 |
| Ti | -0.047027249 | 16.641990440 | 8.872594399 |
| Ti | 6.446487954 | 16.446201884 | 0.002322150 |
| Ti | 9.697674996 | 16.352523874 | 7.358782727 |
| Ti | 9.706795341 | 16.276552474 | 10.340163928 |
| Ti | 6.446204798 | 16.291424783 | 8.877045286 |
| Ti | -0.048481475 | 16.639285442 | 0.002038358 |
| Ti | 6.436638547 | 19.680139217 | 7.377416003 |
| Ti | 6.429021265 | 19.706671628 | 10.371949590 |
| Ti | 3.212444179 | 19.550814742 | 8.879823941 |
| Ti | 3.199177419 | 19.542834409 | 0.007424612 |
| Ti | 6.442244513 | 19.904135760 | 1.570607593 |
| Ti | 6.454819490 | 19.896945531 | 4.395427824 |
| Ti | 3.200982992 | 19.549675307 | 2.965114082 |
| Ti | 3.205273712 | 19.547702548 | 5.904465543 |
| Ti | -0.032395236 | 20.007262868 | 1.481773922 |
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| Ti | 9.707511674 | 19.548513726 | 2.948581388 |
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| O | 6.494400000 | 1.266689833 | 0.000000000 |
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| O | 9.741600000 | 1.980499953 | 8.872200000 |
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| O | 3.247200000 | 8.474889884 | 0.000000000 |
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| O | 3.247200000 | 8.474889884 | 5.914800000 |
| O | 9.741600000 | 8.474889884 | 2.957400000 |
| O | 9.741600000 | 8.474889884 | 0.000000000 |
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| O | 1.269614935 | 9.784335329 | 1.479250550 |
| O | 1.268851193 | 9.784079581 | 4.436722119 |

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| O | 5.211547010 | 9.779205012 | 1.480754447 |
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| O | 7.759349488 | 9.785087927 | 1.479244990 |
| O | 7.757782389 | 9.784794675 | 4.438909057 |
| O | 11.700453527 | 9.777275473 | 1.478635529 |
| O | 11.699372339 | 9.777560154 | 4.435747005 |
| O | 7.756967602 | 9.783316623 | 7.393904336 |
| O | 7.758632376 | 9.782872279 | 10.352913753 |
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| O | 11.700344032 | 9.776706470 | 10.351597237 |
| O | 9.721924826 | 11.071647868 | 2.957014473 |
| O | 9.723428799 | 11.066625066 | 0.000065181 |
| O | 3.240806133 | 11.067882731 | 2.958502046 |
| O | 3.240494532 | 11.067328015 | 0.000277759 |
| O | 3.240852373 | 11.067439816 | 8.872438840 |
| O | 3.240792365 | 11.067398025 | 5.915655398 |
| O | 9.721619978 | 11.071352472 | 8.873976924 |
| O | 9.722366055 | 11.072243661 | 5.915885484 |

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| O | 6.466189625 | 11.800448885 | 8.875780820 |
| O | -0.028829681 | 11.792769663 | 2.956167356 |
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| O | 6.464243773 | 11.804472627 | 5.912111842 |
| O | -0.028907743 | 11.792526774 | -0.001398259 |
| O | -0.028681738 | 11.792900037 | 5.912640270 |
| O | 6.467719056 | 11.814634676 | 2.958313718 |
| O | -0.029151413 | 11.792488554 | 8.870669960 |
| O | 8.436364710 | 13.099938023 | 1.479101260 |
| O | 8.435237802 | 13.099105771 | 4.441712199 |
| O | 10.967558928 | 13.105364807 | 1.480858902 |
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| O | 1.956277978 | 13.091325821 | 1.481378576 |
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| O | 4.487424787 | 13.106709626 | 1.479050748 |
| O | 4.488510911 | 13.106357080 | 4.440809600 |
| O | 1.956165365 | 13.091720158 | 7.395281893 |
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| O | 4.489962669 | 13.104230729 | 7.395714028 |
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| O | 10.967762463 | 13.104286451 | 7.395122075 |
| O | 10.967029245 | 13.107047885 | 10.352163283 |
| O | -0.032632152 | 14.402747954 | 2.964003519 |
| O | -0.033856736 | 14.403841311 | 5.921140666 |
| O | -0.032902189 | 14.402063221 | 8.877891812 |
| O | -0.033474865 | 14.401884626 | 0.006940308 |
| O | 6.452614511 | 14.424878716 | 2.961795761 |
| O | 6.457100583 | 14.424985515 | 5.924199682 |
| O | 6.454335007 | 14.407064592 | 8.870942632 |
| O | 6.458181640 | 14.426559293 | -0.006406202 |
| O | 9.697108294 | 15.111076998 | 8.861613573 |
| O | 3.204952110 | 15.103064875 | 8.875390443 |
| O | 9.698303524 | 15.109695745 | 5.918858026 |
| O | 9.693800956 | 15.107684410 | 2.969837996 |
| O | 3.205592068 | 15.102623031 | 2.964332027 |
| O | 9.696466907 | 15.101207131 | 0.003319504 |
| O | 3.200021951 | 15.101082114 | 0.004775018 |
| O | 3.205371518 | 15.102200475 | 5.921263102 |
| O | 1.237293345 | 16.452694522 | 10.355856011 |
| O | 5.162300624 | 16.464004935 | 4.445103745 |
| O | 5.165374034 | 16.463019092 | 7.396444033 |
| O | 7.726543675 | 16.451752970 | 1.476943304 |

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| O | 3.196340016 | 17.729961458 | 8.876003335 |
| O | 3.196125960 | 17.721625006 | 0.002458782 |
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| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 0.816399334 | 0.932897449 | 2.486099272 |
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TS3-3:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |

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|----|-------------|-------------|--------------|
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 9.741600000 | 6.494389931 | 0.000000000 |

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|----|--------------|--------------|--------------|
| Ti | 6.494400000 | 6.494389931 | 10.350900000 |
| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
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| Ti | 3.225561179 | 9.734088733 | 4.436125907 |
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| Ti | -0.013014388 | 9.836296077 | 0.002614696 |
| Ti | 3.225775494 | 9.735469272 | 7.393866599 |
| Ti | 3.226097097 | 9.735605718 | 10.351182373 |
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| Ti | 9.731137911 | 9.750283359 | 7.391467556 |
| Ti | 9.738381245 | 9.730612206 | 10.344470376 |
| Ti | 6.481191430 | 9.759743886 | 8.879223707 |
| Ti | 6.476040721 | 9.764891705 | 5.916956891 |
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| Ti | 3.202061712 | 19.549212389 | 8.879255647 |
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| Ti | 3.199351859 | 19.548266550 | 2.965311045 |
| Ti | 3.172831586 | 19.546727777 | 5.920858648 |
| Ti | -0.059065399 | 19.987214165 | 1.479401022 |
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| O | 7.757133598 | 9.783978139 | 7.395484179 |
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| O | 3.243960853 | 11.066028559 | 8.873361075 |
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| O | 6.465284436 | 11.800496748 | 8.877739802 |
| O | -0.026629378 | 11.790516867 | 2.958102678 |
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| O | 10.973199964 | 13.103083436 | 4.442767991 |
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| O | -0.026367264 | 14.398908521 | 8.879771062 |
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| O | 6.468384603 | 14.417957093 | 0.001361705 |
| O | 9.690070833 | 15.097723459 | 8.858120410 |
| O | 3.192060855 | 15.098625721 | 8.880270626 |
| O | 9.683732168 | 15.108382716 | 5.921883446 |
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| O | 3.189500763 | 15.100451675 | 5.922392592 |
| O | 1.237850824 | 16.461074551 | 10.353174004 |
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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
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| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
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| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
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| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
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| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
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| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
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| O | 11.658934049 | 16.453539990 | 7.401914276 |
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| H | 0.816399984 | 0.932899949 | 8.400899982 |
| H | 6.457700016 | 0.932899949 | 6.856699960 |
| H | 0.834099951 | 0.932899949 | -0.439200043 |
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| H | 0.834099951 | 0.932899949 | 5.475599957 |
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| H | 7.310799984 | 0.932899949 | 8.400899982 |
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TS4-2:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |

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|----|-------------|-------------|--------------|
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
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| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
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| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | -0.012616021 | 9.836991526 | 8.872383950 |
| Ti | -0.018344732 | 9.836087478 | 5.916658194 |
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| Ti | 6.487143157 | 9.752632596 | 0.005401987 |
| Ti | 9.732189744 | 9.737108773 | 7.394843251 |
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| Ti | 6.478115162 | 9.739473726 | 5.919250177 |
| Ti | -0.033696844 | 13.176443422 | 1.505437499 |
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| Ti | 9.707596231 | 12.995332507 | 5.916417698 |
| Ti | -0.034937924 | 13.175971574 | 7.420068808 |
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| O | 6.464732801 | 11.795481804 | 8.877892285 |
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| O | 6.467678272 | 11.803577153 | 0.005926630 |
| O | 6.464251566 | 11.791984560 | 5.916111548 |
| O | -0.029111538 | 11.798205376 | -0.000756503 |
| O | -0.031499529 | 11.797981775 | 5.912407227 |
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TS5-1:

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| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |

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| Ti | -0.012052697 | 9.801097172 | -0.002297072 |
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5-b:

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| H | 0.834099172 | 0.932897449 | 5.475598892 |
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| H | 7.310799334 | 0.932897449 | 8.400899272 |
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TS5-2:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
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| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
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| O | -0.015145330 | 11.802054096 | 2.952752387 |
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| O | 3.210203741 | 15.100303798 | 2.974840379 |
| O | 9.690616102 | 15.100119845 | 0.006412944 |
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| H | 0.816399334 | 0.932897449 | 8.400899272 |
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| H | 0.834099172 | 0.932897449 | 5.475598892 |
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TS5-3:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |

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| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
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| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
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| Ti | 9.741600000 | 6.494389931 | 0.000000000 |

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|----|--------------|--------------|--------------|
| Ti | 6.494400000 | 6.494389931 | 10.350900000 |
| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
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| Ti | 3.228304673 | 9.733974790 | 1.486625122 |
| Ti | 3.228687193 | 9.752676887 | 4.439949470 |
| Ti | -0.016473565 | 9.827427770 | 2.963964245 |
| Ti | -0.005018872 | 9.822218872 | 0.002962842 |
| Ti | 3.229445739 | 9.751737478 | 7.390404194 |
| Ti | 3.231255339 | 9.734275901 | 10.343210050 |
| Ti | -0.012672523 | 9.833030292 | 8.874925303 |
| Ti | -0.011293112 | 9.822559274 | 5.919083498 |
| Ti | 9.740928479 | 9.739360140 | 1.481061780 |
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| Ti | 6.482576945 | 9.764674534 | 2.964181791 |
| Ti | 6.483810101 | 9.767149501 | 0.010794392 |
| Ti | 9.736530991 | 9.739103677 | 7.395824398 |
| Ti | 9.742002393 | 9.738001033 | 10.354512996 |
| Ti | 6.486847662 | 9.763970513 | 8.887461958 |
| Ti | 6.478079443 | 9.735767168 | 5.926860159 |
| Ti | -0.025972015 | 13.158088870 | 1.494720118 |
| Ti | -0.029887748 | 13.160966390 | 4.456612290 |

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| Ti | 3.218945853 | 13.014842925 | 2.965640144 |
| Ti | 3.218379801 | 13.020726912 | 5.919294775 |
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| Ti | 9.711125028 | 12.994973531 | 2.962118236 |
| Ti | 9.714524976 | 12.997760326 | 5.922326820 |
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| Ti | -0.026736536 | 13.164950842 | 10.374033374 |
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| Ti | 3.214423023 | 12.978426359 | 0.003113314 |
| Ti | 6.469397209 | 13.014967941 | 7.423161539 |
| Ti | 6.465115062 | 13.136938951 | 10.404051812 |
| Ti | 9.714378722 | 12.994497754 | 8.881009858 |
| Ti | 9.714448342 | 12.997531010 | 0.007556512 |
| Ti | 9.702463706 | 16.314100617 | 1.478926182 |
| Ti | 9.696193883 | 16.314345292 | 4.436270110 |
| Ti | 6.439916400 | 16.337950533 | 2.938468381 |
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| Ti | 6.431160650 | 20.122920906 | 10.380000225 |
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| Ti | 3.193848244 | 19.527179140 | 0.006012039 |
| Ti | 6.429855406 | 20.121433925 | 1.460265816 |
| Ti | 6.418306544 | 19.604813258 | 4.238263307 |
| Ti | 3.213845281 | 19.535090535 | 2.958733551 |
| Ti | 3.141700290 | 19.728178736 | 5.921662824 |
| Ti | -0.050958569 | 19.971141698 | 1.468650991 |
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| O | 6.468481629 | 11.792587853 | 8.871509506 |
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| O | 10.972494413 | 13.112212848 | 1.482780266 |
| O | 10.971577403 | 13.116240163 | 4.440861532 |
| O | 1.960556619 | 13.092093422 | 1.483962516 |
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| O | 10.973224383 | 13.111687065 | 10.354993515 |
| O | -0.025904733 | 14.403987402 | 2.961559642 |
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| H | 7.310799984 | 0.932899949 | 8.400899982 |
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TS6-1:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
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| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
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| Ti | -0.014220398 | 9.763374720 | 2.959580550 |
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| Ti | 3.234445388 | 9.740069518 | 7.393120270 |
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| Ti | -0.011942292 | 9.763716551 | 8.880202133 |
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| Ti | 9.728005662 | 9.743662847 | 1.480283510 |
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| Ti | -0.027358959 | 13.139103878 | 1.431884831 |
| Ti | -0.025794458 | 13.020641900 | 4.410937376 |
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| O | 3.206055898 | 17.753303093 | 0.009958276 |
| O | 9.718492925 | 17.738474361 | 2.954829783 |
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| H | 6.457700016 | 0.932899949 | 0.941899960 |
| H | 0.834099951 | 0.932899949 | 5.475599957 |
| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
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TS6-2:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |

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|----|--------------|-------------|--------------|
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
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| Ti | 3.234624763 | 9.746617878 | 4.437142779 |
| Ti | -0.014254688 | 9.761698786 | 2.953720285 |
| Ti | -0.004728573 | 9.773211368 | 0.001461429 |
| Ti | 3.234330957 | 9.742695577 | 7.392389910 |
| Ti | 3.242641970 | 9.741287893 | 10.351733277 |

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| Ti | -0.012439634 | 9.763093969 | 8.879007462 |
| Ti | -0.012333255 | 9.738007462 | 5.916158866 |
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| Ti | 9.727303747 | 9.741637939 | 4.436673262 |
| Ti | 6.483173780 | 9.808928199 | 2.961829475 |
| Ti | 6.484675935 | 9.762124199 | 0.000485487 |
| Ti | 9.728054110 | 9.741872255 | 7.393506506 |
| Ti | 9.728534956 | 9.740600660 | 10.351090457 |
| Ti | 6.483962330 | 9.836435381 | 8.873147314 |
| Ti | 6.478581850 | 9.751691044 | 5.919703842 |
| Ti | -0.023789117 | 13.144918927 | 1.430060589 |
| Ti | -0.023806003 | 13.017232881 | 4.407385184 |
| Ti | 3.222235007 | 13.005137365 | 2.966301892 |
| Ti | 3.221151221 | 13.010284112 | 5.923100712 |
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| Ti | 6.469895590 | 13.095594596 | 4.477768583 |
| Ti | 9.716178710 | 12.998490421 | 2.966558240 |
| Ti | 9.720327723 | 13.002819918 | 5.924613718 |
| Ti | -0.022510889 | 13.017979765 | 7.425697924 |
| Ti | -0.024305032 | 13.145293262 | 10.403052093 |
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| Ti | 6.471454765 | 13.162045818 | 10.400249306 |
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| Ti | 9.710685877 | 16.317389263 | 4.432607429 |
| Ti | 6.459853689 | 16.339237130 | 2.943993514 |
| Ti | -0.036463718 | 16.281403111 | 5.918201128 |
| Ti | 3.215412640 | 16.339627896 | 1.482595724 |
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| Ti | 3.215277556 | 19.627125830 | 2.962214056 |
| Ti | 3.108912663 | 19.556046143 | 5.977032332 |
| Ti | -0.035445136 | 20.133692320 | 1.466394613 |
| Ti | -0.029824493 | 19.614239853 | 4.238256683 |
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| Ti | 9.762148931 | 19.551712360 | 5.936624902 |
| Ti | -0.059646388 | 19.615244627 | 7.620611167 |
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| O | 7.762277293 | 9.788732334 | 10.353060440 |
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| O | -0.019840912 | 11.803607871 | 0.002129565 |
| O | -0.020801953 | 11.801531527 | 5.916888043 |
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| O | -0.020082503 | 11.798817957 | 8.873350665 |
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| O | 10.990035657 | 13.109172806 | 10.352679645 |
| O | -0.019740898 | 14.420458135 | 2.968701645 |
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| O | 6.473256442 | 14.441913451 | 8.876843946 |
| O | 6.476212043 | 14.388865060 | 0.010662018 |
| O | 9.717068703 | 15.118531548 | 8.880203434 |
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7-Ba:

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| O | 5.157599328 | 16.469361353 | 4.463075273 |
| O | 5.157813384 | 16.469633531 | 7.404053186 |
| O | 7.711844510 | 16.452854543 | 1.495799214 |
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| O | 9.656723258 | 17.747205507 | 2.980174109 |
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| O | 9.657184880 | 17.747069060 | 8.890434382 |
| O | 9.644628737 | 17.752236167 | 0.019882600 |
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| O | 10.879327569 | 19.935714191 | 10.378565767 |
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| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
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TS7-B1:

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| Ti | 3.247200000 | 3.247194072 | 4.436100000 |
| Ti | 0.000000000 | 3.247194072 | 2.957400000 |
| Ti | 0.000000000 | 3.247194072 | 0.000000000 |
| Ti | 3.247200000 | 3.247194072 | 7.393500000 |
| Ti | 3.247200000 | 3.247194072 | 10.350900000 |
| Ti | 0.000000000 | 3.247194072 | 8.872200000 |
| Ti | 0.000000000 | 3.247194072 | 5.914800000 |
| Ti | 9.741600000 | 3.247194072 | 1.478700000 |
| Ti | 9.741600000 | 3.247194072 | 4.436100000 |
| Ti | 6.494400000 | 3.247194072 | 2.957400000 |
| Ti | 6.494400000 | 3.247194072 | 0.000000000 |
| Ti | 9.741600000 | 3.247194072 | 7.393500000 |
| Ti | 9.741600000 | 3.247194072 | 10.350900000 |
| Ti | 6.494400000 | 3.247194072 | 8.872200000 |
| Ti | 6.494400000 | 3.247194072 | 5.914800000 |
| Ti | 0.000000000 | 6.494391717 | 4.436100000 |
| Ti | 0.000000000 | 6.494391717 | 1.478700000 |
| Ti | 3.247200000 | 6.494391717 | 2.957400000 |
| Ti | 3.247200000 | 6.494391717 | 0.000000000 |

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| Ti | 0.000000000 | 6.494391717 | 10.350900000 |
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| Ti | 3.247200000 | 6.494391717 | 8.872200000 |
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| Ti | 9.741600000 | 6.494391717 | 0.000000000 |
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| Ti | 6.494400000 | 6.494391717 | 7.393500000 |
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| Ti | 3.219839742 | 9.736245802 | 1.480367974 |
| Ti | 3.224882774 | 9.738206774 | 4.437306619 |
| Ti | -0.020356567 | 9.834040781 | 2.965290343 |
| Ti | -0.019018591 | 9.836169632 | 0.006056755 |
| Ti | 3.225257111 | 9.735595717 | 7.393925866 |
| Ti | 3.223442056 | 9.736970897 | 10.352485166 |
| Ti | -0.015996487 | 9.836980453 | 8.877345876 |
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| Ti | 9.729126206 | 9.738942585 | 4.436395740 |

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| Ti | 6.475495191 | 9.753155165 | 2.963977258 |
| Ti | 6.476671717 | 9.752412210 | 0.011498371 |
| Ti | 9.733656829 | 9.738528245 | 7.392470825 |
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| Ti | 6.480061794 | 9.753748099 | 8.887211762 |
| Ti | 6.478095159 | 9.728080445 | 5.927848049 |
| Ti | -0.041376991 | 13.173336228 | 1.524788122 |
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| Ti | 3.211272330 | 12.991040872 | 2.973440938 |
| Ti | 3.201595934 | 12.992480347 | 5.930545198 |
| Ti | 6.455567125 | 13.116703795 | 1.464977664 |
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| Ti | 9.702503842 | 12.995795068 | 2.974008758 |
| Ti | 9.701974029 | 12.997863196 | 5.931527054 |
| Ti | -0.043914353 | 13.176908126 | 7.437092076 |
| Ti | -0.042278934 | 13.177383188 | 10.394551224 |
| Ti | 3.207053568 | 12.989612113 | 8.887980686 |
| Ti | 3.196187397 | 12.992083866 | 0.016289359 |
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| Ti | -0.061169455 | 16.634540534 | 5.945261220 |
| Ti | 3.162826574 | 16.304422203 | 1.504843416 |
| Ti | 3.176607950 | 16.311883897 | 4.463958708 |
| Ti | -0.067527602 | 16.627339588 | 2.991753158 |
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| Ti | -0.064843467 | 16.629154112 | 0.028698610 |
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| Ti | 6.430709419 | 19.960359212 | 10.551825756 |
| Ti | 3.162589788 | 19.558920806 | 2.972033215 |
| Ti | 3.150518776 | 19.555634660 | 5.962686221 |
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| Ti | 9.638665059 | 19.604269615 | 5.967642823 |
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| O | -0.037999514 | 11.798716515 | 5.926795214 |
| O | 6.458490254 | 11.789601033 | 2.968756416 |
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| O | -0.044228812 | 14.410102133 | 2.981603362 |
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| O | 6.442783678 | 14.404247793 | 8.888867906 |
| O | 6.457883807 | 14.417013755 | 0.025516447 |
| O | 9.677393504 | 15.119563112 | 8.892097387 |
| O | 3.199826859 | 15.108100893 | 8.900957758 |
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7-Bb:

