

Electronic Supplementary Information

Elucidating Metal Hydride Reactivity Using Late Transition Metal Boryl and Borane Hydrides: 2c-2e Terminal Hydride, 3c-2e Bridging Hydride, and 3c-4e Bridging Hydride

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1. Isomers of olefin coordinate intermediate.

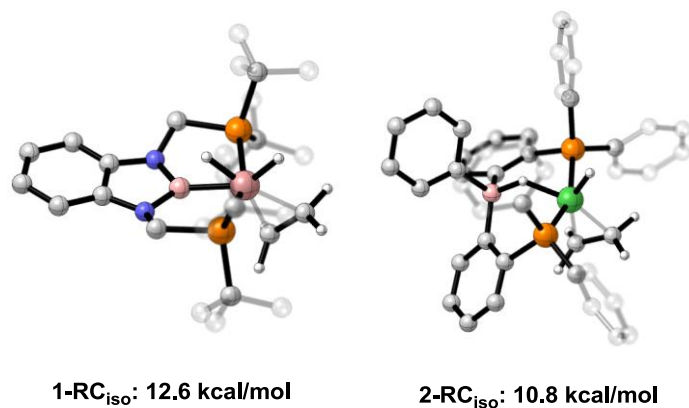


Fig. S1 Key structure for isomers of olefin *trans* coordinated intermediate.

2. Key structure of outer-sphere Concerted Mechanism.

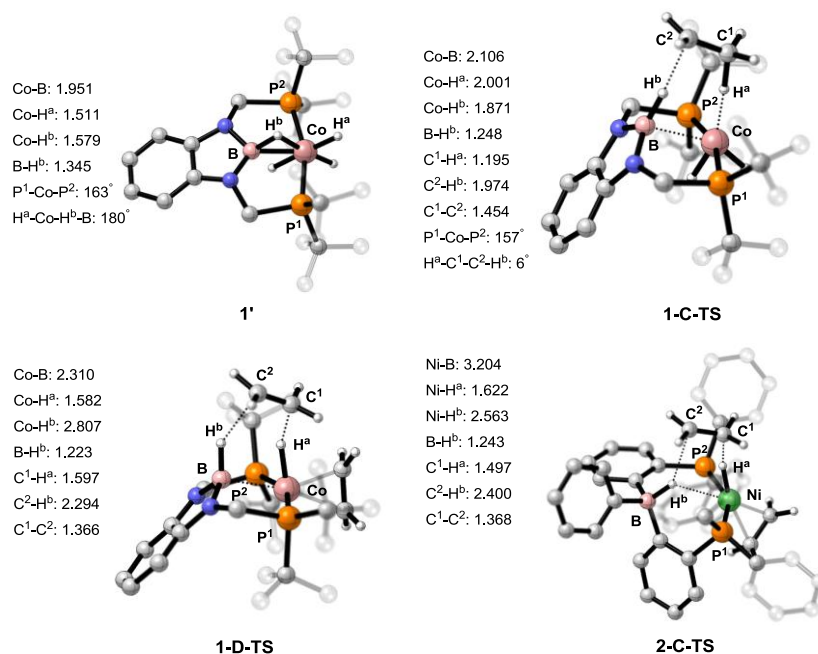


Fig. S2 Key structures for the outer sphere-concerted mechanism by PBP(μ-H)CoH and DBP(μ-H)NiH.

3. Woodward–Hoffmann’s Rule for the Outer-sphere Concerted Mechanism in PBP(μ -H)CoH.

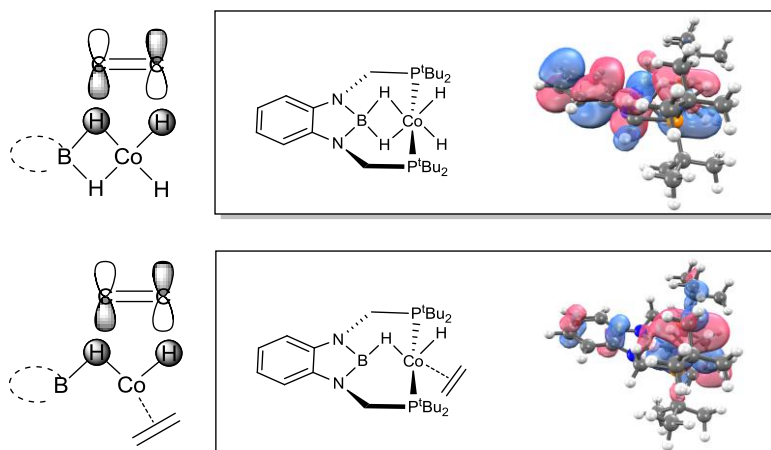


Fig. S3 Woodward–Hoffmann’s rule for the outer-sphere concerted mechanism in PBP(μ -H)CoH hydrides complexes.