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TS7-B2:

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| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |

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| O | 3.207242035 | 17.744627311 | 0.012303257 |
| O | 9.670158872 | 17.734758516 | 2.961524508 |
| O | 9.678817986 | 17.692229719 | 5.937160547 |
| O | 3.209073196 | 17.747576984 | 2.968044156 |
| O | 3.198102726 | 17.745407771 | 5.932401262 |
| O | 9.663103616 | 17.728899175 | 8.899063720 |
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| O | 4.426060630 | 19.984378793 | 1.490911696 |
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| O | 10.893259486 | 19.939253227 | 7.444561285 |
| O | 10.892284676 | 19.914692146 | 10.362514538 |
| O | 1.965560943 | 19.919210596 | 1.498290409 |

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| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
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| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 7.328499172 | 0.932897449 | 5.475598892 |
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TS7-B3:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |

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| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
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| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 3.226121516 | 9.737942453 | 4.436065103 |
| Ti | -0.014061415 | 9.837998086 | 2.961514217 |
| Ti | -0.011576008 | 9.838443859 | 0.002350896 |
| Ti | 3.226471434 | 9.738095688 | 7.393638761 |
| Ti | 3.226371290 | 9.738220347 | 10.351233358 |
| Ti | -0.012120369 | 9.839614370 | 8.873007370 |
| Ti | -0.015315094 | 9.839012148 | 5.917259847 |

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| Ti | 9.740709748 | 9.734112308 | 1.487275869 |
| Ti | 9.734327181 | 9.748623498 | 4.440283656 |
| Ti | 6.481299626 | 9.758236903 | 2.963684238 |
| Ti | 6.482638382 | 9.763063608 | 0.010225861 |
| Ti | 9.735771796 | 9.749555764 | 7.391317675 |
| Ti | 9.742543636 | 9.732527814 | 10.345781214 |
| Ti | 6.483839196 | 9.757228914 | 8.888613688 |
| Ti | 6.478215306 | 9.732647116 | 5.927144661 |
| Ti | -0.034438634 | 13.176440564 | 1.511741374 |
| Ti | -0.032983499 | 13.178432969 | 4.468081324 |
| Ti | 3.211138285 | 12.994000546 | 2.957371964 |
| Ti | 3.210914878 | 12.995871863 | 5.914908714 |
| Ti | 6.460249457 | 13.128868249 | 1.432602770 |
| Ti | 6.458024736 | 13.006288588 | 4.413165481 |
| Ti | 9.706984978 | 13.013210925 | 2.962241027 |
| Ti | 9.708917971 | 13.016785680 | 5.916439819 |
| Ti | -0.033481749 | 13.179784575 | 7.424141740 |
| Ti | -0.035446565 | 13.177184590 | 10.382034561 |
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| Ti | 6.461393641 | 13.136063122 | 10.397975183 |

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| Ti | 9.706940167 | 13.011168871 | 8.872442743 |
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| Ti | 9.696328317 | 16.366834681 | 7.371119698 |
| Ti | 9.702514493 | 16.283730559 | 10.343780355 |
| Ti | 6.434501240 | 16.330556705 | 8.893462996 |
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| Ti | 6.410877989 | 19.556240811 | 7.592838815 |
| Ti | 9.652884807 | 19.562815960 | 2.915822505 |
| Ti | 3.176038911 | 19.564477607 | 0.011345769 |
| Ti | -0.013786962 | 20.027104401 | 4.433526471 |
| Ti | -0.078174911 | 20.003320922 | 1.487405639 |
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| Ti | 9.805505675 | 19.667336465 | 5.803645648 |
| Ti | -0.089886652 | 20.023798610 | 7.409126902 |
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| O | 0.000000000 | 1.266689833 | 5.914800000 |
| O | 6.494400000 | 1.266689833 | 2.957400000 |
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| O | 7.757115934 | 9.781747132 | 4.441849540 |
| O | 11.700482102 | 9.777359770 | 1.478926655 |
| O | 11.699785253 | 9.777935560 | 4.436808711 |
| O | 7.757715107 | 9.781452807 | 7.396187567 |
| O | 7.758944627 | 9.782095392 | 10.356786646 |
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| O | 11.700923332 | 9.777640521 | 10.351976020 |
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| O | 6.463550431 | 11.793787654 | 8.881100946 |
| O | -0.030365347 | 11.795024959 | 2.956067277 |
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| O | -0.030910097 | 11.794687057 | -0.001756814 |
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| O | -0.029936976 | 11.795216770 | 8.869908488 |
| O | 8.434096866 | 13.096550792 | 1.486206236 |
| O | 8.428554025 | 13.093600048 | 4.440846864 |
| O | 10.965641652 | 13.113534807 | 1.482973088 |
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| O | 1.956255118 | 13.093665414 | 1.482197066 |
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| O | -0.031036867 | 14.405908726 | 8.880827682 |
| O | -0.031013877 | 14.405075045 | 0.008683518 |
| O | 6.455713768 | 14.411631620 | 2.971483139 |
| O | 6.460169446 | 14.405305789 | 5.915938362 |
| O | 6.452441240 | 14.406638107 | 8.867146631 |
| O | 6.463886062 | 14.405831215 | 0.004909875 |
| O | 9.680767345 | 15.112348236 | 8.867772536 |
| O | 3.201836486 | 15.113598043 | 8.874667418 |
| O | 9.679458723 | 15.117802881 | 5.918570212 |
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TS7-B4:

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| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |

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| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
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| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
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| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
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| Ti | 3.226478058 | 9.738418230 | 4.436030679 |
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| Ti | -0.010267646 | 9.838034520 | 0.001910480 |
| Ti | 3.226623013 | 9.737931023 | 7.393426538 |
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| Ti | -0.012975941 | 9.839653661 | 8.872004693 |
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| Ti | 6.481545764 | 9.759023792 | 0.009923851 |
| Ti | 9.735035331 | 9.749096417 | 7.394782329 |
| Ti | 9.742629622 | 9.743831084 | 10.347885345 |
| Ti | 6.485438767 | 9.764911350 | 8.887046976 |
| Ti | 6.476634829 | 9.733004305 | 5.925877711 |
| Ti | -0.035920267 | 13.176303046 | 1.508095373 |
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| Ti | 9.707006669 | 12.984241408 | 2.959761898 |
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| O | 7.712492262 | 16.453707512 | 10.377257768 |
| O | 1.243111158 | 16.471697731 | 7.399561014 |
| O | 11.666465864 | 16.458791037 | 7.394394081 |
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| O | 3.222282026 | 17.748952164 | 8.875930346 |
| O | 3.226370641 | 17.747290161 | 0.004390911 |
| O | 9.684044029 | 17.729174211 | 2.961850296 |
| O | 9.692920445 | 17.728492336 | 5.912085580 |
| O | 3.223686245 | 17.743898644 | 2.960890797 |
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| O | 6.398617991 | 18.435775529 | 8.972325734 |
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| H | 0.000000000 | 0.932897449 | 9.814799089 |
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| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
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TS7-B5:

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| Ti | 3.247200000 | 3.247194072 | 1.478700000 |
| Ti | 3.247200000 | 3.247194072 | 4.436100000 |
| Ti | 0.000000000 | 3.247194072 | 2.957400000 |
| Ti | 0.000000000 | 3.247194072 | 0.000000000 |
| Ti | 3.247200000 | 3.247194072 | 7.393500000 |
| Ti | 3.247200000 | 3.247194072 | 10.350900000 |
| Ti | 0.000000000 | 3.247194072 | 8.872200000 |
| Ti | 0.000000000 | 3.247194072 | 5.914800000 |
| Ti | 9.741600000 | 3.247194072 | 1.478700000 |
| Ti | 9.741600000 | 3.247194072 | 4.436100000 |
| Ti | 6.494400000 | 3.247194072 | 2.957400000 |
| Ti | 6.494400000 | 3.247194072 | 0.000000000 |
| Ti | 9.741600000 | 3.247194072 | 7.393500000 |
| Ti | 9.741600000 | 3.247194072 | 10.350900000 |
| Ti | 6.494400000 | 3.247194072 | 8.872200000 |
| Ti | 6.494400000 | 3.247194072 | 5.914800000 |

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|----|--------------|-------------|--------------|
| Ti | 0.000000000 | 6.494391717 | 4.436100000 |
| Ti | 0.000000000 | 6.494391717 | 1.478700000 |
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| Ti | 6.494400000 | 6.494391717 | 7.393500000 |
| Ti | 9.741600000 | 6.494391717 | 8.872200000 |
| Ti | 9.741600000 | 6.494391717 | 5.914800000 |
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| Ti | 3.240980573 | 9.751126327 | 4.436230126 |
| Ti | -0.013106089 | 9.729884253 | 2.972222489 |
| Ti | -0.016597998 | 9.762681415 | 0.010658470 |
| Ti | 3.242469869 | 9.746072092 | 7.382912508 |
| Ti | 3.240936281 | 9.731670202 | 10.338727342 |

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| Ti | -0.014800738 | 9.753248034 | 8.885886847 |
| Ti | -0.014664745 | 9.767346313 | 5.931917431 |
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| Ti | 6.478096848 | 9.833040650 | 0.016147404 |
| Ti | 9.718505654 | 9.734734890 | 7.391169569 |
| Ti | 9.717539157 | 9.736842309 | 10.349066412 |
| Ti | 6.478334153 | 9.836737564 | 8.887140785 |
| Ti | 6.479886315 | 9.834655148 | 5.928676121 |
| Ti | -0.027595355 | 13.013815290 | 1.490363986 |
| Ti | -0.034640610 | 13.019023116 | 4.484033539 |
| Ti | 3.224371015 | 13.006278587 | 2.994012612 |
| Ti | 3.208160863 | 13.014476091 | 5.945627938 |
| Ti | 6.463370796 | 13.169110674 | 1.511065786 |
| Ti | 6.465612403 | 13.168028389 | 4.469956315 |
| Ti | 9.705850276 | 12.996523735 | 2.984217703 |
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| Ti | -0.038825861 | 13.119321996 | 7.474899478 |
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| Ti | 6.462609652 | 13.173493392 | 7.424883929 |
| Ti | 6.460022283 | 13.168971370 | 10.384058369 |
| Ti | 9.697982051 | 12.992305324 | 8.903288189 |
| Ti | 9.716653321 | 12.994048410 | 0.029349238 |
| Ti | 9.692429209 | 16.321899497 | 1.498242499 |
| Ti | 9.691757039 | 16.313001901 | 4.459510778 |
| Ti | 6.444532100 | 16.620452970 | 2.984714546 |
| Ti | -0.053661279 | 16.308579892 | 5.965951190 |
| Ti | 3.210085413 | 16.254397780 | 1.526113037 |
| Ti | 3.202101717 | 16.372138234 | 4.508059457 |
| Ti | -0.046070105 | 16.295513891 | 2.978563154 |
| Ti | 6.446247661 | 16.636840836 | 5.935844858 |
| Ti | 3.203216936 | 16.364240769 | 7.381173557 |
| Ti | 3.212240515 | 16.260398568 | 10.356601867 |
| Ti | -0.065658904 | 16.683029041 | 8.902164377 |
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| Ti | -0.040726642 | 16.306376031 | 0.000189274 |
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| Ti | 3.201321220 | 19.523126822 | 8.904388342 |
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| Ti | 6.428973466 | 19.993992198 | 10.368100238 |
| Ti | 3.136923529 | 19.721631448 | 5.939275442 |
| Ti | -0.048482385 | 19.556981266 | 1.303598261 |
| Ti | -0.071686226 | 19.508582056 | 4.636800994 |
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| Ti | -0.076169570 | 20.002414732 | 7.506945864 |
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| O | -0.035989757 | 11.788647336 | 0.024167873 |
| O | -0.038232403 | 11.787064985 | 5.931053870 |
| O | 6.469066255 | 11.791104801 | 2.974694875 |
| O | -0.036333310 | 11.790361847 | 8.895386016 |
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| O | 6.463074521 | 14.399311431 | 2.982017398 |
| O | 6.462679402 | 14.398664918 | 5.938802258 |
| O | 6.459726658 | 14.399854359 | 8.894912832 |
| O | 6.467011946 | 14.397271878 | 0.022984913 |
| O | 9.680874373 | 15.109604662 | 8.895563460 |
| O | 3.199169496 | 15.095259922 | 8.878611643 |
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| O | 7.731283548 | 16.473322944 | 7.420152089 |
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| O | 11.655256270 | 16.407671470 | 7.434891770 |
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| O | 3.190550907 | 17.698119421 | 0.024593738 |

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| O | 9.715520438 | 17.746693654 | 5.936826715 |
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| O | 4.401992514 | 19.922582825 | 1.481716548 |
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| O | 6.435883118 | 21.102673433 | 8.890961746 |
| O | 6.450346536 | 21.102694865 | 0.021541702 |
| H | 0.000000000 | 0.932897449 | 9.814799089 |
| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
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| H | 6.457698847 | 0.932897449 | 0.941899960 |

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| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 1.368383978 | 21.345794630 | 5.858585741 |

TS7-E2:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |

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|----|-------------|-------------|--------------|
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 3.225486363 | 9.734473070 | 1.478908083 |
| Ti | 3.225377127 | 9.736863740 | 4.437600940 |
| Ti | -0.014798659 | 9.838601737 | 2.962520087 |
| Ti | -0.010387273 | 9.838967142 | 0.002434768 |
| Ti | 3.228077499 | 9.738705411 | 7.393877719 |
| Ti | 3.229496266 | 9.737530614 | 10.350208205 |
| Ti | -0.011353250 | 9.839072513 | 8.874235756 |
| Ti | -0.015709304 | 9.839167168 | 5.918953491 |
| Ti | 9.741635459 | 9.737932452 | 1.482686575 |
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| Ti | 6.481213251 | 9.776295345 | 2.961565794 |
| Ti | 6.484228601 | 9.784764671 | 0.011954402 |
| Ti | 9.735404213 | 9.737543473 | 7.395513161 |
| Ti | 9.741929916 | 9.735593931 | 10.355462440 |
| Ti | 6.484682559 | 9.759725313 | 8.885477306 |
| Ti | 6.477386101 | 9.748534558 | 5.921841569 |
| Ti | -0.036044440 | 13.176930271 | 1.510044891 |
| Ti | -0.035553463 | 13.178500120 | 4.466813309 |
| Ti | 3.210600029 | 12.989559606 | 2.957873539 |
| Ti | 3.210153475 | 12.995176058 | 5.915403191 |
| Ti | 6.458870566 | 13.189027931 | 1.469556074 |
| Ti | 6.457019403 | 13.059441636 | 4.398857225 |

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| Ti | 9.706713122 | 12.995385371 | 2.958793882 |
| Ti | 9.705884047 | 12.995440021 | 5.915607607 |
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| Ti | -0.035748035 | 13.178456186 | 10.381397655 |
| Ti | 3.209826806 | 12.994382739 | 8.873277795 |
| Ti | 3.209268548 | 12.990148255 | 0.001675545 |
| Ti | 6.456987710 | 13.015644816 | 7.410554616 |
| Ti | 6.456661951 | 13.106321718 | 10.408834401 |
| Ti | 9.705770655 | 12.989949658 | 8.874574910 |
| Ti | 9.707772359 | 12.995716843 | 0.002256141 |
| Ti | 9.696055552 | 16.325195287 | 1.493441338 |
| Ti | 9.698063621 | 16.321185832 | 4.446798809 |
| Ti | 6.449403420 | 16.471974910 | 2.951744387 |
| Ti | -0.057334512 | 16.650052927 | 5.924854214 |
| Ti | 3.178528994 | 16.309709683 | 1.484327104 |
| Ti | 3.177950213 | 16.314105617 | 4.444218536 |
| Ti | -0.052005597 | 16.651787083 | 2.963959158 |
| Ti | 6.440481933 | 16.295414235 | 5.919082670 |
| Ti | 3.182139361 | 16.312249659 | 7.402597672 |
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| Ti | 9.698525892 | 16.311549210 | 10.361584022 |
| Ti | 6.435582038 | 16.316710959 | 8.891854880 |
| Ti | -0.055714029 | 16.646619619 | 0.006287787 |
| Ti | 6.234475148 | 19.652342354 | 4.332990249 |
| Ti | 6.447490949 | 19.969376109 | 10.505737871 |
| Ti | 3.123632610 | 19.561273615 | 2.950375465 |
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| Ti | 6.434997931 | 19.569911891 | 7.512527069 |
| Ti | 9.604482694 | 19.588100350 | 3.010925273 |
| Ti | 3.203682974 | 19.560620315 | 0.012569778 |
| Ti | -0.088409306 | 20.020862153 | 4.453291603 |
| Ti | -0.095860591 | 20.011199456 | 1.499389970 |
| Ti | 9.663731884 | 19.560225620 | 8.885931800 |
| Ti | 9.734892454 | 19.538103788 | 5.943705982 |
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| O | 0.000000000 | 1.266689833 | 8.872200000 |
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| O | 5.210652731 | 9.773178507 | 7.397382830 |
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| O | 3.242096051 | 11.069532948 | 0.002273886 |
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| O | 3.241279575 | 11.070314122 | 5.916151295 |
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| O | -0.031609024 | 11.794041615 | 2.958457330 |
| O | 6.463479382 | 11.808699254 | 0.009984774 |
| O | 6.462963077 | 11.798947974 | 5.916337966 |
| O | -0.031195721 | 11.793738004 | 0.001658747 |
| O | -0.031895687 | 11.794319152 | 5.914948935 |
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| O | 10.964813616 | 13.110281166 | 10.354820921 |
| O | -0.034405902 | 14.405253997 | 2.967226730 |
| O | -0.037009767 | 14.405324006 | 5.925012257 |
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| O | -0.036068079 | 14.405441521 | 0.011361739 |
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| O | 7.720941736 | 16.452167310 | 4.451537155 |
| O | 5.159688317 | 16.450211696 | 10.364427148 |
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7-Ec:

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| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
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TS7-E3:

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| Ti | 0.000000000 | 3.247194072 | 0.000000000 |
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| Ti | 3.247200000 | 3.247194072 | 10.350900000 |
| Ti | 0.000000000 | 3.247194072 | 8.872200000 |
| Ti | 0.000000000 | 3.247194072 | 5.914800000 |
| Ti | 9.741600000 | 3.247194072 | 1.478700000 |
| Ti | 9.741600000 | 3.247194072 | 4.436100000 |
| Ti | 6.494400000 | 3.247194072 | 2.957400000 |
| Ti | 6.494400000 | 3.247194072 | 0.000000000 |
| Ti | 9.741600000 | 3.247194072 | 7.393500000 |
| Ti | 9.741600000 | 3.247194072 | 10.350900000 |
| Ti | 6.494400000 | 3.247194072 | 8.872200000 |
| Ti | 6.494400000 | 3.247194072 | 5.914800000 |
| Ti | 0.000000000 | 6.494391717 | 4.436100000 |
| Ti | 0.000000000 | 6.494391717 | 1.478700000 |
| Ti | 3.247200000 | 6.494391717 | 2.957400000 |
| Ti | 3.247200000 | 6.494391717 | 0.000000000 |

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| Ti | 0.000000000 | 6.494391717 | 10.350900000 |
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| Ti | 3.225575337 | 9.736652999 | 4.437058198 |
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| Ti | -0.015589807 | 9.837048319 | 0.010906891 |
| Ti | 3.225522212 | 9.736017201 | 7.393618296 |
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| Ti | -0.016073380 | 9.835301661 | 8.881486236 |
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| Ti | 6.480244936 | 9.739635533 | 5.931515225 |
| Ti | -0.033212491 | 13.174322072 | 1.514874917 |
| Ti | -0.034212889 | 13.172286090 | 4.470914513 |
| Ti | 3.216220153 | 12.990740833 | 2.970519026 |
| Ti | 3.208988379 | 12.991794543 | 5.928628802 |
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| Ti | -0.032367960 | 13.174439944 | 7.429674917 |
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| Ti | 6.460773426 | 13.037271940 | 7.449051802 |
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| Ti | 9.688662717 | 16.311273103 | 1.509823678 |
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| Ti | -0.060568853 | 16.631525852 | 5.952169706 |
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| O | 6.461676797 | 11.800448885 | 5.938163460 |
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| O | 6.462358189 | 11.794926732 | 2.982526070 |
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| O | 8.435015304 | 13.088925149 | 1.500596590 |
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| O | -0.033111698 | 14.400743762 | 2.979888070 |
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| O | 6.459864210 | 14.384173730 | 0.025528277 |
| O | 9.668599827 | 15.109747538 | 8.904021624 |
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| O | 3.204323062 | 17.728587706 | 0.030709642 |
| O | 9.668359664 | 17.736913799 | 2.991847795 |
| O | 9.685509816 | 17.727698303 | 5.943131892 |
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| O | 3.188744165 | 17.722944108 | 5.940564869 |

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| O | 10.888163590 | 19.926186869 | 10.377989784 |
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| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
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| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |

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| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 6.421948863 | 21.278078599 | 6.677608097 |

TS7-F1:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |

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|----|--------------|-------------|--------------|
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
| Ti | 6.494400000 | 6.494389931 | 10.350900000 |
| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
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| Ti | 3.226183732 | 9.734919200 | 1.479117585 |
| Ti | 3.232243786 | 9.737511325 | 4.436765888 |
| Ti | -0.010233356 | 9.837436941 | 2.960401524 |
| Ti | -0.011355718 | 9.836865081 | 0.000969791 |

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| Ti | 3.232626956 | 9.737843869 | 7.393513131 |
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| Ti | -0.009141777 | 9.837194409 | 5.916314544 |
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| Ti | 6.488122513 | 9.772738806 | 2.965241132 |
| Ti | 6.480375473 | 9.772928831 | 0.015859826 |
| Ti | 9.741343731 | 9.737038763 | 7.397059763 |
| Ti | 9.741713912 | 9.735482845 | 10.355415595 |
| Ti | 6.488506981 | 9.753848827 | 8.888613570 |
| Ti | 6.482476541 | 9.741301109 | 5.925421916 |
| Ti | -0.031229751 | 13.172632207 | 1.509476479 |
| Ti | -0.030922046 | 13.174505667 | 4.466508697 |
| Ti | 3.214471861 | 12.989244922 | 2.961057357 |
| Ti | 3.214327425 | 12.993938753 | 5.917913787 |
| Ti | 6.461272975 | 13.173714492 | 1.468396655 |
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| Ti | 9.709728862 | 12.992172092 | 2.966675944 |
| Ti | 9.714283904 | 12.995574682 | 5.923852483 |
| Ti | -0.030371191 | 13.172246799 | 7.422722424 |
| Ti | -0.032132862 | 13.172122497 | 10.380493874 |

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| Ti | 3.215000765 | 12.991983139 | 8.876268791 |
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| Ti | 6.463058285 | 13.006234295 | 7.428063607 |
| Ti | 6.464844375 | 13.099955882 | 10.421284582 |
| Ti | 9.710699385 | 12.989584967 | 8.881450274 |
| Ti | 9.714087384 | 12.989170984 | 0.010622389 |
| Ti | 9.695036451 | 16.309654319 | 1.488486746 |
| Ti | 9.694572231 | 16.318917320 | 4.444343812 |
| Ti | 6.433453953 | 16.415989347 | 2.940067507 |
| Ti | -0.061375067 | 16.636877626 | 5.932098661 |
| Ti | 3.175737830 | 16.306775369 | 1.489538753 |
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| Ti | -0.058983180 | 16.636975139 | 2.971197454 |
| Ti | 6.443137103 | 16.282712925 | 5.917878653 |
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| Ti | 3.175062153 | 16.305140869 | 10.363936574 |
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| Ti | 6.418925980 | 19.579582089 | 7.594496734 |
| Ti | 6.413097256 | 19.995238433 | 10.566012877 |
| Ti | 3.190254633 | 19.559014390 | 8.889069364 |
| Ti | 3.182129229 | 19.555665379 | 0.019941866 |
| Ti | 6.421280200 | 20.081463322 | 1.659723992 |
| Ti | 6.423445563 | 19.545923028 | 4.391883439 |
| Ti | 3.188583624 | 19.559402655 | 2.972777770 |
| Ti | 3.189179940 | 19.556002923 | 5.927995801 |
| Ti | -0.074662870 | 19.996333576 | 1.491823522 |
| Ti | -0.073323465 | 20.004202823 | 4.451906712 |
| Ti | 9.667469152 | 19.563194224 | 2.975030836 |
| Ti | 9.649089740 | 19.561587227 | 5.930514441 |
| Ti | -0.072822616 | 20.000752728 | 7.409213613 |
| Ti | -0.071734155 | 19.996342149 | 10.364391541 |
| Ti | 9.670581918 | 19.556819459 | 8.893021516 |
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| O | 1.266699988 | 3.247190143 | 4.436100000 |
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| O | 0.000000000 | 5.227600085 | 5.914800000 |
| O | 6.494400000 | 5.227600085 | 0.000000000 |
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| O | 7.760933082 | 9.782158614 | 1.483660624 |
| O | 7.760847096 | 9.781871791 | 4.441977064 |
| O | 11.702006208 | 9.776249267 | 1.480352004 |
| O | 11.702465622 | 9.775654546 | 4.437465018 |
| O | 7.760846577 | 9.778887828 | 7.396046795 |
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| O | 6.465024140 | 11.784998286 | 8.879766685 |
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| O | 6.463988413 | 11.794869581 | 5.916972861 |
| O | -0.029584070 | 11.792228520 | 0.002936343 |
| O | -0.029272469 | 11.792565707 | 5.916751766 |
| O | 6.465983623 | 11.803038153 | 2.960857437 |
| O | -0.029170377 | 11.792379612 | 8.873981419 |
| O | 8.437975711 | 13.093540397 | 1.489273178 |
| O | 8.435343531 | 13.090453206 | 4.444924645 |
| O | 10.968834299 | 13.108325552 | 1.486996927 |
| O | 10.968984060 | 13.111057339 | 4.443318304 |

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| O | -0.030908798 | 14.402123586 | 2.968508113 |
| O | -0.030732800 | 14.401480644 | 5.926117378 |
| O | -0.031397826 | 14.400488728 | 8.884330545 |
| O | -0.030776572 | 14.401159531 | 0.011869584 |
| O | 6.460197113 | 14.426805040 | 2.975580676 |
| O | 6.463350144 | 14.408319042 | 5.916706695 |
| O | 6.460979298 | 14.388212474 | 8.870000641 |
| O | 6.466369520 | 14.393490310 | -0.000568649 |
| O | 9.686971185 | 15.103688528 | 8.881331268 |
| O | 3.187206551 | 15.103825689 | 8.881419280 |

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| O | 9.688123422 | 15.104263603 | 0.011957715 |
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| O | 7.721094354 | 16.449545180 | 1.473853176 |
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| O | 5.153644369 | 16.411388029 | 10.362641351 |
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| O | 1.228845170 | 16.467332515 | 4.448743713 |
| O | 1.229437849 | 16.471495561 | 1.492461965 |
| O | 5.156187056 | 16.434000640 | 1.470033044 |
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| O | 11.645735220 | 16.453400686 | 10.362858898 |

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| O | 6.438834173 | 18.458116318 | 3.057252589 |
| O | -0.061394031 | 18.509521280 | 5.920496780 |
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| O | 6.442638983 | 21.176837454 | 5.923361200 |
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| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
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| H | 7.259705292 | 21.682054481 | 9.015467221 |

TS8-1:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |

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| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
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| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |

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|----|--------------|-------------|--------------|
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| Ti | 6.481343139 | 9.733865133 | 2.971562397 |
| Ti | 6.479367542 | 9.741388263 | 0.008234703 |
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| Ti | 6.478495864 | 9.748259522 | 8.875483779 |
| Ti | 6.488606606 | 9.759671020 | 5.927370251 |
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| Ti | 3.215199364 | 12.995244638 | 5.918732987 |
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| Ti | -0.026966437 | 13.173396950 | 7.424357038 |
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| Ti | 9.715513554 | 12.998903690 | 0.008505837 |
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| Ti | 3.199352118 | 16.318632997 | 4.438187924 |
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| Ti | 9.705140438 | 16.333739266 | 10.357511209 |
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| Ti | 3.216368485 | 19.582562123 | 8.878296621 |
| Ti | 3.224932781 | 19.587654220 | 0.004451597 |
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| O | 3.243414154 | 11.072529055 | 2.957631269 |
| O | 3.242433240 | 11.072664073 | 0.003076287 |
| O | 3.246231945 | 11.073435960 | 8.871353474 |
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| O | 6.466819322 | 11.778774612 | 2.962829432 |
| O | -0.026024490 | 11.797413844 | 8.869440864 |
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| O | 1.962183596 | 13.100407727 | 4.438215842 |
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| O | 4.496303541 | 13.100857429 | 4.438874396 |
| O | 1.963104502 | 13.101623244 | 7.398886727 |
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| O | 4.498273812 | 13.099532612 | 10.358007815 |
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| O | -0.026173861 | 14.407428211 | 0.006681358 |
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| O | 6.468515919 | 14.427752307 | 5.886805725 |
| O | 6.466492394 | 14.422425894 | 8.910208978 |
| O | 6.469037290 | 14.385687500 | -0.001704645 |
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| O | 9.690358275 | 15.114345284 | 5.908707165 |
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| O | 3.217747117 | 15.115122529 | 2.961107633 |
| O | 9.688900022 | 15.121391566 | -0.005059402 |
| O | 3.207937066 | 15.118081131 | -0.005024268 |
| O | 3.205021080 | 15.113414447 | 5.911365749 |
| O | 1.245791657 | 16.481501518 | 10.358249376 |
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8-b:

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| O | 3.223279436 | 17.729298156 | 5.923228235 |
| O | 9.669565154 | 17.743210339 | 8.883275108 |
| O | 9.673046672 | 17.743894358 | 0.000789744 |
| O | 6.457092789 | 18.672701627 | -0.012825297 |
| O | 6.444641466 | 18.541552270 | 5.917695413 |
| O | -0.055086800 | 18.500986231 | 0.008396295 |
| O | 6.419949757 | 18.466012712 | 3.083706295 |
| O | -0.062512627 | 18.498678428 | 5.928802224 |
| O | 6.422847948 | 18.452738112 | 8.792131116 |
| O | -0.062671090 | 18.499515681 | 8.884457240 |
| O | -0.065291710 | 18.501312345 | 2.962726632 |
| O | 1.970295621 | 19.915442959 | 4.437111431 |
| O | 4.478089477 | 19.953211845 | 1.457440908 |
| O | 4.436092530 | 20.011054080 | 4.472005084 |
| O | 1.981973851 | 19.936396066 | 7.409491135 |
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| O | 4.460693317 | 19.986895552 | 7.394036709 |
| O | 4.493861907 | 19.980750817 | 10.366044254 |
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| O | 10.880243799 | 19.950934403 | 1.483665948 |

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| O | 8.409694937 | 19.984005172 | 7.410289515 |
| O | 8.380149833 | 20.015249631 | 10.361592302 |
| O | 10.887394912 | 19.947473235 | 7.412637099 |
| O | 10.880626059 | 19.951065849 | 10.362749237 |
| O | 1.988213151 | 19.942880489 | 1.488375430 |
| O | 6.442576247 | 21.048158421 | 2.893013617 |
| O | 6.419222254 | 21.283885076 | 5.948876701 |
| O | -0.057366594 | 21.101325399 | 2.963732621 |
| O | -0.055494648 | 21.099777339 | 5.923133835 |
| O | -0.058133582 | 21.101027860 | 8.881137736 |
| O | -0.053657512 | 21.101171451 | 0.006647407 |
| O | 6.436196927 | 21.165264863 | 8.943032569 |
| H | 0.000000000 | 0.932897449 | 9.814799089 |
| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |

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| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
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| H | 5.650693273 | 21.878668859 | 6.020583241 |
| H | 7.267256201 | 21.670665843 | 8.946719146 |

TS8-2:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |

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|----|-------------|-------------|--------------|
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |
| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
| Ti | 6.494400000 | 6.494389931 | 4.436100000 |
| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
| Ti | 6.494400000 | 6.494389931 | 10.350900000 |
| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
| Ti | 9.741600000 | 6.494389931 | 5.914800000 |
| Ti | 3.227118666 | 9.738738629 | 1.478583833 |
| Ti | 3.226613401 | 9.738116048 | 4.436137736 |

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| Ti | -0.011876309 | 9.836860080 | 2.958614545 |
| Ti | -0.012713957 | 9.836969737 | 0.001305870 |
| Ti | 3.226521441 | 9.738317146 | 7.393822357 |
| Ti | 3.227263231 | 9.739692326 | 10.351166876 |
| Ti | -0.015801265 | 9.835441679 | 8.876117372 |
| Ti | -0.010701213 | 9.836691486 | 5.917274752 |
| Ti | 9.738108091 | 9.740354556 | 1.480670456 |
| Ti | 9.741546746 | 9.737154493 | 4.438852275 |
| Ti | 6.485549951 | 9.744822285 | 2.971651356 |
| Ti | 6.478786293 | 9.737196284 | 0.013307472 |
| Ti | 9.737508268 | 9.739304418 | 7.396356730 |
| Ti | 9.733239759 | 9.739264056 | 10.353362568 |
| Ti | 6.482296776 | 9.731122987 | 8.880718495 |
| Ti | 6.480581995 | 9.747979128 | 5.921445633 |
| Ti | -0.029653041 | 13.178280806 | 1.508251524 |
| Ti | -0.027579249 | 13.176098019 | 4.465488039 |
| Ti | 3.213949841 | 12.996240483 | 2.960013159 |
| Ti | 3.216436807 | 12.996001523 | 5.919676753 |
| Ti | 6.468239907 | 13.035239531 | 1.518609522 |
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| Ti | 9.715921532 | 12.996513376 | 2.965405090 |
| Ti | 9.716625525 | 12.995884722 | 5.924254808 |

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| Ti | -0.027252191 | 13.174486736 | 7.425670715 |
| Ti | -0.025903824 | 13.177605360 | 10.381800926 |
| Ti | 3.216535132 | 12.996302991 | 8.877101713 |
| Ti | 3.218737253 | 12.997938920 | 0.006956869 |
| Ti | 6.467026234 | 13.027379213 | 7.369332364 |
| Ti | 6.463568875 | 13.000785723 | 10.353135203 |
| Ti | 9.715616555 | 12.996994511 | 8.881551181 |
| Ti | 9.714783583 | 12.998368263 | 0.008042354 |
| Ti | 9.700356663 | 16.336762877 | 1.481749789 |
| Ti | 9.716841399 | 16.302763414 | 4.437347076 |
| Ti | 6.443663409 | 16.379420262 | 2.972273119 |
| Ti | -0.047208053 | 16.626755226 | 5.925130316 |
| Ti | 3.195482235 | 16.333257060 | 1.481887722 |
| Ti | 3.176270371 | 16.306994684 | 4.440310155 |
| Ti | -0.048474072 | 16.639376883 | 2.957263368 |
| Ti | 6.454464765 | 16.353606516 | 5.902981047 |
| Ti | 3.196457304 | 16.320000677 | 7.401475990 |
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| Ti | -0.043385320 | 16.637276250 | 8.878453363 |
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| Ti | 9.707220984 | 16.320912225 | 10.357671026 |

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| Ti | 6.447781898 | 16.259102684 | 8.876837203 |
| Ti | -0.045731746 | 16.640624189 | 0.003883776 |
| Ti | 6.455127454 | 19.496652990 | 7.276547014 |
| Ti | 6.418206790 | 19.692414042 | 10.257460592 |
| Ti | 3.207058373 | 19.577040684 | 8.883293444 |
| Ti | 3.212383651 | 19.587879607 | 0.014120875 |
| Ti | 6.432581625 | 19.695981653 | 1.743271133 |
| Ti | 6.437313704 | 20.139104459 | 4.512886643 |
| Ti | 3.205893408 | 19.576234507 | 2.965648307 |
| Ti | 3.200376805 | 19.551101565 | 5.922833955 |
| Ti | -0.069968068 | 20.000873101 | 1.482063510 |
| Ti | -0.048596296 | 19.995044479 | 4.439051840 |
| Ti | 9.664576936 | 19.578553740 | 2.964444882 |
| Ti | 9.700732299 | 19.545191861 | 5.913445156 |
| Ti | -0.045636149 | 20.003173045 | 7.400470355 |
| Ti | -0.053271875 | 20.002811569 | 10.361041516 |
| Ti | 9.694439096 | 19.568788530 | 8.882123142 |
| Ti | 9.638744680 | 19.593685012 | 0.006109279 |
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| O | 0.000000000 | 1.266689833 | 5.914800000 |

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| O | 9.741600000 | 1.980499953 | 0.000000000 |
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| O | 1.266699988 | 3.247190143 | 1.478700000 |
| O | 1.266699988 | 3.247190143 | 4.436100000 |
| O | 5.227599998 | 3.247190143 | 1.478700000 |
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| O | 0.000000000 | 5.227600085 | 0.000000000 |
| O | 0.000000000 | 5.227600085 | 8.872200000 |
| O | 0.000000000 | 5.227600085 | 5.914800000 |
| O | 6.494400000 | 5.227600085 | 0.000000000 |
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| O | 6.494400000 | 5.227600085 | 8.872200000 |
| O | 6.494400000 | 5.227600085 | 5.914800000 |

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| O | 8.474900012 | 6.494389931 | 7.393500000 |
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| O | 6.494400000 | 7.761090122 | 8.872200000 |
| O | 6.494400000 | 7.761090122 | 5.914800000 |
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| O | 9.741600000 | 8.474889884 | 2.957400000 |
| O | 9.741600000 | 8.474889884 | 0.000000000 |
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| O | 9.741600000 | 8.474889884 | 5.914800000 |
| O | 1.269903286 | 9.787755778 | 1.479898220 |
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| O | 5.211533502 | 9.776340351 | 1.485103717 |
| O | 5.211226187 | 9.769518027 | 4.439140089 |
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| O | 1.268677143 | 9.786281655 | 10.351424051 |
| O | 5.211517526 | 9.776713614 | 7.396791704 |
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| O | 7.759223756 | 9.783762753 | 1.483326557 |
| O | 7.760415608 | 9.776972934 | 4.440140282 |
| O | 11.701274809 | 9.781429233 | 1.480336980 |
| O | 11.702486924 | 9.780878803 | 4.437281067 |

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| O | 7.758911635 | 9.783597017 | 7.396680388 |
| O | 7.758454949 | 9.779323599 | 10.355829868 |
| O | 11.701140245 | 9.781432805 | 7.393424172 |
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| O | 9.723931465 | 11.074167842 | 2.961381962 |
| O | 9.725451025 | 11.073738142 | 0.001262810 |
| O | 3.244129188 | 11.074193917 | 2.960563945 |
| O | 3.242712499 | 11.073648488 | 0.000764784 |
| O | 3.243423896 | 11.073053052 | 8.875163551 |
| O | 3.244000209 | 11.073488824 | 5.914198938 |
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| O | 6.466190275 | 11.781153138 | 8.878938258 |
| O | -0.024903686 | 11.799095850 | 2.958080439 |
| O | 6.466338737 | 11.786923181 | 0.006549813 |
| O | 6.467666582 | 11.793376171 | 5.898086550 |
| O | -0.025399209 | 11.798410046 | -0.001513479 |
| O | -0.024774967 | 11.799719504 | 5.913493302 |
| O | 6.467311728 | 11.796863772 | 2.979682708 |
| O | -0.025988511 | 11.798763664 | 8.872256900 |
| O | 8.434780466 | 13.086944889 | 1.481859923 |
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| O | 10.970824313 | 13.113150114 | 1.482814098 |
| O | 10.970949005 | 13.116395540 | 4.439682713 |
| O | 1.961710414 | 13.099157206 | 1.481213672 |
| O | 1.961834976 | 13.102639092 | 4.438638750 |
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| O | 4.496976621 | 13.127305544 | 4.439334804 |
| O | 1.962226459 | 13.099141132 | 7.398982901 |
| O | 1.963561058 | 13.103545282 | 10.355474743 |
| O | 4.498063134 | 13.101474653 | 7.398313464 |
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| O | 10.970269431 | 13.117870377 | 10.356533847 |
| O | -0.027751740 | 14.409372752 | 2.964008961 |
| O | -0.027184389 | 14.410146425 | 5.924039154 |
| O | -0.026531832 | 14.408172594 | 8.881030678 |
| O | -0.027366752 | 14.409167010 | 0.009796920 |
| O | 6.465649811 | 14.425881347 | 2.935372220 |
| O | 6.468568134 | 14.415685366 | 5.944679559 |
| O | 6.465891662 | 14.389450851 | 8.873902043 |
| O | 6.467018960 | 14.402112156 | 0.010954919 |