4. The NBO Analysis of the Co-boryl and the Ni-borane Systems.

Boryl hydrides complex

The NBO analysis of the M-H terminal hydride hydrogenation in Co-boryl hydrides complex is shown in Fig. S4. This process contains mainly two stages. In stage I, the occupancies of the C¹-C² bond and the Co-H^a bond are 1.74 and 1.67, respectively, in the **1-RC**. Then in **1-A-TS_I**, accompanied with the disappears of the C¹-C² bond and the Co-H^a bond occupancies, the C¹-H^a bond and the Co-C² bond form. The orbital occupancies of the C¹-H^a bond and the Co-C² bond increases to 1.72 and 1.81, respectively to intermediate **1-A-IM** in stage II. In this electron evolution, two electrons transfer from Co-H^a to C1-H^a, and another two electrons transfer from π_{C1-C2} to Co-C², indicating a classical two-electron transfer process for the **2c-2e** terminal hydride in the boryl cobalt hydrides complexes.

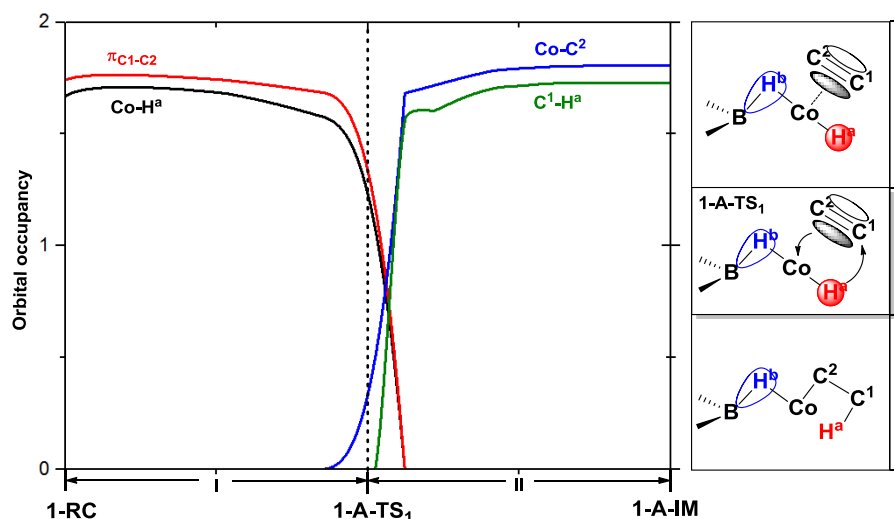


Fig. S4 NBO analysis along the terminal hydride hydrogenation process in the Co-boryl hydrides complex.

As shown in Fig. S5, the hydrogenation reaction by the B-H-Co bridging hydride contains three stages in total. In stage I, with the B-H^b bond occupancy drops from 1.62 to 0, the occupancy of the lone pair (LP) H appears. Meanwhile the occupancies of the C¹-C² bond and the d_{x²-y²} (Co) orbital keep above 1.74 and 1.64. Then in stage II, with the occupancies of the lone pair (LP) H^b and the d_{x²-y²} (Co) drop to 0, the Co-B bond and the Co-H^a bond form and their occupancies become higher than 1.74 and 1.51, respectively. In stage III which is after transition state **1-B-TS₁**, accompanied with the occupancies of the Co-H^b bond and the C¹-C² bond drop to 0, the Co-C¹ bond and the C²-H^b bond appears to generate intermediate **1-B-IM**.