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| O | 9.680204150 | 15.113036898 | 8.881062973 |
| O | 3.217289261 | 15.115624738 | 8.880003869 |
| O | 9.691809254 | 15.107466524 | 5.928081802 |
| O | 9.687734018 | 15.116513068 | 2.941930432 |
| O | 3.207236190 | 15.118005050 | 2.946116928 |
| O | 9.681268583 | 15.121838767 | 0.013577305 |
| O | 3.214245596 | 15.121386565 | 0.012094938 |
| O | 3.201282254 | 15.111053423 | 5.929527261 |
| O | 1.244305349 | 16.470695099 | 10.359643849 |
| O | 5.163306087 | 16.403649513 | 4.441990076 |
| O | 5.174601278 | 16.476078663 | 7.399973039 |
| O | 7.718513220 | 16.510304227 | 1.476491295 |
| O | 7.736425295 | 16.415748244 | 4.436446607 |
| O | 5.177599872 | 16.449651266 | 10.366698786 |
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| O | 1.244735278 | 16.482038017 | 1.481748251 |
| O | 5.178382188 | 16.499188482 | 1.473030191 |
| O | 7.726301694 | 16.486088905 | 7.403240611 |
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| O | 11.656730629 | 16.458166669 | 7.404365251 |
| O | 11.655710358 | 16.459096434 | 10.359429615 |
| O | 3.214746574 | 17.749300067 | 8.897545273 |
| O | 3.233347185 | 17.762708256 | -0.005042485 |
| O | 9.667816082 | 17.752189732 | 2.970501755 |
| O | 9.692537925 | 17.723380237 | 5.909910353 |
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| O | 6.434606709 | 18.595024288 | -0.003564495 |
| O | 6.434982345 | 18.508153957 | 5.847741665 |
| O | -0.058934991 | 18.518813928 | 0.000857528 |
| O | 6.430883079 | 18.475675766 | 3.088766525 |
| O | -0.060694065 | 18.507749619 | 5.929703522 |
| O | 6.433964932 | 18.500742628 | 8.843986759 |

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| O | -0.057904980 | 18.514776255 | 8.889276737 |
| O | -0.063003084 | 18.512051612 | 2.954270124 |
| O | 1.969491614 | 19.911006305 | 4.446917578 |
| O | 4.488327119 | 19.946934592 | 1.456502939 |
| O | 4.428812957 | 20.005302968 | 4.446450663 |
| O | 1.987031170 | 19.942195399 | 7.412059696 |
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| O | 10.878651632 | 19.967723035 | 1.471736388 |
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| O | 8.399255838 | 19.980940842 | 7.440732517 |
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| O | 10.886505699 | 19.955443566 | 7.410240304 |
| O | 10.870755091 | 19.982616419 | 10.358186679 |
| O | 1.992115636 | 19.950605074 | 1.474399940 |
| O | 6.440692091 | 21.080857713 | 2.876329858 |
| O | 6.441128775 | 21.132597004 | 5.988850693 |
| O | -0.053511778 | 21.110544824 | 2.962507666 |
| O | -0.054109652 | 21.109631490 | 5.920788853 |

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| O | -0.054614137 | 21.116464529 | 8.876541108 |
| O | -0.053582437 | 21.120046428 | 0.004770286 |
| O | 6.438241754 | 21.429635635 | 9.004867781 |
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| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 7.239082194 | 21.948617326 | 8.797348916 |

TS8-3:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |

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|----|--------------|-------------|--------------|
| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
| Ti | 9.741600000 | 6.494389931 | 5.914800000 |
| Ti | 3.231109215 | 9.738427874 | 1.478756545 |
| Ti | 3.232752428 | 9.738369652 | 4.436224447 |
| Ti | -0.007144100 | 9.838361348 | 2.956922321 |
| Ti | -0.011716937 | 9.837249060 | -0.000016680 |
| Ti | 3.228277786 | 9.739428006 | 7.393581388 |
| Ti | 3.228677322 | 9.739060100 | 10.350827603 |
| Ti | -0.013311961 | 9.837176193 | 8.874173769 |
| Ti | -0.005794953 | 9.838850341 | 5.915103074 |
| Ti | 9.740296054 | 9.740000938 | 1.481707439 |
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| Ti | 6.483165208 | 9.736756584 | 0.010491081 |

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| Ti | 9.741865491 | 9.737247005 | 7.396089263 |
| Ti | 9.734354588 | 9.738242850 | 10.354041114 |
| Ti | 6.479604848 | 9.748804951 | 8.877275017 |
| Ti | 6.489047316 | 9.754883963 | 5.924002956 |
| Ti | -0.024008498 | 13.177183876 | 1.506666712 |
| Ti | -0.024290874 | 13.179771716 | 4.464784414 |
| Ti | 3.220929892 | 12.996987724 | 2.965857927 |
| Ti | 3.218338497 | 12.998253605 | 5.922417198 |
| Ti | 6.470794155 | 13.015023306 | 1.507076963 |
| Ti | 6.468665161 | 13.102738748 | 4.470385611 |
| Ti | 9.718234188 | 12.996776268 | 2.967621957 |
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| Ti | -0.023792884 | 13.178584417 | 7.422722897 |
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| Ti | 3.220677650 | 12.997495648 | 8.880555128 |
| Ti | 3.221994974 | 12.995927585 | 0.009023619 |
| Ti | 6.467637487 | 13.102305834 | 7.371501558 |
| Ti | 6.469730112 | 13.017712587 | 10.334374404 |
| Ti | 9.718247436 | 12.993649429 | 8.882277873 |
| Ti | 9.717998052 | 12.997013442 | 0.009885878 |
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| Ti | 6.463721623 | 16.316311264 | 2.972496936 |
| Ti | -0.041847965 | 16.641128898 | 5.918444463 |
| Ti | 3.202987683 | 16.313253363 | 1.478295546 |
| Ti | 3.197030500 | 16.324746300 | 4.440293238 |
| Ti | -0.036546067 | 16.638271380 | 2.957089710 |
| Ti | 6.450641772 | 16.456814349 | 5.918961062 |
| Ti | 3.196391711 | 16.333372789 | 7.397103769 |
| Ti | 3.199273926 | 16.319275224 | 10.350621176 |
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| Ti | 9.716199622 | 16.304186815 | 7.397391702 |
| Ti | 9.709040715 | 16.321978794 | 10.357623353 |
| Ti | 6.457238264 | 16.321955219 | 8.867506015 |
| Ti | -0.040780286 | 16.642320483 | 0.003383620 |
| Ti | 6.418980013 | 19.939615060 | 7.289031501 |
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| Ti | 3.203062759 | 19.579018444 | 8.875758817 |
| Ti | 3.221756889 | 19.562184806 | -0.022273599 |
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| Ti | 3.216902715 | 19.613117920 | 5.912492400 |

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| Ti | -0.070648291 | 20.013660851 | 1.466930494 |
| Ti | -0.046832287 | 20.000792376 | 4.435745112 |
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| Ti | 9.754791166 | 19.563398537 | 5.968072356 |
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| Ti | -0.069599056 | 20.006785663 | 10.350349450 |
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| O | 0.000000000 | 1.266689833 | 5.914800000 |
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| O | 3.247200000 | 4.513899978 | 8.872200000 |
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| O | 8.474900012 | 6.494389931 | 7.393500000 |
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| O | 1.980500012 | 6.494389931 | 4.436100000 |
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| O | 6.494400000 | 7.761090122 | 5.914800000 |
| O | 3.247200000 | 8.474889884 | 2.957400000 |
| O | 3.247200000 | 8.474889884 | 0.000000000 |
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| O | 3.247200000 | 8.474889884 | 5.914800000 |
| O | 9.741600000 | 8.474889884 | 2.957400000 |
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| O | 9.741600000 | 8.474889884 | 5.914800000 |

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| O | 1.271872648 | 9.787147841 | 1.478350435 |
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| O | 5.213369209 | 9.775989590 | 1.483142370 |
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| O | 1.270734050 | 9.787037826 | 10.350731192 |
| O | 5.212993183 | 9.776384642 | 7.394876965 |
| O | 5.212343613 | 9.775575607 | 10.355098680 |
| O | 7.760815534 | 9.782617246 | 1.482055466 |
| O | 7.762223909 | 9.781916440 | 4.440132592 |
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| O | 7.759582377 | 9.782698328 | 10.353737803 |
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| O | 9.727576772 | 11.072913391 | 2.958960561 |
| O | 9.727041893 | 11.073202001 | 0.002047940 |
| O | 3.245883845 | 11.074010321 | 2.959449833 |
| O | 3.245017752 | 11.073249507 | 0.001517264 |
| O | 3.246016071 | 11.074466809 | 8.873457605 |
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| O | 9.726603781 | 11.072231516 | 8.874013478 |
| O | 9.725940962 | 11.072510124 | 5.917209690 |
| O | 6.469144577 | 11.796604095 | 8.866729993 |
| O | -0.020499703 | 11.799975251 | 2.955698549 |
| O | 6.469067034 | 11.791846685 | 0.004199271 |
| O | 6.471290587 | 11.806665772 | 5.919608614 |
| O | -0.020761038 | 11.800072407 | -0.001155989 |
| O | -0.020203429 | 11.800334941 | 5.913254108 |
| O | 6.470464759 | 11.795382506 | 2.973015190 |
| O | -0.021512570 | 11.800187065 | 8.870742712 |
| O | 8.438473961 | 13.093793288 | 1.482741819 |
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| O | 10.974592623 | 13.116178369 | 1.482791504 |
| O | 10.975480668 | 13.111882805 | 4.440101007 |
| O | 1.966585240 | 13.103623507 | 1.482399944 |
| O | 1.965670829 | 13.103926403 | 4.440018555 |
| O | 4.502566611 | 13.109314968 | 1.483472179 |
| O | 4.499127436 | 13.119098038 | 4.439766348 |
| O | 1.965654203 | 13.102462640 | 7.397593515 |
| O | 1.966845796 | 13.104739367 | 10.355058696 |
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| O | 8.441080813 | 13.101921140 | 7.400690149 |
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| O | 10.974706925 | 13.114379204 | 10.356417444 |
| O | -0.021737926 | 14.411717702 | 2.964832064 |
| O | -0.022386846 | 14.412414580 | 5.922074849 |
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| O | 6.474417251 | 14.408146876 | 2.951251684 |
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| O | 6.472070304 | 14.412223483 | 8.888800123 |
| O | 6.469226537 | 14.406454154 | 0.005335623 |
| O | 9.690508166 | 15.113072260 | 8.887090864 |
| O | 3.214550573 | 15.121768044 | 8.868044262 |
| O | 9.704861309 | 15.110318684 | 5.915960247 |
| O | 9.691943168 | 15.115228614 | 2.960531532 |
| O | 3.214522777 | 15.118396173 | 2.960720924 |
| O | 9.690256572 | 15.117433904 | 0.002959766 |
| O | 3.219312397 | 15.112672564 | 0.000683396 |
| O | 3.203458917 | 15.128838258 | 5.920167799 |
| O | 1.248213029 | 16.471839892 | 10.353969899 |
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| O | 1.251756763 | 16.489484351 | 4.441451948 |
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| O | 3.230767739 | 17.753946391 | 8.875906332 |
| O | 3.217981435 | 17.740032065 | -0.004357670 |
| O | 9.689526212 | 17.751598226 | 2.954811092 |
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| O | 9.677842917 | 17.739721310 | 8.879102572 |
| O | 9.671855080 | 17.756872847 | 0.008508913 |

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| Ti | 3.247200000 | 3.247194072 | 10.350900000 |
| Ti | 0.000000000 | 3.247194072 | 8.872200000 |
| Ti | 0.000000000 | 3.247194072 | 5.914800000 |
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| O | 6.427802915 | 18.454653007 | 8.782092754 |
| O | -0.065082850 | 18.516471121 | 8.880798226 |
| O | -0.054184728 | 18.508126811 | 2.957210253 |
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| O | 4.464195228 | 19.960012738 | 1.476666255 |
| O | 4.411362504 | 20.253466255 | 4.449897572 |
| O | 1.955399675 | 19.928597900 | 7.443402813 |
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| O | 8.398444948 | 19.921192642 | 1.481432046 |

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| O | 6.453830652 | 21.202106842 | 5.905202172 |
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| O | 6.427723554 | 21.161102174 | 8.943395265 |
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| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 0.834099172 | 0.932897449 | 5.475598892 |
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| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 7.242643594 | 21.693887820 | 8.971360676 |

TS8-4:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |

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|----|-------------|-------------|--------------|
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
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| Ti | 3.230601223 | 9.739012951 | 1.478678588 |
| Ti | 3.232781003 | 9.738240350 | 4.435989512 |
| Ti | -0.007725478 | 9.838144177 | 2.957002762 |
| Ti | -0.011771620 | 9.837356216 | 0.000042941 |
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| Ti | -0.005595055 | 9.838681033 | 5.915185645 |
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| Ti | 6.481423150 | 9.731712707 | 0.011324358 |
| Ti | 9.741903808 | 9.736175436 | 7.395694273 |
| Ti | 9.732480953 | 9.737870658 | 10.353472820 |
| Ti | 6.480161418 | 9.755987679 | 8.876551637 |
| Ti | 6.487284346 | 9.754799309 | 5.924613718 |
| Ti | -0.023759113 | 13.178155432 | 1.507477395 |
| Ti | -0.024172806 | 13.179310941 | 4.464791867 |
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| Ti | 6.426481695 | 19.572839419 | 10.175647907 |
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| Ti | 3.228970869 | 19.619542334 | 2.960802666 |
| Ti | 3.124912526 | 19.557248086 | 5.961349358 |
| Ti | -0.037434891 | 20.005798033 | 1.481339420 |
| Ti | -0.043921367 | 19.999071078 | 4.438783426 |
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| Ti | 9.740933934 | 19.567187605 | 5.947061212 |
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| O | 6.474553243 | 11.802819911 | 5.919236455 |
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| O | -0.023602858 | 14.411512318 | 2.965322047 |
| O | -0.021068743 | 14.412011669 | 5.922237388 |
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| O | -0.048481735 | 18.511187927 | 5.933618054 |
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| O | 6.189864595 | 21.177357165 | 5.819045185 |
| O | -0.042901357 | 21.114493556 | 2.961775769 |
| O | -0.040587272 | 21.113348763 | 5.920398476 |
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| H | 0.000000000 | 0.932899949 | 9.814800036 |

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| H | 6.457700016 | 0.932899949 | 0.941899960 |
| H | 0.834099951 | 0.932899949 | 5.475599957 |
| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
| H | -0.036699984 | 0.932899949 | 6.856699960 |
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| H | 7.255558617 | 21.688911095 | 8.957015393 |

TS8-5:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |

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|----|-------------|-------------|--------------|
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
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|----|--------------|-------------|--------------|
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| Ti | 6.488282275 | 9.754404614 | 2.971257312 |
| Ti | 6.483067921 | 9.733483297 | 0.012463667 |
| Ti | 9.741368150 | 9.738406443 | 7.397334565 |
| Ti | 9.735999359 | 9.739197975 | 10.354047383 |
| Ti | 6.482468099 | 9.745076604 | 8.878749931 |
| Ti | 6.483640208 | 9.751410650 | 5.924343885 |

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| Ti | -0.025620798 | 13.179339516 | 1.507084889 |
| Ti | -0.025245941 | 13.175986933 | 4.463428150 |
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| Ti | -0.024463496 | 13.178815876 | 7.422890168 |
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| Ti | 9.716643839 | 12.996734834 | 0.009406425 |
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| Ti | 3.212109458 | 19.575334032 | 0.002635635 |
| Ti | 6.431677474 | 19.634314630 | 1.715378829 |
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| Ti | 3.209175937 | 19.567347983 | 2.933037767 |
| Ti | 3.128761887 | 19.553517597 | 5.876349541 |
| Ti | -0.072223833 | 20.006052352 | 1.479520028 |
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| O | 9.741600000 | 8.474889884 | 2.957400000 |
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| O | 1.272155284 | 9.787994737 | 4.436063210 |
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| O | 1.271132416 | 9.787778638 | 7.394090534 |
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| O | 9.726055264 | 11.073253436 | 0.002037530 |
| O | 3.246003472 | 11.073733142 | 2.958797312 |
| O | 3.244302329 | 11.074543248 | 0.001463203 |
| O | 3.245165045 | 11.075117252 | 8.874418760 |
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| O | 9.727584046 | 11.072635498 | 8.874994388 |
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| O | -0.023048626 | 11.799929174 | 8.871124689 |
| O | 8.436909201 | 13.092974609 | 1.484445873 |
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| O | 10.974140873 | 13.114085951 | 4.440794932 |
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| O | -0.025755881 | 14.411246569 | 2.964966449 |
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| O | 6.479321432 | 14.427219023 | 5.928995047 |
| O | 6.467762699 | 14.396642152 | 8.887381990 |
| O | 6.473748717 | 14.410610057 | 0.005026634 |
| O | 9.693434672 | 15.112902595 | 8.879855526 |
| O | 3.214792295 | 15.128521787 | 8.882249127 |
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| O | 3.217966368 | 15.124676640 | -0.004728409 |
| O | 3.199185212 | 15.116272323 | 5.923732413 |
| O | 1.252673643 | 16.488739611 | 10.349476781 |
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| O | 9.668752055 | 17.755219416 | 2.971677617 |
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| O | 9.691619357 | 17.749013958 | 8.885817644 |
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| O | -0.043107489 | 18.517336591 | -0.001901253 |
| O | 6.432432643 | 18.487086192 | 3.106145627 |

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| O | 8.483214143 | 20.026446815 | 7.419228552 |

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| O | 6.451625803 | 21.184159843 | 5.954991776 |
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| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |

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| H | 7.251117876 | 21.717632722 | 8.998592415 |

TS8-6:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |

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|----|--------------|-------------|--------------|
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
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| Ti | 6.486734400 | 9.737092342 | 0.012858420 |
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| Ti | 9.741067979 | 9.739239052 | 10.354231570 |
| Ti | 6.484508769 | 9.738632187 | 8.882664582 |
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| Ti | 9.720305382 | 12.996849849 | 2.967013443 |
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| Ti | 9.724280604 | 16.308035178 | 4.436497120 |
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| Ti | 6.457928229 | 20.091796464 | 4.426216606 |
| Ti | 3.223557007 | 19.577848290 | 2.968643917 |
| Ti | 3.221322674 | 19.608553392 | 5.915942148 |
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| Ti | 9.738926775 | 19.560717470 | 5.893244813 |
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| O | -0.019786618 | 11.802131606 | 5.913143501 |
| O | 6.472754554 | 11.797122377 | 2.972501431 |
| O | -0.019912220 | 11.801524026 | 8.871438292 |
| O | 8.439749851 | 13.093269290 | 1.481682242 |
| O | 8.440982748 | 13.106901794 | 4.439907475 |
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| O | 1.967846323 | 13.105351233 | 1.483639449 |
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| O | -0.021124075 | 14.413044662 | 8.880192551 |
| O | -0.022690135 | 14.412907859 | 0.008810923 |
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| O | 6.474160332 | 14.415924326 | 5.929816376 |
| O | 6.474035380 | 14.399375725 | 8.877566735 |
| O | 6.471766496 | 14.409216303 | 0.006595475 |
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| O | 9.687641407 | 17.754588619 | 8.886443666 |
| O | 9.682495764 | 17.758511276 | -0.010919312 |
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| O | -0.042738997 | 18.523432391 | 0.003022463 |
| O | 6.452971313 | 18.475079973 | 3.072604807 |
| O | -0.054475417 | 18.513338209 | 5.931231433 |
| O | 6.442245812 | 18.480711784 | 8.823126324 |
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| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
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| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
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TS9-B1:

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| Ti | 0.000000000 | 3.247190143 | 2.957400000 |

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|----|-------------|-------------|--------------|
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
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| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 6.494400000 | 6.494389931 | 4.436100000 |

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| Ti | 6.480795271 | 9.741036074 | 0.015020161 |
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| Ti | -0.027903449 | 13.182123096 | 10.390578608 |
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| O | 3.242583261 | 11.073555618 | 0.002758899 |
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TS9-B2:

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| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
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| H | 6.457698847 | 0.932897449 | 6.856699960 |
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TS9-B3:

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| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |

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| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
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| O | 2.018655261 | 19.947092470 | 1.495528789 |
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| H | 6.457700016 | 0.932899949 | 0.941899960 |
| H | 0.834099951 | 0.932899949 | 5.475599957 |
| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
| H | -0.036699984 | 0.932899949 | 6.856699960 |
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TS9-E1:

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| Ti | 3.247200000 | 3.247194072 | 1.478700000 |
| Ti | 3.247200000 | 3.247194072 | 4.436100000 |
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| Ti | 0.000000000 | 3.247194072 | 0.000000000 |
| Ti | 3.247200000 | 3.247194072 | 7.393500000 |
| Ti | 3.247200000 | 3.247194072 | 10.350900000 |
| Ti | 0.000000000 | 3.247194072 | 8.872200000 |
| Ti | 0.000000000 | 3.247194072 | 5.914800000 |
| Ti | 9.741600000 | 3.247194072 | 1.478700000 |
| Ti | 9.741600000 | 3.247194072 | 4.436100000 |
| Ti | 6.494400000 | 3.247194072 | 2.957400000 |
| Ti | 6.494400000 | 3.247194072 | 0.000000000 |
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| Ti | 9.741600000 | 3.247194072 | 10.350900000 |
| Ti | 6.494400000 | 3.247194072 | 8.872200000 |
| Ti | 6.494400000 | 3.247194072 | 5.914800000 |
| Ti | 0.000000000 | 6.494391717 | 4.436100000 |
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| Ti | 3.247200000 | 6.494391717 | 0.000000000 |
| Ti | 0.000000000 | 6.494391717 | 10.350900000 |
| Ti | 0.000000000 | 6.494391717 | 7.393500000 |

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|----|--------------|-------------|--------------|
| Ti | 3.247200000 | 6.494391717 | 8.872200000 |
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| Ti | 3.225286466 | 9.738071042 | 4.435780601 |
| Ti | -0.019392538 | 9.837230486 | 2.962167329 |
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| Ti | -0.018244328 | 9.837019744 | 8.877274898 |
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| O | 9.717201578 | 11.079804296 | 2.963137356 |
| O | 9.715074922 | 11.076757467 | 0.003477902 |
| O | 3.235001698 | 11.073139135 | 2.963515903 |
| O | 3.236996648 | 11.072885530 | 0.004010234 |
| O | 3.236465406 | 11.072335458 | 8.877736253 |
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| O | 9.715655911 | 11.075203692 | 8.877523320 |
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| O | -0.040017454 | 11.805381675 | 0.008280720 |
| O | -0.039647013 | 11.803456423 | 5.921613850 |
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| O | 8.421585144 | 13.094472305 | 1.494551664 |
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| O | 6.449189754 | 14.381969869 | 2.976670418 |
| O | 6.444320772 | 14.388424288 | 5.931893772 |
| O | 6.451304720 | 14.392014045 | 8.873560404 |
| O | 6.444924622 | 14.378855175 | 0.039155976 |
| O | 9.690248519 | 15.120373932 | 8.873028072 |
| O | 3.170338906 | 15.112222862 | 8.878363222 |
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| O | 9.691934596 | 15.123292172 | 0.034495114 |
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| O | 6.426475330 | 18.447342761 | 9.034206372 |
| O | -0.067422003 | 18.516962614 | 8.878055652 |
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| O | 4.456611067 | 20.036640653 | 10.382626987 |
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9-Eb:

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| O | 6.438669086 | 21.247915354 | 8.841118081 |
| O | 6.463668110 | 21.125920770 | 0.120105456 |
| H | 0.000000000 | 0.932897449 | 9.814799089 |
| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |

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| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 7.310799334 | 0.932897449 | 2.486099272 |
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| H | 8.230171796 | 21.195070561 | 1.359529793 |

TS9-E2:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |

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|----|-------------|-------------|--------------|
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
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| Ti | 3.226672111 | 9.739556951 | 4.436469793 |

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| Ti | -0.011633678 | 9.839118591 | 0.001868840 |
| Ti | 3.227046838 | 9.739586955 | 7.393522831 |
| Ti | 3.226537417 | 9.738546461 | 10.350799567 |
| Ti | -0.012103483 | 9.839867975 | 8.871604380 |
| Ti | -0.014486019 | 9.840371255 | 5.914374134 |
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| Ti | 6.477660164 | 9.752125386 | 0.005119496 |
| Ti | 9.736901172 | 9.740327767 | 7.394151929 |
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| Ti | 6.487793377 | 9.750199419 | 8.883475738 |
| Ti | 6.475177485 | 9.734178031 | 5.924362102 |
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| Ti | -0.032757883 | 13.183804745 | 4.473687253 |
| Ti | 3.211282721 | 12.995950445 | 2.957543138 |
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| Ti | 6.455768581 | 16.269447256 | 5.921057740 |
| Ti | 3.194780710 | 16.328698961 | 7.393706781 |
| Ti | 3.180312876 | 16.317703232 | 10.350879298 |
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| Ti | -0.086168608 | 20.008686983 | 1.488876295 |
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| O | 6.464703577 | 11.787012836 | 5.919859875 |
| O | -0.027501706 | 11.803765749 | -0.003618083 |
| O | -0.028372345 | 11.803557865 | 5.911220008 |
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| O | -0.028623678 | 11.803781822 | 8.869046938 |
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| O | -0.034890644 | 14.419532657 | 2.965030447 |
| O | -0.029154401 | 14.417957807 | 5.922544603 |
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| O | -0.030543943 | 14.419184039 | 0.007940264 |
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| O | 1.237261003 | 16.484975902 | 10.349843025 |
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| O | 3.221131998 | 17.757283972 | 0.000965532 |
| O | 9.671367610 | 17.753696001 | 2.966503114 |
| O | 9.660873309 | 17.765075709 | 5.923863603 |
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| O | -0.045250381 | 18.520568444 | 0.006855371 |
| O | 6.363226498 | 18.405732300 | 2.812428015 |
| O | -0.041690801 | 18.535665426 | 5.915410289 |
| O | 6.449327695 | 18.461332097 | 8.971541432 |
| O | -0.057002128 | 18.524611832 | 8.870413376 |
| O | -0.078674980 | 18.529441037 | 2.983402762 |
| O | 2.024722849 | 20.010554014 | 4.453148583 |
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| O | 2.016929050 | 19.974950412 | 7.380817486 |

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| O | 10.888048119 | 19.922313146 | 10.400437160 |
| O | 1.958130960 | 19.914251731 | 1.501208890 |
| O | -0.063905675 | 21.127551342 | 2.967574047 |
| O | -0.036002616 | 21.139242519 | 5.931668655 |
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| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 7.328499172 | 0.932897449 | 5.475598892 |
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| H | 6.430062577 | 20.830786675 | 3.051096110 |

TS9-E3:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |

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| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
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| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |

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|----|--------------|-------------|--------------|
| Ti | 6.494400000 | 6.494389931 | 4.436100000 |
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| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 3.230292999 | 9.738938298 | 4.436014472 |
| Ti | -0.011977882 | 9.837452300 | 2.957396451 |
| Ti | -0.011835784 | 9.837271920 | 0.000333003 |
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| Ti | -0.008189958 | 9.837887000 | 5.914500475 |
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| Ti | 6.481664611 | 9.742414469 | 0.001783667 |
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| Ti | 3.214825156 | 12.997019157 | 5.918192374 |
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| Ti | 9.714028804 | 12.998185024 | 5.921857776 |
| Ti | -0.029577965 | 13.183365045 | 7.429791083 |
| Ti | -0.028551201 | 13.175961216 | 10.387020856 |
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| Ti | -0.038160965 | 16.643497781 | 2.958444435 |
| Ti | 6.463490163 | 16.293021421 | 5.922322916 |
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| Ti | 6.459239448 | 16.320260354 | -0.011884489 |
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| Ti | 6.463653562 | 19.542869056 | 4.432963263 |
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| Ti | 3.223740798 | 19.583672269 | 0.004537716 |
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| Ti | 6.440584284 | 20.074103070 | 10.419104742 |
| Ti | 3.224132281 | 19.574212456 | 5.906812063 |
| Ti | -0.034965590 | 20.007407887 | 1.476063064 |
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| Ti | -0.035972741 | 20.001820011 | 10.350591721 |
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| O | 0.000000000 | 1.266689833 | 5.914800000 |
| O | 6.494400000 | 1.266689833 | 2.957400000 |
| O | 6.494400000 | 1.266689833 | 0.000000000 |
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| O | 1.270502589 | 9.787922585 | 4.434239677 |

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| O | 7.759408976 | 9.782884424 | 1.479895736 |
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| O | 9.724693518 | 11.075774838 | 2.958079611 |
| O | 9.723263841 | 11.076114169 | 0.000712733 |
| O | 3.242213859 | 11.075357641 | 2.957455244 |
| O | 3.242224770 | 11.076120955 | 0.000006861 |
| O | 3.243346613 | 11.075469441 | 8.872376734 |
| O | 3.241979152 | 11.074846145 | 5.914547556 |
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| O | 6.468843887 | 11.791009789 | 8.878403087 |
| O | -0.023462059 | 11.801652614 | 2.952743869 |
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| O | 6.470129388 | 11.794171633 | 5.912231794 |
| O | -0.022998489 | 11.801205770 | -0.004212166 |
| O | -0.022767678 | 11.801238632 | 5.909764021 |
| O | 6.468528129 | 11.795223913 | 2.959353895 |
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| O | 8.435074922 | 13.100362721 | 1.481761974 |
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| O | 4.499582824 | 13.110219729 | 1.479663758 |
| O | 4.500480610 | 13.110477263 | 4.437331698 |
| O | 1.963100995 | 13.107157899 | 7.393985132 |
| O | 1.962818488 | 13.104488620 | 10.351709736 |
| O | 4.499609581 | 13.108969923 | 7.393584108 |
| O | 4.499470990 | 13.115679732 | 10.352934928 |
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| O | -0.027775510 | 14.414130519 | 8.880052134 |
| O | -0.026639120 | 14.413538656 | 0.005574462 |
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| O | 6.468829859 | 14.413489721 | 5.913990027 |
| O | 6.463996337 | 14.411954519 | 8.863207730 |
| O | 6.469045083 | 14.414215887 | 0.010674203 |
| O | 9.704587765 | 15.119271645 | 8.872218691 |
| O | 3.213667464 | 15.118468325 | 8.872009780 |
| O | 9.688234476 | 15.120290350 | 5.911278683 |
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| O | 3.230218443 | 15.120869354 | 2.958656067 |
| O | 9.700734637 | 15.121704464 | 0.002005827 |
| O | 3.212000222 | 15.120508236 | 0.000810682 |
| O | 3.225346474 | 15.118530119 | 5.910523954 |
| O | 1.250324748 | 16.479834870 | 10.351281031 |
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| O | 3.222169154 | 17.747891311 | 2.952683657 |
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| O | -0.034074688 | 18.520134816 | 5.915163405 |
| O | 6.451887917 | 18.506794136 | 8.959035652 |
| O | -0.037005741 | 18.515567430 | 8.863260371 |
| O | -0.040196829 | 18.519053960 | 2.960038711 |
| O | 2.016933856 | 19.969915466 | 4.435955087 |
| O | 4.508771361 | 19.976099135 | 1.505547514 |
| O | 4.510421977 | 19.901847246 | 4.443101704 |
| O | 2.017140118 | 19.970401244 | 7.389963896 |
| O | 2.001558623 | 19.932004418 | 10.351954964 |
| O | 4.524430918 | 19.972095752 | 7.374932970 |
| O | 4.474114385 | 20.023359266 | 10.321479193 |
| O | 8.415834873 | 19.982169932 | 1.509736493 |
| O | 8.414585999 | 19.917482870 | 4.432277856 |
| O | 10.906606127 | 19.955072446 | 1.465882747 |
| O | 10.903330481 | 19.969572207 | 4.444729338 |
| O | 8.393996933 | 20.024025068 | 7.378682480 |
| O | 8.445358025 | 20.052909574 | 10.317262059 |
| O | 10.899439946 | 19.967098668 | 7.389003214 |
| O | 10.915760244 | 19.929890212 | 10.350268299 |
| O | 2.011608967 | 19.950691871 | 1.473433344 |

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| O | -0.032317433 | 21.121913459 | 5.914768770 |
| O | -0.035984172 | 21.116413094 | 8.873138679 |
| O | -0.033320688 | 21.116983526 | -0.003414141 |
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| H | 0.000000000 | 0.932899949 | 9.814800036 |
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| O | 10.850613878 | 19.983026115 | 4.458420444 |

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| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |

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TS9-E4:

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| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |

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| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 3.230034911 | 9.738783992 | 10.351153982 |
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| Ti | 6.484120664 | 9.750982379 | 0.009698734 |
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| Ti | 9.702442535 | 16.331065343 | 4.442828558 |
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| Ti | 3.196746955 | 19.576032695 | 0.013608890 |
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| Ti | 6.420817409 | 20.106164421 | 10.306835213 |
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| Ti | 9.651072350 | 19.592568079 | 5.929865942 |
| Ti | -0.070887935 | 20.012087787 | 7.402477247 |
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| O | -0.026335961 | 11.801825851 | 8.870809904 |
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| O | -0.028211933 | 14.413912990 | 0.010479251 |
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| O | 6.467276658 | 14.390081648 | 5.922355920 |
| O | 6.466054152 | 14.423734994 | 8.852608526 |
| O | 6.467106764 | 14.417657768 | 0.030974033 |
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| O | 9.681773198 | 17.737180262 | 8.887840624 |
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| O | 2.007651020 | 19.981944188 | 4.446069041 |
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| H | 6.457700016 | 0.932899949 | 6.856699960 |
| H | 0.834099951 | 0.932899949 | -0.439200043 |
| H | 0.000000000 | 0.932899949 | 3.900000036 |
| H | 0.816399984 | 0.932899949 | 2.486099982 |

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| H | 6.457700016 | 0.932899949 | 0.941899960 |
| H | 0.834099951 | 0.932899949 | 5.475599957 |
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| H | 7.310799984 | 0.932899949 | 8.400899982 |
| H | -0.036699984 | 0.932899949 | 6.856699960 |
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| H | 6.431255468 | 21.286103581 | 6.600889592 |

TS9-F1:

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| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |

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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
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TS9-G1

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| Ti | 0.000000000 | 3.247190143 | 0.000000000 |

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9-Ge:

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| O | 10.885797420 | 19.931597936 | 10.366952294 |
| O | 1.960766647 | 19.921719140 | 1.497538638 |
| O | -0.067059226 | 21.120570425 | 2.970810626 |
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| O | -0.065749695 | 21.116883156 | 8.885009446 |
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| O | 6.427450010 | 21.096459404 | 0.051928632 |
| H | 0.000000000 | 0.932897449 | 9.814799089 |
| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
| H | 0.000000000 | 0.932897449 | 3.899999089 |
| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
| H | 6.494400000 | 0.932897449 | 3.899999089 |

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| H | 7.310799334 | 0.932897449 | 2.486099272 |
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| H | 6.428841890 | 20.819695576 | 5.863091044 |
| H | 6.427990084 | 20.822278415 | 3.039808069 |

TS9-G2:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |

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| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
| Ti | 6.494400000 | 6.494389931 | 4.436100000 |
| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
| Ti | 9.741600000 | 6.494389931 | 5.914800000 |
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| Ti | 3.232271972 | 9.737472392 | 4.435798937 |
| Ti | -0.008574167 | 9.838083455 | 2.957331388 |
| Ti | -0.009223087 | 9.837760198 | 0.000268769 |
| Ti | 3.231758655 | 9.737372021 | 7.393803784 |
| Ti | 3.231565901 | 9.737835297 | 10.351061474 |

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| Ti | -0.008791859 | 9.838015589 | 8.872187816 |
| Ti | -0.008786793 | 9.837595176 | 5.914688329 |
| Ti | 9.741534277 | 9.736181865 | 1.482368359 |
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| Ti | 6.480866320 | 9.743408885 | 2.964817277 |
| Ti | 6.489713641 | 9.781965375 | 0.005205734 |
| Ti | 9.742399850 | 9.735875039 | 7.398485467 |
| Ti | 9.741946931 | 9.737423814 | 10.354561143 |
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| Ti | -0.032453426 | 13.176310190 | 4.469867830 |
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| Ti | 3.212928142 | 12.991027299 | 5.916131303 |
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| Ti | 6.459377779 | 13.061233300 | 4.464717340 |
| Ti | 9.709947853 | 12.992615007 | 2.960869030 |
| Ti | 9.708186442 | 12.989107047 | 5.917389381 |
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| Ti | -0.051902206 | 16.641753623 | 2.960398449 |
| Ti | 6.437907812 | 16.382614967 | 5.935572423 |
| Ti | 3.181749177 | 16.311811745 | 7.396746042 |
| Ti | 3.179340014 | 16.317159947 | 10.350519560 |
| Ti | -0.054074712 | 16.642157605 | 8.873780671 |
| Ti | 6.440197867 | 16.326843718 | -0.017156469 |
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| Ti | 9.701089881 | 16.317419624 | 10.350576342 |
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| Ti | 3.189925757 | 19.552681773 | 2.955460774 |
| Ti | 3.200307185 | 19.563824664 | 5.909077313 |
| Ti | -0.071094586 | 20.003871709 | 1.479790334 |
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| Ti | 9.656598695 | 19.561818686 | 5.906792544 |
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| O | 7.761416915 | 9.781697482 | 4.434371932 |
| O | 11.702732152 | 9.775848857 | 1.477846258 |
| O | 11.702624215 | 9.776406073 | 4.435258087 |
| O | 7.761477313 | 9.781457808 | 7.396786026 |
| O | 7.761051280 | 9.783478430 | 10.352123181 |
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| O | 11.702372882 | 9.776818270 | 10.349997638 |

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| O | 3.245503013 | 11.070369843 | 2.956894403 |
| O | 3.243575995 | 11.069490085 | 0.001545656 |
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| O | 6.464973224 | 11.797914624 | 8.872002801 |
| O | -0.028932812 | 11.793329022 | 2.952838033 |
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| O | -0.028482360 | 11.793187932 | -0.002817456 |
| O | -0.028596272 | 11.793367598 | 5.911014291 |
| O | 6.464090635 | 11.803742889 | 2.959542577 |
| O | -0.028874232 | 11.793000765 | 8.867374115 |
| O | 8.435788917 | 13.096169671 | 1.480536545 |
| O | 8.436223132 | 13.091916613 | 4.436825983 |
| O | 10.968281625 | 13.111880662 | 1.481344270 |
| O | 10.968569847 | 13.110218658 | 4.436938127 |
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| O | 10.969644150 | 13.105857014 | 10.353215289 |
| O | -0.029551858 | 14.404485324 | 2.964912151 |
| O | -0.029231944 | 14.404061340 | 5.922261284 |
| O | -0.029507436 | 14.404557477 | 8.880018301 |
| O | -0.029155050 | 14.404588195 | 0.005619415 |
| O | 6.463747471 | 14.427187233 | 2.959585400 |
| O | 6.463981399 | 14.409179155 | 5.909336736 |
| O | 6.466260674 | 14.389942701 | 8.882674283 |
| O | 6.463862682 | 14.407446070 | 0.002448609 |
| O | 9.698160387 | 15.110090797 | 8.877835385 |
| O | 3.180280274 | 15.110956268 | 8.877233377 |
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| O | -0.070865594 | 18.508650808 | 0.004984520 |
| O | 6.427332721 | 18.515294538 | 2.883647412 |
| O | -0.068824534 | 18.512237708 | 5.905290303 |
| O | 6.425097089 | 18.529180646 | 8.870515702 |
| O | -0.068971567 | 18.507869277 | 8.871787147 |
| O | -0.069401496 | 18.511110774 | 2.960773565 |
| O | 1.981004367 | 19.955628948 | 4.434790700 |
| O | 4.453041875 | 19.942910136 | 1.498284376 |
| O | 4.463491754 | 19.883057637 | 4.418198858 |
| O | 1.959211498 | 19.911524587 | 7.383926068 |
| O | 1.960165006 | 19.911281698 | 10.350070863 |
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| O | 4.409998940 | 19.974833611 | 10.335317341 |
| O | 8.403766849 | 19.933624631 | 1.496454692 |

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| O | 10.871966946 | 19.968688162 | 4.432970834 |
| O | 8.428205016 | 20.012003490 | 7.360133312 |
| O | 8.440072493 | 19.956805174 | 10.336068284 |
| O | 10.891627573 | 19.923111823 | 7.383885256 |
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| H | 6.457700016 | 0.932899949 | 0.941899960 |
| H | 0.834099951 | 0.932899949 | 5.475599957 |

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TS10-1:

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| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |

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| O | -0.044797332 | 21.117179623 | 2.963687669 |
| O | -0.045969571 | 21.112565089 | 5.929192483 |
| O | -0.045064901 | 21.128955455 | 8.885880578 |
| O | -0.044459104 | 21.125110664 | 0.004798204 |
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| H | 0.816399984 | 0.932899949 | 8.400899982 |
| H | 6.457700016 | 0.932899949 | 6.856699960 |

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| H | 0.834099951 | 0.932899949 | -0.439200043 |
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| H | 6.457700016 | 0.932899949 | 0.941899960 |
| H | 0.834099951 | 0.932899949 | 5.475599957 |
| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
| H | -0.036699984 | 0.932899949 | 6.856699960 |
| H | 7.328499951 | 0.932899949 | -0.439200043 |
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| H | 6.387741560 | 21.682101987 | 4.428698929 |

TS10-2:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |

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|----|-------------|-------------|--------------|
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
| Ti | 6.494400000 | 6.494389931 | 4.436100000 |
| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |