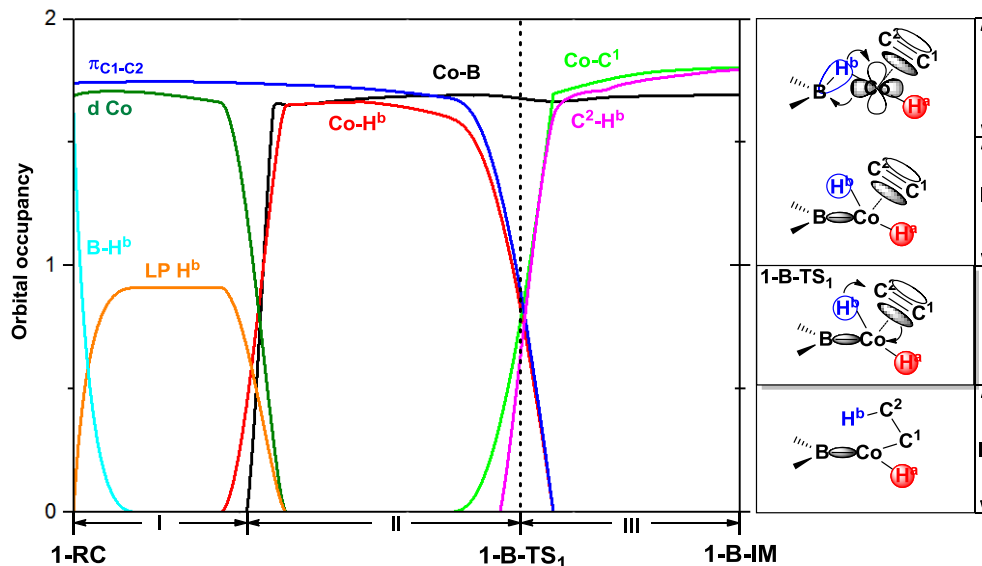


Fig. S5 NBO analysis along the bridging hydride hydrogenation process in the Co-boryl hydrides complex.

Borane hydrides complex

As for the M-H terminal hydride hydrogenation in the Ni-borane hydrides complex, electron evolution process is quite similarity to that in the Co-boryl system. As shown in Fig. S6, the C¹-C² and Ni-H^a continuous dropping from 1.85 and 1.77, respectively, to 0 in stage I, and the Ni-C² and C¹-H^a bond form in stage II. The hydrogenation process shows a typical two-electron transfer mode as well for the terminal hydride in the borane nickel hydrides complexes.

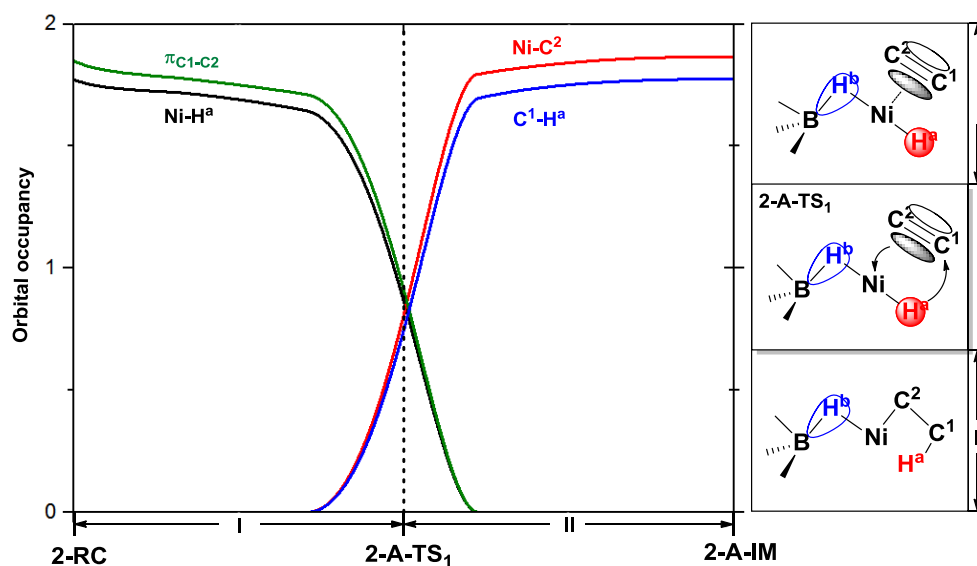


Fig. S6 NBO analysis along the terminal hydride hydrogenation process in the Ni-borane intermediate.

As for the B-H-Ni bridging hydride, the electron evolution includes three stages in hydrogenation reaction as well. However, the electronic structure is quite different from which in the boryl B-H-Co bridging hydride. As shown in Fig. S7, in stage I, occupancies of the B-H^b bond continuously drops from 1.63 to 1.53, indicating the weakness of the B-H^b bond. Then in stage II, with the breaking of the B-H^b bond, the lone pair (LP) H^b and the p_z orbital of boron atom appears. Meanwhile, the occupancy of the C¹-C² bond drops from 1.85 to 1.62, suggesting the activation of the C-C bond. After 2-B-TS, with the occupancies of the lone pair (LP) H^b and the C¹-C² bond drop from 0.83 and 1.32 to 0, the C²-H^b bond forms finally.

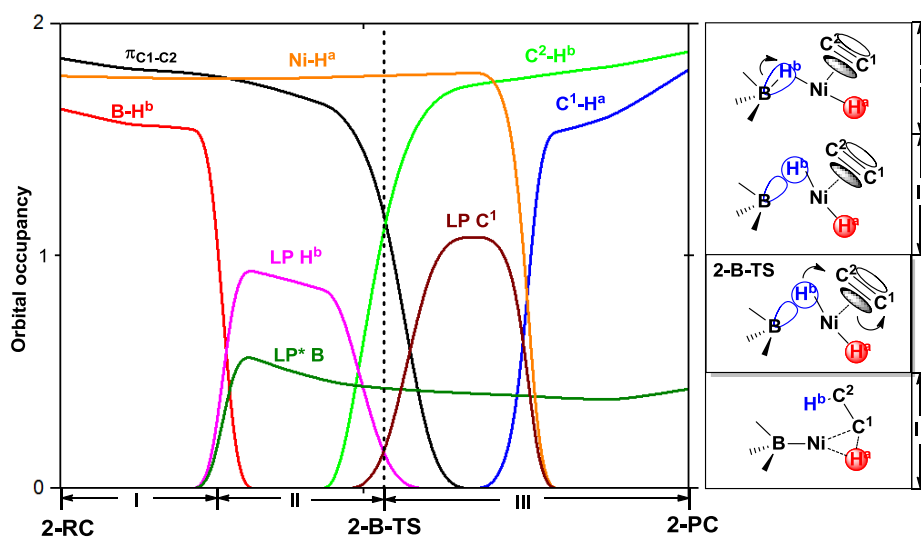


Fig. S7 NBO analysis along the bridging hydride hydrogenation process in the Ni-borane hydrides complexes.

5. The Calculated Results of Orbital Occupancy for M-H and M-H-B

Hydrogenation Reaction in Co-boryl and Ni-borane System.

Table S1 M-H hydride hydrogenation reaction in Co-boryl hydride complex

Irc	Co-H ^a	C ¹ -C ²	Co-C ²	C ¹ -H ^a
1-RC	1.66788	1.74	0	0
1	1.70924	1.7667	0	0
3	1.71001	1.7658	0	0
5	1.70875	1.76298	0	0
7	1.70424	1.7577	0	0
9	1.69519	1.74995	0	0
11	1.67971	1.73936	0	0
13	1.65632	1.72569	0	0
15	1.6241	1.70862	0	0
17	1.58449	1.68921	0	0
19	1.55252	1.67438	0	0
21	1.51602	1.65644	0	0
23	0	0	1.68193	1.55917
25	0	0	1.71571	1.60361
27	0	0	1.75577	1.66256
29	0	0	1.78332	1.70318
31	0	0	1.79476	1.71596
33	0	0	1.80232	1.72551
35	0	0	1.804	1.72637
37	0	0	1.80535	1.72801
39	0	0	1.80604	1.72804
41	0	0	1.8068	1.72817
1-A-IM	0	0	1.81259	1.72211