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|----|--------------|--------------|--------------|
| Ti | 6.494400000 | 6.494389931 | 10.350900000 |
| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
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| Ti | 3.230357163 | 9.740697458 | 4.436274723 |
| Ti | -0.006555188 | 9.839176098 | 2.957417863 |
| Ti | -0.008912915 | 9.842841936 | -0.000134976 |
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| Ti | -0.010292585 | 9.839619371 | 8.872512065 |
| Ti | -0.012295588 | 9.840848461 | 5.916313834 |
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| Ti | 6.484837256 | 9.737400597 | 0.016321063 |
| Ti | 9.735264193 | 9.739538377 | 7.396594978 |
| Ti | 9.738935737 | 9.740873552 | 10.353231496 |
| Ti | 6.485179641 | 9.735681800 | 8.885048129 |
| Ti | 6.480463407 | 9.741914046 | 5.924304137 |
| Ti | -0.025689638 | 13.186825856 | 1.513829535 |
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| Ti | 9.719348237 | 12.998900118 | 5.925364424 |
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| Ti | 9.718295495 | 12.999382681 | 8.882570537 |
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| Ti | 9.720890917 | 16.319415957 | 4.442341179 |
| Ti | 6.454124719 | 16.342943688 | 2.960973604 |
| Ti | -0.030204415 | 16.651375958 | 5.922676621 |
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| Ti | 3.206391528 | 16.332850935 | 10.361963279 |
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| Ti | 3.284409795 | 19.634526801 | 2.957369006 |
| Ti | 3.183761921 | 19.578730549 | 5.960200704 |
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| O | 11.703482775 | 9.785711938 | 10.351165693 |
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| O | 3.244044241 | 11.076531723 | 0.001892381 |
| O | 3.244401563 | 11.075573026 | 8.874416394 |
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| O | 9.724811197 | 11.075676254 | 5.916954998 |
| O | 6.470742070 | 11.773544639 | 8.877903878 |
| O | -0.020748439 | 11.807399797 | 2.954436449 |
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| O | 8.442364626 | 13.103188807 | 1.482530543 |
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| O | 10.975394812 | 13.117407459 | 10.355651595 |
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| O | -0.024816661 | 14.421598285 | 8.881103667 |
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| O | 6.475230609 | 14.383373268 | -0.010322154 |
| O | 9.709899275 | 15.132110473 | 8.882850899 |
| O | 3.219174716 | 15.128597512 | 8.885203096 |
| O | 9.721919760 | 15.124415177 | 5.923714432 |
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| O | 1.256574439 | 16.492856580 | 10.354177272 |
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| O | 5.182043081 | 16.414305198 | 7.389104830 |
| O | 7.744998812 | 16.410118934 | 1.484052066 |
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| O | 9.653739990 | 17.795782597 | 8.871701382 |
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| O | 10.926101407 | 19.951998829 | 1.465738071 |
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| O | 8.251275739 | 20.055080216 | 10.356333454 |
| O | 10.887966809 | 19.992750963 | 7.432674430 |
| O | 10.858463789 | 20.018543992 | 10.336157124 |
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| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
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11-Ea:

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| H | 0.816399334 | 0.932897449 | 8.400899272 |
| H | 6.457698847 | 0.932897449 | 6.856699960 |
| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |

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| H | -0.036701153 | 0.932897449 | 6.856699960 |
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| H | 7.310799334 | 0.932897449 | 2.486099272 |
| H | -0.036701153 | 0.932897449 | 0.941899960 |
| H | 7.328499172 | 0.932897449 | 5.475598892 |
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| H | 7.276697889 | 21.636874979 | 8.782728358 |

TS11-E1:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |

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|----|--------------|-------------|--------------|
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
| Ti | 9.741600000 | 6.494389931 | 5.914800000 |
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| Ti | -0.016857384 | 9.839624014 | 2.961886376 |

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| Ti | -0.009021241 | 9.840575568 | 0.001045618 |
| Ti | 3.229142321 | 9.738921153 | 7.392947084 |
| Ti | 3.231675397 | 9.738044967 | 10.350593377 |
| Ti | -0.011012424 | 9.840201233 | 8.871842391 |
| Ti | -0.015991031 | 9.842215783 | 5.916265214 |
| Ti | 9.739955228 | 9.735866110 | 1.482939019 |
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| Ti | 6.475518701 | 9.753375908 | 2.960764930 |
| Ti | 6.487877155 | 9.756467385 | 0.009461787 |
| Ti | 9.734345625 | 9.741282892 | 7.391614362 |
| Ti | 9.742047594 | 9.735248886 | 10.349701307 |
| Ti | 6.482389906 | 9.757442513 | 8.887274696 |
| Ti | 6.479437422 | 9.728441206 | 5.926823960 |
| Ti | -0.035983652 | 13.182979994 | 1.515277833 |
| Ti | -0.035253162 | 13.187644535 | 4.471987694 |
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| Ti | 3.210475467 | 12.999602353 | 5.914890851 |
| Ti | 6.455353459 | 13.100946012 | 1.426148303 |
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| Ti | -0.034716335 | 13.186167555 | 7.429952676 |

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| Ti | -0.035887535 | 13.186944443 | 10.386611670 |
| Ti | 3.210251020 | 12.995823286 | 8.872043258 |
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| Ti | -0.051218475 | 16.652356086 | 5.917756335 |
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| Ti | 6.451688150 | 16.249722524 | 5.923166958 |
| Ti | 3.194216217 | 16.330087358 | 7.397647339 |
| Ti | 3.187512437 | 16.329776960 | 10.358302609 |
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| Ti | 6.446472237 | 16.563163665 | 0.008343417 |
| Ti | 9.693308031 | 16.340002231 | 7.396361344 |
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| Ti | 6.442910319 | 16.286877043 | 8.889417983 |

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| Ti | 6.414249882 | 19.610746537 | 7.573643396 |
| Ti | 6.425084489 | 19.763905211 | 10.322406279 |
| Ti | 3.249708267 | 19.607596123 | 8.894476083 |
| Ti | 3.206700792 | 19.595063050 | 0.003363155 |
| Ti | 6.430803328 | 19.812805916 | 1.593436947 |
| Ti | 6.269703112 | 19.495707866 | 4.299818868 |
| Ti | 3.185678679 | 19.599125369 | 2.956131157 |
| Ti | 3.145711492 | 19.573759897 | 5.952255944 |
| Ti | -0.036595295 | 20.016824123 | 1.481607242 |
| Ti | -0.080146481 | 20.013043984 | 4.445667544 |
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| Ti | 9.644587692 | 19.622453074 | 5.956469056 |
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| O | 0.000000000 | 1.266689833 | 0.000000000 |
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| O | 9.741600000 | 1.980499953 | 2.957400000 |
| O | 9.741600000 | 1.980499953 | 0.000000000 |
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| O | 1.266699988 | 3.247190143 | 4.436100000 |
| O | 5.227599998 | 3.247190143 | 1.478700000 |
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| O | 0.000000000 | 5.227600085 | 8.872200000 |
| O | 0.000000000 | 5.227600085 | 5.914800000 |
| O | 6.494400000 | 5.227600085 | 0.000000000 |
| O | 6.494400000 | 5.227600085 | 2.957400000 |
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| O | 8.474900012 | 6.494389931 | 7.393500000 |

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| O | 11.008299988 | 6.494389931 | 7.393500000 |
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| O | 7.761298197 | 9.775213774 | 10.354047738 |
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| O | 6.461270507 | 11.772452353 | 8.878152891 |
| O | -0.031600971 | 11.805282377 | 2.954501748 |
| O | 6.463770072 | 11.778910701 | 0.002081063 |
| O | 6.461521710 | 11.776582895 | 5.921818738 |
| O | -0.031026087 | 11.805195937 | -0.002959056 |
| O | -0.031146363 | 11.805647782 | 5.911624462 |
| O | 6.459233993 | 11.770401727 | 2.956570154 |
| O | -0.030882690 | 11.805431682 | 8.867482592 |
| O | 8.433452491 | 13.101361424 | 1.485252652 |
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| O | 1.953660735 | 13.104000342 | 1.481385792 |
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| O | -0.034598137 | 14.423442098 | 5.922301386 |
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| O | -0.033660995 | 14.421724016 | 0.007370905 |
| O | 6.454886772 | 14.367486182 | 2.978716939 |
| O | 6.454635178 | 14.392753070 | 5.914640774 |
| O | 6.456212928 | 14.379267014 | 8.861750796 |
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| O | 3.192998777 | 15.132013317 | 8.876907589 |
| O | 9.685342650 | 15.137156135 | 5.917795728 |
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| O | 9.701829853 | 15.123414689 | 0.003011816 |
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| O | 3.203207324 | 15.127672033 | 5.919164294 |
| O | 1.237959541 | 16.505347148 | 10.352901095 |
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| O | 11.645638323 | 16.493470946 | 4.444690301 |
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| O | 11.649219206 | 16.487526951 | 10.353815405 |
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| O | 3.245853711 | 17.765456474 | 0.011815759 |
| O | 9.644226214 | 17.777564849 | 2.955592201 |
| O | 9.629308966 | 17.796123356 | 5.916971086 |
| O | 3.234487732 | 17.774531951 | 2.951938865 |
| O | 3.202311357 | 17.755508025 | 5.927582001 |
| O | 9.629017368 | 17.776362905 | 8.880983596 |
| O | 9.639632205 | 17.757984779 | 0.000544398 |
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| O | -0.057261644 | 18.528895966 | 0.005045916 |
| O | 6.410574052 | 18.361062865 | 2.841626662 |
| O | -0.052202767 | 18.530392948 | 5.922219998 |
| O | 6.467601248 | 18.378492296 | 8.992119258 |
| O | -0.064707474 | 18.532458576 | 8.874662213 |
| O | -0.070582178 | 18.527472922 | 2.962794061 |
| O | 1.974059775 | 19.965993880 | 4.429621283 |
| O | 4.501079783 | 20.102148537 | 1.460972753 |
| O | 4.451731305 | 19.976276658 | 4.486472684 |
| O | 1.985279371 | 19.980998706 | 7.447528267 |
| O | 1.995057729 | 19.956704446 | 10.354827545 |

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| O | 4.513933629 | 20.105436468 | 10.424368914 |
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| O | 8.359206562 | 20.180381305 | 4.405803921 |
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| O | 8.347790316 | 20.086184298 | 7.390625171 |
| O | 8.362557283 | 20.126742479 | 10.398293045 |
| O | 10.863245356 | 19.970574838 | 7.396367850 |
| O | 10.878563957 | 19.959848787 | 10.341499963 |
| O | 1.985911016 | 19.966115681 | 1.485756593 |
| O | -0.055147457 | 21.130144182 | 0.004833693 |
| O | 6.567245477 | 21.008444994 | 3.137277349 |
| O | -0.076791604 | 21.124527373 | 2.964769604 |
| O | -0.068523064 | 21.124208046 | 5.924275273 |
| O | -0.075831732 | 21.134068268 | 8.881919318 |
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11-Eb:

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| H | 0.000000000 | 0.932897449 | 3.899999089 |
| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |
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| H | 7.310799334 | 0.932897449 | 2.486099272 |
| H | -0.036701153 | 0.932897449 | 0.941899960 |
| H | 7.328499172 | 0.932897449 | 5.475598892 |
| H | 8.226203848 | 21.176538129 | 4.285370076 |
| H | 7.274202091 | 21.682574549 | 8.775117548 |

TS11-E2:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |

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|----|-------------|-------------|--------------|
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
| Ti | 6.494400000 | 6.494389931 | 4.436100000 |

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|----|--------------|-------------|--------------|
| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
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| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 3.226627689 | 9.738104975 | 1.478798777 |
| Ti | 3.225916682 | 9.738551819 | 4.436676220 |
| Ti | -0.014745795 | 9.840589855 | 2.958607920 |
| Ti | -0.011032427 | 9.843275208 | 0.000225590 |
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| Ti | 3.230770986 | 9.738712197 | 10.351054258 |
| Ti | -0.011357537 | 9.839345763 | 8.873020146 |
| Ti | -0.015604485 | 9.840494843 | 5.915030204 |
| Ti | 9.737930274 | 9.739344423 | 1.482382081 |
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| Ti | 6.487602571 | 9.733989077 | 0.007783285 |
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| Ti | 6.482263785 | 9.752704391 | 5.921790347 |
| Ti | -0.033902846 | 13.184451973 | 1.515132802 |
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| Ti | 3.210137239 | 12.995876150 | 2.957788129 |
| Ti | 3.209723545 | 12.997245258 | 5.915593766 |
| Ti | 6.457918487 | 13.007809502 | 1.505364273 |
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| Ti | -0.033415896 | 13.187319849 | 10.386591204 |
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| Ti | 6.439331644 | 16.480818214 | 5.913286521 |
| Ti | 3.183142875 | 16.321019382 | 7.396179523 |
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| Ti | 9.697331832 | 16.325197430 | 10.354968436 |
| Ti | 6.447645645 | 16.293377182 | 8.863172122 |
| Ti | -0.050686844 | 16.652676485 | 0.001776096 |
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| Ti | 6.444844351 | 19.573319124 | 10.188854354 |
| Ti | 3.237437098 | 19.600664142 | 8.894751121 |
| Ti | 3.224593253 | 19.574567503 | 0.002710043 |
| Ti | 6.455030947 | 19.641118023 | 1.696240193 |
| Ti | 6.232464222 | 19.829612050 | 4.409528589 |
| Ti | 3.153354102 | 19.584702761 | 2.929822955 |
| Ti | 3.125807195 | 19.572292561 | 5.938391298 |
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| O | 0.000000000 | 1.266689833 | 5.914800000 |
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| O | 1.980500012 | 6.494389931 | 1.478700000 |
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| O | 6.494400000 | 7.761090122 | 5.914800000 |
| O | 3.247200000 | 8.474889884 | 2.957400000 |
| O | 3.247200000 | 8.474889884 | 0.000000000 |
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| O | 9.741600000 | 8.474889884 | 2.957400000 |
| O | 9.741600000 | 8.474889884 | 0.000000000 |
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| O | 9.722265132 | 11.075595886 | 0.001204253 |
| O | 3.239861458 | 11.073904236 | 2.957235569 |
| O | 3.241660926 | 11.074047826 | 0.000597395 |
| O | 3.240555579 | 11.074214991 | 8.872989626 |
| O | 3.241617414 | 11.074932585 | 5.915440691 |
| O | 9.721970546 | 11.074601827 | 8.874243800 |
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| O | 6.465607857 | 11.784883628 | 8.868604275 |

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| O | -0.028092177 | 11.804005066 | 2.953636531 |
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| O | -0.029011784 | 11.803459637 | -0.002298610 |
| O | -0.029555235 | 11.804038285 | 5.911480023 |
| O | 6.465448354 | 11.785514068 | 2.964564479 |
| O | -0.028692129 | 11.802963501 | 8.869426195 |
| O | 8.430327516 | 13.099639055 | 1.478556507 |
| O | 8.433923205 | 13.105339803 | 4.436683909 |
| O | 10.965878308 | 13.121201528 | 1.481091709 |
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| O | 1.956015604 | 13.103832820 | 4.437295736 |
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| O | 4.487916933 | 13.114638524 | 4.432951315 |
| O | 1.956061065 | 13.102934130 | 7.394728031 |
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| O | 4.488602612 | 13.116240163 | 7.399928678 |
| O | 4.491751097 | 13.108614876 | 10.351627047 |
| O | 8.433769028 | 13.104220371 | 7.398080421 |
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| O | -0.032733594 | 14.419105815 | 2.965704379 |
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| O | -0.030560698 | 14.415934684 | 8.880651539 |
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| O | 6.465616819 | 14.391275019 | 2.943466387 |
| O | 6.449573963 | 14.403615567 | 5.915756778 |
| O | 6.467213013 | 14.391242158 | 8.890486551 |
| O | 6.450961166 | 14.403333388 | 0.000059739 |
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| O | 3.190443750 | 15.124428393 | 8.884156650 |
| O | 9.705665965 | 15.116367335 | 5.916584377 |
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| O | 9.692598063 | 15.130734221 | 0.009700627 |
| O | 3.210349476 | 15.125363516 | -0.000710722 |
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| O | 11.648147759 | 16.493371647 | 1.486074691 |
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| O | 3.218481763 | 17.754219642 | 0.001174561 |
| O | 9.625626901 | 17.791317725 | 2.976418330 |
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| O | 9.661635752 | 17.764492418 | 0.001886585 |
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| O | 6.482839448 | 18.426356078 | 8.764067756 |
| O | -0.048029725 | 18.532441431 | 8.882490806 |
| O | -0.056593630 | 18.523726359 | 2.959721204 |
| O | 1.944271001 | 19.920131074 | 4.437179096 |
| O | 4.484598944 | 19.944782524 | 1.467592242 |
| O | 4.367777417 | 20.082851718 | 4.485950171 |
| O | 1.986870758 | 19.981221950 | 7.431665484 |
| O | 2.007753372 | 19.973183038 | 10.344408389 |
| O | 4.487681186 | 20.041686315 | 7.346645202 |
| O | 4.527835542 | 19.994719079 | 10.360443057 |
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| O | 10.869085770 | 19.951009770 | 1.516732164 |
| O | 10.881313167 | 19.945073634 | 4.419081464 |
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| O | 10.913956229 | 19.977080335 | 7.460230064 |
| O | 10.882389029 | 19.965639548 | 10.356539525 |
| O | 1.972928710 | 19.963607852 | 1.468327925 |
| O | -0.074126952 | 21.127866026 | 0.013805380 |

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| O | -0.064870613 | 21.125979707 | 2.965900514 |
| O | -0.067923111 | 21.124910281 | 5.926019311 |
| O | -0.047161034 | 21.140027979 | 8.892975617 |
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| H | 0.816399984 | 0.932899949 | 8.400899982 |
| H | 6.457700016 | 0.932899949 | 6.856699960 |
| H | 0.834099951 | 0.932899949 | -0.439200043 |
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| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
| H | 7.328499172 | 0.932897449 | -0.439201108 |

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| H | 6.419440206 | 20.984161807 | 5.952407836 |
| H | 7.239568755 | 21.666902492 | 8.867168753 |

TS11-E3:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |

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| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
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| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
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| Ti | 3.232246774 | 9.737715995 | 4.435973896 |
| Ti | -0.007751716 | 9.838602809 | 2.956770547 |
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| Ti | 3.229090106 | 9.737965671 | 7.393921607 |

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| Ti | -0.010886043 | 9.838180610 | 8.874315014 |
| Ti | -0.009204643 | 9.838295625 | 5.914783084 |
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| Ti | 6.483864265 | 9.754417116 | 8.872066680 |
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| Ti | 3.178220640 | 19.571656406 | 5.915458909 |
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| O | 6.464724229 | 11.779568644 | 8.869442402 |
| O | -0.027218420 | 11.799713074 | 2.953241068 |
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| O | -0.027589250 | 11.799932031 | -0.004523048 |
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| O | 6.465117010 | 11.781214932 | 2.964452689 |
| O | -0.027754987 | 11.799756651 | 8.869201788 |
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| O | 8.436081424 | 13.102965563 | 4.433754900 |
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| O | 1.957995097 | 13.102005080 | 4.435322677 |
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| O | -0.029623296 | 14.411767709 | 2.962415159 |
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| O | 6.465242742 | 14.423089909 | 5.917618284 |
| O | 6.464932569 | 14.398353448 | 8.882542619 |
| O | 6.464682015 | 14.404797151 | 0.004649979 |
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| O | 9.671044579 | 17.753273446 | 8.876447181 |
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| O | 6.429774875 | 18.452950640 | 3.051037554 |
| O | -0.064964263 | 18.517910238 | 5.918795093 |
| O | 6.428414558 | 18.421048596 | 8.822435594 |
| O | -0.065807106 | 18.517779864 | 8.869783568 |
| O | -0.065743071 | 18.517329805 | 2.959501647 |
| O | 1.972530863 | 19.936868628 | 4.427298541 |
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| O | 10.886496087 | 19.950707230 | 10.349896968 |
| O | 1.981797593 | 19.938817098 | 1.489957284 |
| O | -0.058355561 | 21.118205829 | 0.006719686 |
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| O | -0.058777957 | 21.121234441 | 2.961220961 |
| O | -0.059807059 | 21.119469924 | 5.918942844 |
| O | -0.058964086 | 21.121890241 | 8.880397795 |
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| H | 6.457700016 | 0.932899949 | 0.941899960 |

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TS11-F1:

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| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |

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| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
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| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 6.421461913 | 19.784798311 | 1.715806114 |
| Ti | 6.421583229 | 19.672222463 | 4.376106065 |
| Ti | 3.203593741 | 19.582967534 | 2.951501761 |
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| Ti | -0.076996048 | 20.005466918 | 4.441195482 |
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| O | 6.462915668 | 11.788474099 | 5.910880499 |
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| O | 10.965661265 | 13.120861483 | 10.352408747 |
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| O | 10.863867520 | 19.969537202 | 10.336449079 |
| O | 1.962492339 | 19.930886772 | 1.484788340 |
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| H | 7.268061116 | 21.664010684 | 8.914243108 |