Table S2 M-H-B bridging hydride hydrogenation reaction in Co-boryl hydride complex

irc	Co-B	Co-H ^b	Co-C ¹	C ¹ -C ²	C ² -H ^b	d _{x2-y2} Co	LP H ^b	B-H ^b
1-RC	0	0	0	1.74	0	1.68844	0	1.6179
1	0	0	0	1.74435	0	1.71098	0.91114	0
3	0	0	0	1.74504	0	1.70833	0.91092	0
5	0	0	0	1.74609	0	1.70368	0.91068	0
7	0	0	0	1.74675	0	1.69553	0.91005	0
9	0	0	0	1.7458	0	1.68039	0.90984	0
11	0	0	0	1.74359	0	1.66221	0.91153	0
13	0	0	0	1.7404	0	1.64384	0.91443	0

15	1.64194	1.64289	0	1.73626	0	0	0	0
16	1.65025	1.65115	0	1.73382	0	0	0	0
18	1.65746	1.65732	0	1.73113	0	0	0	0
20	1.66919	1.6639	0	1.72491	0	0	0	0
22	1.67802	1.6628	0	1.71728	0	0	0	0
24	1.68431	1.65316	0	1.70778	0	0	0	0
26	1.6885	1.63408	0	1.69591	0	0	0	0
28	1.69059	1.60496	0	1.68144	0	0	0	0
30	1.6906	1.56523	0	1.66451	0	0	0	0
32	1.68822	1.51398	0	1.64456	0	0	0	0
36	1.66584	0	1.69721	0	1.60243	0	0	0
40	1.68199	0	1.75964	0	1.71279	0	0	0
42	1.68606	0	1.77758	0	1.74349	0	0	0
44	1.68848	0	1.78855	0	1.76088	0	0	0
46	1.69031	0	1.79571	0	1.77386	0	0	0
48	1.69214	0	1.80103	0	1.78703	0	0	0
50	1.6934	0	1.80377	0	1.79489	0	0	0
52	1.69412	0	1.8052	0	1.79879	0	0	0
1-B-IM	1.69504	0	1.80573	0	1.8	0	0	0

Table S3 M-H hydride hydrogenation reaction in Ni-borane hydride complex

irc	Ni-H ^a	Ni-C ²	C ¹ -C ²	C ¹ -H ^a
2-RC	1.77395	0	1.85022	0
1	1.73483	0	1.80478	0
3	1.72912	0	1.79339	0
5	1.71868	0	1.77863	0
7	1.70185	0	1.76014	0
9	1.67722	0	1.73762	0
11	1.64395	0	1.71046	0
15	1.55154	0	1.6448	0
17	0	1.78363	0	1.63504
19	0	1.79465	0	1.69631
21	0	1.82395	0	1.73454
23	0	1.84072	0	1.75089
25	0	1.85336	0	1.76196
27	0	1.86297	0	1.77172
29	0	1.86565	0	1.77463
31	0	1.8663	0	1.77635
2-A-IM	0	1.8326	0	1.987

Table S4 M-H-B bridging hydride hydrogenation reaction in Ni-borane hydride complex

	Ni-H	C ¹ -C ²	B-H ^b	C ² -H ^b	C ¹ -H ^a	LP H ^b	LP*B	LP C ¹
2-RC	1.77395	1.85022	1.63319	0	0	0	0	0
1	1.76682	1.80447	1.56505	0	0	0	0	0
2	1.76564	1.79958	1.56116	0	0	0	0	0
3	1.76436	1.79387	1.55573	0	0	0	0	0
4	1.76305	1.78636	1.54727	0	0	0	0	0
5	1.76203	1.7754	1.53024	0	0	0	0	0
6	1.76203	1.75995	0	0	0	0.9534	0.58346	0
7	1.76299	1.74029	0	0	0	0.93134	0.55731	0
8	1.76379	1.71552	0	0	0	0.9095	0.52345	0
9	1.76529	1.68759	0	0	0	0.88446	0.49499	0
10	1.76744	1.65737	0	0	0	0.85744	0.47005	0
11	1.77055	1.62445	0	0	0	0.83071	0.44701	0
12	1.77549	1.31624	0	1.28635	0	0	0.42898	0
13	1.78159	0	0	1.69292	0	0	0.41711	1.07484
14	1.78642	0	0	1.73767	0	0	0.40791	1.08094
15	1.78928	0	0	1.75904	0	0	0.40029	1.08425
16	0	0	0	1.77363	1.51504	0	0.39418	0
17	0	0	0	1.78672	1.53493	0	0.38898	0
18	0	0	0	1.7994	1.55891	0	0.38502	0
19	0	0	0	1.8102	1.58799	0	0.38222	0
20	0	0	0	1.82121	1.62192	0	0.38027	0
2-PC	0	0	0	1.9352	1.9813	0	0.47262	0