TS12-1:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |

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| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
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| Ti | 3.226927081 | 9.738634330 | 4.436567269 |
| Ti | -0.011832277 | 9.837262276 | 2.957775117 |
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| Ti | 9.740099794 | 9.740425637 | 10.354319109 |
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| Ti | 6.400378883 | 19.682888149 | 10.214254043 |
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| Ti | -0.073580253 | 20.004369631 | 4.444855560 |
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| O | 6.462729409 | 11.781646417 | 8.877182036 |
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| O | 6.462594455 | 11.788871294 | 5.911110584 |
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| O | 6.462860596 | 14.420577794 | 5.931118460 |
| O | 6.462786949 | 14.383369696 | 8.874569114 |
| O | 6.462916058 | 14.400235481 | 0.015170161 |
| O | 9.677739136 | 15.116856328 | 8.875325854 |
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| O | 3.195083479 | 15.120800417 | 0.013166463 |
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| O | 1.233659468 | 16.482857767 | 10.356589446 |
| O | 5.160667153 | 16.422865607 | 4.439094663 |
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| O | 10.874069573 | 19.947540029 | 4.438342419 |
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| O | 10.871733277 | 19.959498027 | 10.358138532 |
| O | 1.976194484 | 19.946457744 | 1.499144388 |
| O | -0.068589566 | 21.119352051 | 0.012119780 |
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| H | 0.834099951 | 0.932899949 | -0.439200043 |
| H | 0.000000000 | 0.932899949 | 3.900000036 |
| H | 0.816399984 | 0.932899949 | 2.486099982 |
| H | 6.457700016 | 0.932899949 | 0.941899960 |
| H | 0.834099951 | 0.932899949 | 5.475599957 |
| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
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| H | 7.227079504 | 21.902411976 | 8.907152683 |
| H | 5.619225826 | 21.901619014 | 8.909219550 |

13-Ea:

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| Ti | 3.247200000 | 3.247194072 | 4.436100000 |
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| Ti | 3.247200000 | 3.247194072 | 10.350900000 |
| Ti | 0.000000000 | 3.247194072 | 8.872200000 |
| Ti | 0.000000000 | 3.247194072 | 5.914800000 |
| Ti | 9.741600000 | 3.247194072 | 1.478700000 |
| Ti | 9.741600000 | 3.247194072 | 4.436100000 |
| Ti | 6.494400000 | 3.247194072 | 2.957400000 |
| Ti | 6.494400000 | 3.247194072 | 0.000000000 |
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| Ti | 9.741600000 | 3.247194072 | 10.350900000 |
| Ti | 6.494400000 | 3.247194072 | 8.872200000 |
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| Ti | 0.000000000 | 6.494391717 | 4.436100000 |

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| Ti | 6.494400000 | 6.494391717 | 7.393500000 |
| Ti | 9.741600000 | 6.494391717 | 8.872200000 |
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| Ti | -0.016314842 | 9.737530257 | 2.970009526 |
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| O | -0.034217695 | 11.804261171 | 2.964879856 |
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| O | -0.033513312 | 14.394997293 | 8.878271187 |
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| O | 6.453975477 | 14.419466934 | 8.869095085 |
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| O | 1.218999659 | 16.505941868 | 1.492923320 |
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| O | -0.066835169 | 21.084633923 | 5.846530550 |
| O | -0.068455522 | 21.272692535 | 8.884900850 |
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| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 6.494400000 | 0.932897449 | 9.814799089 |

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TS13-E1:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |

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| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |
| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
| Ti | 6.494400000 | 6.494389931 | 4.436100000 |
| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
| Ti | 9.741600000 | 6.494389931 | 5.914800000 |
| Ti | 3.227754078 | 9.749855446 | 1.479395226 |
| Ti | 3.229909569 | 9.746836835 | 4.435768061 |

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| Ti | -0.019292135 | 9.739745547 | 2.964839517 |
| Ti | -0.017583458 | 9.763950153 | 0.002383073 |
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| Ti | -0.013038028 | 9.772362328 | 8.877115672 |
| Ti | -0.016246911 | 9.763592249 | 5.925084654 |
| Ti | 9.725552078 | 9.747965198 | 1.481265012 |
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| Ti | 6.475203463 | 9.756811716 | 2.956156827 |
| Ti | 6.477662502 | 9.761328023 | 0.004409365 |
| Ti | 9.724622989 | 9.749397171 | 7.391779621 |
| Ti | 9.727674578 | 9.742605566 | 10.350460530 |
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| Ti | 9.705516984 | 13.017021782 | 5.915974679 |

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| Ti | -0.035958713 | 13.151681957 | 10.302364098 |
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| Ti | 3.207975772 | 13.009564375 | 0.001054609 |
| Ti | 6.458516751 | 13.015327274 | 7.425022572 |
| Ti | 6.458865371 | 13.134405047 | 10.396677831 |
| Ti | 9.704818186 | 13.009162179 | 8.872957686 |
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| Ti | 9.689249551 | 16.359177962 | 4.449685349 |
| Ti | 6.431382629 | 16.320630402 | 2.943530977 |
| Ti | -0.052691016 | 16.348666225 | 5.940713922 |
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| Ti | -0.054616215 | 16.287244949 | 2.962405695 |
| Ti | 6.452832593 | 16.263474686 | 5.921069333 |
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| Ti | 3.182615270 | 16.335269824 | 10.352708273 |
| Ti | -0.054469052 | 16.784595229 | 8.870382855 |
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| Ti | 9.691977199 | 16.332700558 | 10.353448451 |

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| Ti | 6.432649426 | 16.331879736 | 8.894102978 |
| Ti | -0.057088504 | 16.355631068 | -0.022043750 |
| Ti | 6.419973137 | 19.600482333 | 7.586503828 |
| Ti | 6.431693321 | 19.966722190 | 10.528849361 |
| Ti | 3.206372565 | 19.595257361 | 8.889810844 |
| Ti | 3.211659526 | 19.596443945 | 0.005916693 |
| Ti | 6.462776818 | 20.064589678 | 1.501916536 |
| Ti | 6.267850909 | 19.500383837 | 4.286434740 |
| Ti | 3.140554548 | 19.581548776 | 2.943756331 |
| Ti | 3.146859702 | 19.590960368 | 5.946025530 |
| Ti | -0.039839767 | 19.619022980 | 1.264679468 |
| Ti | -0.071028084 | 19.644859943 | 4.656697553 |
| Ti | 9.788054833 | 19.585088884 | 2.921272165 |
| Ti | 9.651290043 | 19.643618352 | 5.952779995 |
| Ti | -0.060352719 | 20.146425420 | 7.424160667 |
| Ti | -0.050156381 | 20.133737683 | 10.328779121 |
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| Ti | 9.672990950 | 19.594485831 | -0.018060369 |
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| O | 0.000000000 | 1.266689833 | 5.914800000 |

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| O | 6.494400000 | 1.266689833 | 5.914800000 |
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| O | 9.741600000 | 1.980499953 | 2.957400000 |
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| O | 3.247200000 | 1.980499953 | 5.914800000 |
| O | 3.247200000 | 1.980499953 | 2.957400000 |
| O | 3.247200000 | 1.980499953 | 0.000000000 |
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| O | 1.266699988 | 3.247190143 | 4.436100000 |
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| O | 7.761099988 | 3.247190143 | 4.436100000 |

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| O | 9.741600000 | 4.513899978 | 5.914800000 |
| O | 9.741600000 | 4.513899978 | 2.957400000 |
| O | 9.741600000 | 4.513899978 | 0.000000000 |
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| O | 3.247200000 | 4.513899978 | 2.957400000 |
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| O | 0.000000000 | 5.227600085 | 0.000000000 |
| O | 0.000000000 | 5.227600085 | 8.872200000 |
| O | 0.000000000 | 5.227600085 | 5.914800000 |
| O | 6.494400000 | 5.227600085 | 0.000000000 |
| O | 6.494400000 | 5.227600085 | 2.957400000 |
| O | 6.494400000 | 5.227600085 | 8.872200000 |
| O | 6.494400000 | 5.227600085 | 5.914800000 |

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| O | 8.474900012 | 6.494389931 | 7.393500000 |
| O | 11.008299988 | 6.494389931 | 7.393500000 |
| O | 8.474900012 | 6.494389931 | 10.350900000 |
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| O | 8.474900012 | 6.494389931 | 1.478700000 |
| O | 11.008299988 | 6.494389931 | 1.478700000 |
| O | 8.474900012 | 6.494389931 | 4.436100000 |
| O | 11.008299988 | 6.494389931 | 4.436100000 |
| O | 1.980500012 | 6.494389931 | 1.478700000 |
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| O | 1.980500012 | 6.494389931 | 7.393500000 |
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| O | 1.980500012 | 6.494389931 | 10.350900000 |
| O | 4.513899988 | 6.494389931 | 10.350900000 |
| O | 0.000000000 | 7.761090122 | 8.872200000 |
| O | 0.000000000 | 7.761090122 | 5.914800000 |
| O | 6.494400000 | 7.761090122 | 2.957400000 |
| O | 6.494400000 | 7.761090122 | 0.000000000 |
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| O | 0.000000000 | 7.761090122 | 0.000000000 |

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| O | 6.494400000 | 7.761090122 | 8.872200000 |
| O | 6.494400000 | 7.761090122 | 5.914800000 |
| O | 3.247200000 | 8.474889884 | 2.957400000 |
| O | 3.247200000 | 8.474889884 | 0.000000000 |
| O | 3.247200000 | 8.474889884 | 8.872200000 |
| O | 3.247200000 | 8.474889884 | 5.914800000 |
| O | 9.741600000 | 8.474889884 | 2.957400000 |
| O | 9.741600000 | 8.474889884 | 0.000000000 |
| O | 9.741600000 | 8.474889884 | 8.872200000 |
| O | 9.741600000 | 8.474889884 | 5.914800000 |
| O | 1.261023753 | 9.788065461 | 1.483129239 |
| O | 1.261463164 | 9.787478955 | 4.436627837 |
| O | 5.207589972 | 9.778412765 | 1.479136749 |
| O | 5.208193822 | 9.780677706 | 4.438773490 |
| O | 1.262942069 | 9.788318709 | 7.395822742 |
| O | 1.262806466 | 9.789993571 | 10.354314259 |
| O | 5.209126547 | 9.780187998 | 7.395743484 |
| O | 5.208418528 | 9.782121824 | 10.354375536 |
| O | 7.756473767 | 9.786978533 | 1.480105948 |
| O | 7.756192300 | 9.787994737 | 4.437627556 |
| O | 11.701694997 | 9.780514113 | 1.482527230 |
| O | 11.702001662 | 9.779331815 | 4.438212057 |

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| O | 7.757530666 | 9.787778995 | 7.395579170 |
| O | 7.757784987 | 9.788438367 | 10.354809446 |
| O | 11.702985044 | 9.781790709 | 7.396555704 |
| O | 11.702565636 | 9.781794281 | 10.353221441 |
| O | 9.727786411 | 11.084410972 | 2.958348379 |
| O | 9.724673515 | 11.082508936 | 0.002619665 |
| O | 3.232376922 | 11.081433438 | 2.958226534 |
| O | 3.234579173 | 11.081269845 | 0.003121358 |
| O | 3.233137676 | 11.080184703 | 8.872989508 |
| O | 3.232873743 | 11.079928241 | 5.914930007 |
| O | 9.728214002 | 11.082621808 | 8.873449442 |
| O | 9.725683265 | 11.084497412 | 5.915374800 |
| O | 6.461696540 | 11.803297473 | 8.885853961 |
| O | -0.036469043 | 11.807772346 | 2.960755229 |
| O | 6.463960098 | 11.818004404 | 0.005732033 |
| O | 6.462342343 | 11.796777332 | 5.919727383 |
| O | -0.034791280 | 11.804527992 | 0.003348605 |
| O | -0.033283670 | 11.804614075 | 5.915720106 |
| O | 6.459526631 | 11.801272565 | 2.947261796 |
| O | -0.034632297 | 11.810145872 | 8.874076766 |
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| O | 8.431025144 | 13.108568798 | 4.437605671 |

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| O | 10.979320287 | 13.126150749 | 1.482596907 |
| O | 10.978908282 | 13.129076847 | 4.439839100 |
| O | 1.937214316 | 13.105995604 | 1.484047452 |
| O | 1.937863496 | 13.108895984 | 4.437871364 |
| O | 4.481647499 | 13.133632803 | 1.484378799 |
| O | 4.485386715 | 13.117859304 | 4.438259967 |
| O | 1.943765607 | 13.107658322 | 7.390640904 |
| O | 1.942536997 | 13.102393702 | 10.356318903 |
| O | 4.486590257 | 13.116954185 | 7.394358947 |
| O | 4.483011583 | 13.124445168 | 10.352495576 |
| O | 8.431428317 | 13.108194464 | 7.395313833 |
| O | 8.436324055 | 13.112345723 | 10.349237350 |
| O | 10.974407014 | 13.127983132 | 7.388747458 |
| O | 10.974717446 | 13.125821420 | 10.357911404 |
| O | -0.039362299 | 14.431827842 | 2.960842414 |
| O | -0.036120424 | 14.431283485 | 5.908141828 |
| O | -0.034722959 | 14.396871111 | 8.873655396 |
| O | -0.035239654 | 14.429833652 | 0.013215083 |
| O | 6.447897758 | 14.416980179 | 2.979132986 |
| O | 6.456974202 | 14.410625059 | 5.917124635 |
| O | 6.449634231 | 14.423911446 | 8.865752986 |
| O | 6.466497979 | 14.440112144 | 0.001676136 |

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| O | 9.682444978 | 15.133336705 | 8.869590863 |
| O | 3.205407497 | 15.125569257 | 8.877550410 |
| O | 9.686460596 | 15.142638640 | 5.919717801 |
| O | 9.696721228 | 15.136906459 | 2.973088179 |
| O | 3.188536345 | 15.128037081 | 2.968970177 |
| O | 9.700599944 | 15.131008542 | 0.003941386 |
| O | 3.169134714 | 15.126968012 | -0.000947078 |
| O | 3.193615355 | 15.127059810 | 5.918603571 |
| O | 1.225828651 | 16.485117349 | 10.332220115 |
| O | 5.161485447 | 16.509914176 | 4.458815198 |
| O | 5.165153874 | 16.493055891 | 7.389078924 |
| O | 7.726095562 | 16.460159788 | 1.486320510 |
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| O | 11.657732714 | 16.503519408 | 1.483341698 |
| O | 11.655591251 | 16.503670499 | 4.444670072 |
| O | 1.222294658 | 16.505092471 | 4.437982089 |
| O | 1.218688837 | 16.510079197 | 1.485952491 |
| O | 5.151471732 | 16.431503884 | 1.466613224 |
| O | 7.715660620 | 16.485963532 | 7.404371639 |
| O | 7.723678866 | 16.471222311 | 10.361651923 |
| O | 1.226650842 | 16.477062364 | 7.416668863 |

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| O | 11.651326249 | 16.485576695 | 7.409455410 |
| O | 11.654102345 | 16.473220431 | 10.331255766 |
| O | 3.196336639 | 17.768246840 | 8.874407167 |
| O | 3.208627940 | 17.770797175 | 0.011263672 |
| O | 9.683074675 | 17.774001524 | 2.963000606 |
| O | 9.652497481 | 17.815231221 | 5.917938156 |
| O | 3.197283912 | 17.761764560 | 2.957235923 |
| O | 3.171971988 | 17.770057792 | 5.929281205 |
| O | 9.674123574 | 17.772349878 | 8.872855715 |
| O | 9.674554282 | 17.770064578 | 0.001753738 |
| O | 6.456547649 | 18.598203277 | 0.045587020 |
| O | 6.527546249 | 18.663194307 | 5.945216859 |
| O | -0.054309550 | 18.472207454 | -0.117177275 |
| O | 6.380153113 | 18.444921372 | 2.842711082 |
| O | -0.054738960 | 18.493500606 | 6.031097034 |
| O | 6.435756347 | 18.484282967 | 8.980993401 |
| O | -0.061941899 | 18.643906061 | 8.865272231 |
| O | -0.083594748 | 18.759927719 | 2.969907554 |
| O | 1.934603178 | 19.981814885 | 4.442627573 |
| O | 4.434070694 | 20.031085281 | 1.527696429 |
| O | 4.430077936 | 19.963016346 | 4.460566570 |
| O | 1.978143584 | 20.037094998 | 7.421682602 |

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| O | 4.465513331 | 19.994785873 | 10.352535324 |
| O | 8.470605785 | 19.999769742 | 1.512492672 |
| O | 8.402624224 | 20.169184478 | 4.387020527 |
| O | 10.955573903 | 19.974837183 | 1.462267621 |
| O | 10.903227610 | 19.994854096 | 4.460174892 |
| O | 8.367378595 | 20.067416121 | 7.400322840 |
| O | 8.422031180 | 20.037268592 | 10.343416122 |
| O | 10.878821265 | 20.032365449 | 7.384826656 |
| O | 10.906802388 | 19.996455735 | 10.340448075 |
| O | 1.930643672 | 19.957412753 | 1.482737206 |
| O | -0.052942219 | 21.078770296 | 0.081885911 |
| O | 6.596682514 | 21.053138717 | 3.172042177 |
| O | -0.064355348 | 21.100924632 | 5.845791319 |
| O | -0.066769576 | 21.283645401 | 8.877627066 |
| O | 6.420755582 | 21.189052628 | 8.821843404 |
| O | 6.442973704 | 21.212040646 | 0.054088007 |
| H | 0.000000000 | 0.932899949 | 9.814800036 |
| H | 0.816399984 | 0.932899949 | 8.400899982 |
| H | 6.457700016 | 0.932899949 | 6.856699960 |
| H | 0.834099951 | 0.932899949 | -0.439200043 |

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| H | 0.000000000 | 0.932899949 | 3.900000036 |
| H | 0.816399984 | 0.932899949 | 2.486099982 |
| H | 6.457700016 | 0.932899949 | 0.941899960 |
| H | 0.834099951 | 0.932899949 | 5.475599957 |
| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
| H | -0.036699984 | 0.932899949 | 6.856699960 |
| H | 7.328499951 | 0.932899949 | -0.439200043 |
| H | 6.494400000 | 0.932899949 | 3.900000036 |
| H | 7.310799984 | 0.932899949 | 2.486099982 |
| H | -0.036699984 | 0.932899949 | 0.941899960 |
| H | 7.328499951 | 0.932899949 | 5.475599957 |
| H | 7.734872614 | 20.897141456 | 3.771201835 |
| H | 7.248906403 | 21.702150333 | 8.780167013 |

13-Eb:

| | | | |
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| Ti | 3.247200000 | 3.247194072 | 4.436100000 |
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| Ti | 0.000000000 | 3.247194072 | 0.000000000 |
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| Ti | 3.247200000 | 3.247194072 | 10.350900000 |
| Ti | 0.000000000 | 3.247194072 | 8.872200000 |

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| Ti | 0.000000000 | 6.494391717 | 7.393500000 |
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| O | 5.207777920 | 9.778420624 | 4.439629006 |
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| O | 3.204281498 | 15.122198100 | 8.876054439 |
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| O | 1.222417272 | 16.471244457 | 10.330401196 |
| O | 5.158767281 | 16.500863702 | 4.454789348 |
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| O | 9.665522131 | 17.765367533 | 0.006557975 |
| O | 6.454974446 | 18.590712651 | 0.029453456 |
| O | 6.512677709 | 18.707884459 | 5.925610362 |
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| O | 10.911316645 | 19.988577558 | 10.354370923 |
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| H | 0.834099172 | 0.932897449 | -0.439201108 |
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| H | 0.816399334 | 0.932897449 | 2.486099272 |
| H | 6.457698847 | 0.932897449 | 0.941899960 |
| H | 0.834099172 | 0.932897449 | 5.475598892 |
| H | 6.494400000 | 0.932897449 | 9.814799089 |
| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |
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| H | 6.494400000 | 0.932897449 | 3.899999089 |
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| H | 7.252298558 | 21.693495983 | 8.785868999 |

TS13-E2:

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| H | 7.310799334 | 0.932897449 | 8.400899272 |
| H | -0.036701153 | 0.932897449 | 6.856699960 |

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| H | 7.328499172 | 0.932897449 | -0.439201108 |
| H | 6.494400000 | 0.932897449 | 3.899999089 |
| H | 7.310799334 | 0.932897449 | 2.486099272 |
| H | -0.036701153 | 0.932897449 | 0.941899960 |
| H | 7.328499172 | 0.932897449 | 5.475598892 |
| H | 6.429441842 | 20.851783002 | 5.952716589 |
| H | 7.117792780 | 21.772254535 | 8.750421602 |

TS13-E3:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |

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|----|--------------|-------------|--------------|
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
| Ti | 0.000000000 | 6.494389931 | 4.436100000 |
| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |
| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
| Ti | 6.494400000 | 6.494389931 | 4.436100000 |
| Ti | 6.494400000 | 6.494389931 | 1.478700000 |
| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
| Ti | 6.494400000 | 6.494389931 | 10.350900000 |
| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |
| Ti | 9.741600000 | 6.494389931 | 5.914800000 |
| Ti | 3.230787872 | 9.748258093 | 1.480886702 |
| Ti | 3.233965192 | 9.744802997 | 4.436591283 |
| Ti | -0.013754100 | 9.738748988 | 2.967065848 |
| Ti | -0.015683327 | 9.766985908 | 0.004210628 |

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| Ti | 3.235675817 | 9.748467406 | 7.393138251 |
| Ti | 3.233173265 | 9.739202619 | 10.351050473 |
| Ti | -0.012429632 | 9.768361803 | 8.878440351 |
| Ti | -0.015537722 | 9.766542636 | 5.925783902 |
| Ti | 9.729666410 | 9.748259879 | 1.480135640 |
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| Ti | 6.483280158 | 9.765325691 | 2.957718098 |
| Ti | 6.476632361 | 9.774637627 | 0.004640989 |
| Ti | 9.725071103 | 9.748838527 | 7.392886635 |
| Ti | 9.728334409 | 9.740090235 | 10.351209936 |
| Ti | 6.484585403 | 9.771735818 | 8.881155835 |
| Ti | 6.475562343 | 9.743145994 | 5.919114492 |
| Ti | -0.035061317 | 13.024438827 | 1.453453149 |
| Ti | -0.034190029 | 13.024244516 | 4.463759024 |
| Ti | 3.213186489 | 13.010331976 | 2.958696406 |
| Ti | 3.212337931 | 13.008878213 | 5.916271129 |
| Ti | 6.459917464 | 13.137371508 | 1.429479874 |
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| Ti | 9.705994972 | 13.010035151 | 2.958975821 |
| Ti | 9.708517267 | 13.009262907 | 5.916634889 |
| Ti | -0.033014023 | 13.140769811 | 7.445671848 |
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| Ti | 3.215168710 | 13.005012349 | 8.874377948 |
| Ti | 3.210312328 | 13.002843493 | 0.000925548 |
| Ti | 6.460356485 | 13.035409553 | 7.427276820 |
| Ti | 6.460325442 | 13.159688008 | 10.395330203 |
| Ti | 9.704445018 | 13.005487768 | 8.873361194 |
| Ti | 9.708650791 | 13.004467992 | 0.001307289 |
| Ti | 9.695192966 | 16.332173346 | 1.481165170 |
| Ti | 9.696395989 | 16.333201338 | 4.440465122 |
| Ti | 6.445444304 | 16.341848544 | 2.944751792 |
| Ti | -0.050936618 | 16.339160692 | 5.945061181 |
| Ti | 3.196049196 | 16.331406817 | 1.480830629 |
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| Ti | 3.199406541 | 16.324885604 | 10.355314097 |
| Ti | -0.045170500 | 16.773635576 | 8.876827030 |
| Ti | 6.444339736 | 16.761595425 | 0.011113199 |
| Ti | 9.690903934 | 16.331639347 | 7.400388968 |
| Ti | 9.694846425 | 16.326098620 | 10.355318001 |
| Ti | 6.448217412 | 16.385421049 | 8.901787486 |
| Ti | -0.051404345 | 16.342862249 | -0.018450154 |

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| Ti | 6.431745406 | 19.540850934 | 7.429978819 |
| Ti | 6.430462242 | 20.105077850 | 10.304845001 |
| Ti | 3.189907572 | 19.577350011 | 8.876383775 |
| Ti | 3.179124920 | 19.582474969 | 0.001523298 |
| Ti | 6.431450560 | 20.107392082 | 1.419696439 |
| Ti | 6.427595614 | 19.684371558 | 4.215390658 |
| Ti | 3.178732398 | 19.578329068 | 2.957858634 |
| Ti | 3.184546575 | 19.577559324 | 5.916909809 |
| Ti | -0.064353269 | 19.594740507 | 1.278285874 |
| Ti | -0.064247151 | 19.602303286 | 4.644309241 |
| Ti | 9.686945078 | 19.579958210 | 2.958166913 |
| Ti | 9.675903948 | 19.577603973 | 5.915758789 |
| Ti | -0.063024645 | 20.130327592 | 7.419192235 |
| Ti | -0.060127883 | 20.125508031 | 10.332738607 |
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| Ti | 9.684225353 | 19.583751208 | 0.000528665 |
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| O | 0.000000000 | 1.266689833 | 0.000000000 |
| O | 0.000000000 | 1.266689833 | 8.872200000 |
| O | 0.000000000 | 1.266689833 | 5.914800000 |
| O | 6.494400000 | 1.266689833 | 2.957400000 |
| O | 6.494400000 | 1.266689833 | 0.000000000 |

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| O | 9.741600000 | 1.980499953 | 2.957400000 |
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| O | 0.000000000 | 5.227600085 | 5.914800000 |
| O | 6.494400000 | 5.227600085 | 0.000000000 |
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| O | 11.008299988 | 6.494389931 | 7.393500000 |

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| O | 1.980500012 | 6.494389931 | 1.478700000 |
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| O | 4.513899988 | 6.494389931 | 4.436100000 |
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| O | 0.000000000 | 7.761090122 | 5.914800000 |
| O | 6.494400000 | 7.761090122 | 2.957400000 |
| O | 6.494400000 | 7.761090122 | 0.000000000 |
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| O | 1.263766857 | 9.783875625 | 4.437739701 |
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| O | 5.209685066 | 9.776234622 | 4.438843284 |
| O | 1.264305763 | 9.785221159 | 7.395637017 |
| O | 1.264131713 | 9.785815523 | 10.354506608 |
| O | 5.209460230 | 9.778078436 | 7.395738042 |
| O | 5.209471530 | 9.780026192 | 10.351813363 |
| O | 7.758490928 | 9.786155567 | 1.480208629 |
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| O | 11.703776582 | 9.777025798 | 1.484281087 |
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| O | 11.703825679 | 9.778000568 | 7.396494545 |
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| O | 3.236091848 | 11.076427067 | 0.002081536 |
| O | 3.233413298 | 11.076726392 | 8.873109223 |
| O | 3.236278368 | 11.077627581 | 5.914278196 |
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| O | 6.464795407 | 11.804091506 | 8.873791554 |
| O | -0.031218581 | 11.803570009 | 2.960888076 |
| O | 6.463214541 | 11.806052478 | 0.000523105 |
| O | 6.462744736 | 11.804254742 | 5.917890483 |
| O | -0.030770078 | 11.798186802 | 0.006137670 |
| O | -0.030366905 | 11.799406605 | 5.913570076 |
| O | 6.464244033 | 11.798964404 | 2.963724577 |
| O | -0.030522121 | 11.801896575 | 8.874083864 |
| O | 8.440723232 | 13.101373568 | 1.486631510 |
| O | 8.436321457 | 13.105703422 | 4.438744625 |
| O | 10.982062612 | 13.114441712 | 1.482591110 |
| O | 10.982104436 | 13.120860769 | 4.438469469 |

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| O | 1.940890017 | 13.098879312 | 1.482623760 |
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| O | -0.032569416 | 14.426342836 | 2.959037453 |
| O | -0.032107664 | 14.418190338 | 5.909668793 |
| O | -0.028192320 | 14.384632361 | 8.875575458 |
| O | -0.032323018 | 14.417265216 | 0.011992375 |
| O | 6.462626278 | 14.418674687 | 2.967114231 |
| O | 6.462039704 | 14.420611727 | 5.922141686 |
| O | 6.463031009 | 14.433424480 | 8.866526760 |
| O | 6.465061808 | 14.392505181 | 0.005202776 |
| O | 9.676818230 | 15.118924099 | 8.876717724 |
| O | 3.208849399 | 15.117853244 | 8.876331015 |

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| O | 3.188136030 | 15.121644813 | 2.959357917 |
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| O | 3.186553215 | 15.119140199 | 0.005009008 |
| O | 3.194583410 | 15.121134746 | 5.920874026 |
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| O | 1.227739953 | 16.486099264 | 4.441441774 |
| O | 1.227714105 | 16.493058392 | 1.480081579 |
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| O | 7.725387413 | 16.500762260 | 7.400551033 |
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| O | 3.198846594 | 17.753886026 | 0.004615910 |
| O | 9.681035304 | 17.754859011 | 2.962265869 |
| O | 9.709145015 | 17.751519287 | 5.916030397 |
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| O | 9.710618075 | 17.750807408 | 8.878748867 |
| O | 9.693359857 | 17.754539326 | 0.004636257 |
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| O | 6.430789170 | 18.569726325 | 5.872924399 |
| O | -0.064954261 | 18.456184993 | -0.110058576 |
| O | 6.429285067 | 18.484152236 | 2.882984363 |
| O | -0.063411711 | 18.462635840 | 6.030447116 |
| O | 6.430151550 | 18.511946598 | 8.969974365 |
| O | -0.062113740 | 18.625570798 | 8.866083505 |
| O | -0.064202340 | 18.685816920 | 2.967069870 |
| O | 1.935419134 | 19.944532849 | 4.425633052 |
| O | 4.395125076 | 20.003850277 | 1.473067691 |
| O | 4.435029137 | 19.963632498 | 4.458347456 |
| O | 1.977976807 | 20.009797486 | 7.400450363 |
| O | 1.955238614 | 19.970621987 | 10.345496475 |
| O | 4.453439722 | 19.888884830 | 7.384396176 |

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| O | 10.942106855 | 19.937514427 | 1.499111383 |
| O | 10.927507704 | 19.954558093 | 4.426245943 |
| O | 8.411669234 | 19.880418719 | 7.385279019 |
| O | 8.448997747 | 19.955106022 | 10.355488938 |
| O | 10.885637788 | 20.017943913 | 7.399192758 |
| O | 10.907624709 | 19.984624539 | 10.345699471 |
| O | 1.922454234 | 19.928063901 | 1.499622895 |
| O | -0.058129426 | 21.056288417 | 0.090473964 |
| O | 6.434583848 | 21.085805505 | 3.005364178 |
| O | -0.058907066 | 21.062390646 | 5.831686177 |
| O | -0.058329583 | 21.265269775 | 8.874452474 |
| O | 6.433844786 | 21.211129097 | 8.851065592 |
| O | 6.434980267 | 21.224373693 | -0.029744110 |
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| H | 6.457700016 | 0.932899949 | 6.856699960 |
| H | 0.834099951 | 0.932899949 | -0.439200043 |
| H | 0.000000000 | 0.932899949 | 3.900000036 |
| H | 0.816399984 | 0.932899949 | 2.486099982 |

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| H | 6.457700016 | 0.932899949 | 0.941899960 |
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| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
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| H | -0.036699984 | 0.932899949 | 0.941899960 |
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| H | 6.435230561 | 21.488261187 | 7.674709584 |

TS13-F1:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |

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|----|-------------|-------------|--------------|
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
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| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
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| Ti | 6.494400000 | 6.494389931 | 7.393500000 |
| Ti | 9.741600000 | 6.494389931 | 8.872200000 |

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| Ti | 3.230258968 | 9.749536118 | 1.478906427 |
| Ti | 3.233736459 | 9.741810104 | 4.435941010 |
| Ti | -0.012495615 | 9.737980316 | 2.966247594 |
| Ti | -0.017087416 | 9.766656222 | 0.002625343 |
| Ti | 3.235675427 | 9.748847456 | 7.393706545 |
| Ti | 3.233644499 | 9.741362188 | 10.350919046 |
| Ti | -0.013144925 | 9.767820661 | 8.878347015 |
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| Ti | 6.485693997 | 9.774425099 | 2.956469484 |
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| Ti | 9.723903020 | 9.748060210 | 7.393625985 |
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| Ti | 6.476087221 | 9.746302122 | 5.915166599 |
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| Ti | 6.458044349 | 13.182463140 | 1.458649065 |

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| Ti | 9.683839716 | 16.328306410 | 7.396536422 |
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| Ti | 6.435273554 | 20.092552277 | 1.644505803 |
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| Ti | 3.179488087 | 19.577548608 | 2.958072040 |
| Ti | 3.187320073 | 19.582611773 | 5.913175441 |
| Ti | -0.060939163 | 19.591333632 | 1.270978612 |
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| Ti | 9.702271862 | 19.577074617 | 2.956994481 |
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| O | -0.031903740 | 11.804334038 | 2.959499517 |
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| O | -0.032176375 | 11.799171575 | 0.005004512 |
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| O | 4.481122362 | 13.115471847 | 10.348335461 |
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| O | 10.976677326 | 13.117363524 | 7.387356061 |
| O | 10.977162458 | 13.112416089 | 10.355170367 |
| O | -0.034870252 | 14.428796015 | 2.957947592 |
| O | -0.033456811 | 14.419854485 | 5.907315767 |
| O | -0.031218451 | 14.386116842 | 8.872515377 |
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| O | 9.689972767 | 15.116194455 | 8.871788685 |
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| O | 3.198423549 | 17.754583261 | -0.005187280 |
| O | 9.688788578 | 17.752041499 | 2.955485852 |
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| O | 3.202797657 | 17.752308319 | 2.954863734 |
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| O | -0.060483906 | 18.455831733 | -0.120465904 |
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| O | 10.902882108 | 19.986534076 | 10.338455497 |
| O | 1.920383689 | 19.922013464 | 1.492832941 |
| O | -0.056787423 | 21.054552117 | 0.085644293 |
| O | 6.439464650 | 21.305905823 | 2.960135004 |
| O | -0.057514926 | 21.068447870 | 5.837873767 |
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| H | 0.834099951 | 0.932899949 | 5.475599957 |
| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
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TS14-E1:

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| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
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| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
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| O | 6.463871644 | 14.430305499 | 0.004539491 |
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14-Eb:

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| H | 7.328499172 | 0.932897449 | 5.475598892 |
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| H | 7.272684869 | 21.684610174 | 8.779315874 |
| H | 0.535051015 | 21.875970291 | 2.975849799 |
| H | 0.673165342 | 21.790595871 | 5.886236130 |

TS14-E2:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |

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| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
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| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |

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| Ti | 3.231220009 | 9.740227396 | 4.437850781 |
| Ti | -0.010633151 | 9.779850097 | 2.958037261 |
| Ti | -0.017702046 | 9.794598819 | -0.001347391 |
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| Ti | -0.035578921 | 13.105909164 | 1.472260912 |
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| Ti | -0.037874042 | 13.179944596 | 10.368723422 |
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| Ti | 6.233526836 | 19.656331449 | 4.326369932 |
| Ti | 3.132017919 | 19.560663177 | 2.939624961 |
| Ti | 3.148138839 | 19.557473830 | 5.949359940 |
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| O | 7.758251155 | 9.786344878 | 1.481897896 |
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| O | 3.235409936 | 11.073979603 | 0.001976490 |
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| O | -0.034669185 | 14.433471629 | 8.877741694 |
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| O | 6.449250542 | 14.410846517 | 5.920525763 |
| O | 6.456399707 | 14.409269167 | 8.868842760 |
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| O | 3.205264101 | 15.114101323 | 2.961199431 |
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| O | 1.236390623 | 16.474227706 | 10.355333024 |
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| O | 9.635658022 | 17.762211762 | 2.978284094 |
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| O | -0.033447719 | 18.524418592 | 8.873807879 |
| O | -0.018517742 | 18.501624886 | 2.972180139 |
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| O | 1.981199199 | 19.950957978 | 10.357301706 |
| O | 4.480222238 | 19.949759963 | 7.376263681 |
| O | 4.457097108 | 19.967066521 | 10.346936493 |
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| O | -0.049560845 | 21.152188147 | 5.914188055 |
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| H | 6.457700016 | 0.932899949 | 6.856699960 |
| H | 0.834099951 | 0.932899949 | -0.439200043 |
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| H | 0.694881317 | 21.745593892 | 5.900431886 |

TS14-E3:

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| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |

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|----|-------------|-------------|--------------|
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
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| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 3.247200000 | 6.494389931 | 8.872200000 |
| Ti | 3.247200000 | 6.494389931 | 5.914800000 |
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| Ti | 9.741600000 | 6.494389931 | 2.957400000 |
| Ti | 9.741600000 | 6.494389931 | 0.000000000 |
| Ti | 6.494400000 | 6.494389931 | 10.350900000 |
| Ti | 6.494400000 | 6.494389931 | 7.393500000 |

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| Ti | 3.233285228 | 9.742240518 | 4.437249009 |
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| Ti | 3.234441881 | 9.739388715 | 10.351422395 |
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| Ti | 6.480348067 | 9.740929274 | 5.923724487 |
| Ti | -0.034299005 | 13.108885983 | 1.469320310 |
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| O | 10.974760309 | 13.117383170 | 10.353319271 |
| O | -0.031542262 | 14.431212404 | 2.961214809 |
| O | -0.032528761 | 14.432344338 | 5.914440262 |
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| O | 3.205295923 | 15.109694316 | 8.878137513 |
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| O | 5.163819924 | 16.462059680 | 10.370705116 |
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| O | 10.902648180 | 19.957069137 | 7.387518126 |
| O | 10.909625244 | 19.938712442 | 10.353566392 |
| O | 1.946216724 | 19.933955032 | 1.500285826 |
| O | -0.056044854 | 21.097668848 | 0.029577667 |
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| O | -0.061309994 | 21.147137484 | 5.899164818 |
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| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
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TS14-F1:

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| Ti | 3.247200000 | 3.247190143 | 1.478700000 |
| Ti | 3.247200000 | 3.247190143 | 4.436100000 |
| Ti | 0.000000000 | 3.247190143 | 2.957400000 |
| Ti | 0.000000000 | 3.247190143 | 0.000000000 |
| Ti | 3.247200000 | 3.247190143 | 7.393500000 |
| Ti | 3.247200000 | 3.247190143 | 10.350900000 |
| Ti | 0.000000000 | 3.247190143 | 8.872200000 |
| Ti | 0.000000000 | 3.247190143 | 5.914800000 |
| Ti | 9.741600000 | 3.247190143 | 1.478700000 |
| Ti | 9.741600000 | 3.247190143 | 4.436100000 |
| Ti | 6.494400000 | 3.247190143 | 2.957400000 |
| Ti | 6.494400000 | 3.247190143 | 0.000000000 |
| Ti | 9.741600000 | 3.247190143 | 7.393500000 |
| Ti | 9.741600000 | 3.247190143 | 10.350900000 |
| Ti | 6.494400000 | 3.247190143 | 8.872200000 |
| Ti | 6.494400000 | 3.247190143 | 5.914800000 |
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| Ti | 0.000000000 | 6.494389931 | 1.478700000 |
| Ti | 3.247200000 | 6.494389931 | 2.957400000 |
| Ti | 3.247200000 | 6.494389931 | 0.000000000 |
| Ti | 0.000000000 | 6.494389931 | 10.350900000 |
| Ti | 0.000000000 | 6.494389931 | 7.393500000 |

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| Ti | -0.011217517 | 9.787528605 | 8.874711661 |
| Ti | -0.017929350 | 9.788943433 | 5.918656213 |
| Ti | 9.736041443 | 9.741140730 | 1.481273411 |
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| Ti | -0.090475305 | 19.672602156 | 4.445321528 |
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| Ti | 9.648053623 | 19.564361877 | 5.925224953 |
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| O | 6.494400000 | 7.761090122 | 0.000000000 |
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| O | 5.209679740 | 9.771944059 | 7.393532058 |
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| O | 9.730342477 | 11.073624199 | 2.958710246 |
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| O | 9.730276104 | 11.071736094 | 8.871332772 |
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| O | -0.031036867 | 11.820407576 | 2.961400416 |
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| O | 6.461639779 | 11.796106887 | 5.912322882 |
| O | -0.031422635 | 11.821219111 | 0.005198399 |
| O | -0.032614877 | 11.817093213 | 5.913723152 |
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| O | -0.031431597 | 11.819754633 | 8.872960998 |
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| O | 1.945825631 | 13.100308786 | 1.481402590 |
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| O | 9.693585472 | 15.108931002 | 0.002529997 |
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| O | 3.202947029 | 17.747453753 | 8.867850493 |
| O | 3.207917193 | 17.741347595 | 0.000730478 |
| O | 9.677163472 | 17.739865257 | 2.959128659 |
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| O | 6.423212544 | 18.490464850 | 2.800660284 |
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| O | 4.390504310 | 19.986193317 | 1.494491333 |
| O | 4.449744408 | 19.895647503 | 4.465458583 |
| O | 1.967266373 | 19.982048844 | 7.393559858 |
| O | 1.957804682 | 19.938537062 | 10.350994637 |
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| O | 8.393696892 | 20.008533035 | 7.403115335 |
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| O | -0.053096526 | 21.158539338 | 5.905119838 |
| O | -0.061717972 | 21.110885226 | 8.867488389 |
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| H | 6.457700016 | 0.932899949 | 6.856699960 |
| H | 0.834099951 | 0.932899949 | -0.439200043 |
| H | 0.000000000 | 0.932899949 | 3.900000036 |
| H | 0.816399984 | 0.932899949 | 2.486099982 |
| H | 6.457700016 | 0.932899949 | 0.941899960 |
| H | 0.834099951 | 0.932899949 | 5.475599957 |
| H | 6.494400000 | 0.932899949 | 9.814800036 |
| H | 7.310799984 | 0.932899949 | 8.400899982 |
| H | -0.036699984 | 0.932899949 | 6.856699960 |
| H | 7.328499951 | 0.932899949 | -0.439200043 |
| H | 6.494400000 | 0.932899949 | 3.900000036 |

| | | | |
|---|--------------|--------------|-------------|
| H | 7.310799984 | 0.932899949 | 2.486099982 |
| H | -0.036699984 | 0.932899949 | 0.941899960 |
| H | 7.328499951 | 0.932899949 | 5.475599957 |
| H | 6.426998129 | 21.292693375 | 4.362950249 |
| H | 7.188151421 | 21.764053101 | 8.800592001 |
| H | 0.541918064 | 21.858519429 | 2.958300233 |
| H | 0.738193250 | 21.725526258 | 5.896144603 |