6. The Cartesian Coordinates (xyz) for All Optimized Structures.

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 1 -2.391849 -1.020258 3.805770
 1 -1.038843 -1.286016 2.672888
 1 -1.752662 0.327924 2.848513
 1 -4.551312 -0.629628 3.155846
 1 -4.271103 0.682926 2.016053
 1 -5.178404 -0.758776 1.518221
 1 -1.964410 0.178859 -2.587163
 1 -3.414716 -0.370789 -3.460895

1 -3.498732 1.019151 -2.374973
 1 -2.385089 -2.623101 -2.296385
 1 -3.504257 -3.099675 -1.009360
 1 -4.126109 -2.573792 -2.578502
 1 -5.498549 -0.661598 -1.943415
 1 -5.334580 -1.428963 -0.362454
 1 -5.065643 0.324423 -0.539038
 27 -0.000043 -0.995429 -0.130257
 7 1.154587 1.832414 -0.317712
 7 -1.154478 1.832425 -0.318597
 5 0.000055 0.945072 -0.364967
 6 0.711964 3.141266 -0.170313
 6 -0.711946 3.141275 -0.170915
 6 1.418188 4.328459 -0.012411
 6 -1.418307 4.328474 -0.013662
 1 2.511196 4.327628 0.002406
 1 -2.511327 4.327637 0.000191
 6 0.697246 5.520995 0.137800
 6 -0.697489 5.521005 0.137176
 1 1.237822 6.462281 0.261578
 1 -1.238163 6.462299 0.260468
 6 -2.391355 1.299491 0.171306
 6 2.390933 1.299289 0.173341
 1 -3.280555 1.645266 -0.384775
 1 -2.555384 1.596519 1.225011
 1 3.280793 1.645766 -0.381250
 1 2.553541 1.595368 1.227545
 1 -0.000093 0.090587 0.924154
 1 -0.000089 -2.033846 0.998758
 6 0.000467 -2.752796 -1.120527
 1 0.908343 -3.336678 -0.941071
 1 -0.906898 -3.337450 -0.941005
 6 -0.000014 -1.682389 -2.047759
 1 -0.902255 -1.447159 -2.612831
 1 0.901803 -1.446438 -2.613226

1-A-TS₁

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 15 2.194721 -0.285385 0.083562
 15 -2.029410 -0.748372 -0.084281
 7 -1.344899 1.570937 -1.055556
 7 0.883823 1.908374 -0.592719
 6 2.179841 1.591297 -0.080703

1 2.360696 2.077881 0.896406
1 2.993402 1.933849 -0.743254
6 -2.552688 0.804879 -0.991597
1 -2.949119 0.546348 -1.991371
1 -3.360071 1.338941 -0.458836
6 0.224289 3.122337 -0.498243
6 -2.059722 3.967949 -0.709642
1 -3.120268 3.810749 -0.924354
6 -1.157498 2.912382 -0.783796
6 -1.579289 5.237012 -0.351512
1 -2.277292 6.075309 -0.291589
5 -0.084026 0.854256 -0.872076
6 -0.228581 5.442019 -0.075327
1 0.122680 6.439026 0.200566
6 0.690102 4.383619 -0.145945
1 1.748708 4.542508 0.076613
1 0.145873 -0.110569 -1.802601
6 2.746132 -0.561578 1.888754
6 3.671910 -0.677092 -1.092377
6 -3.401694 -1.974553 -0.643461
6 -2.413806 -0.260454 1.736831
1 0.179946 -2.091368 0.584150
6 0.346957 -3.128123 -0.480734
1 1.235062 -3.564602 -0.002664
1 -0.555311 -3.697924 -0.221264
6 0.477630 -2.628529 -1.808443
1 -0.331309 -2.770989 -2.527774
1 1.466842 -2.643045 -2.274854
6 3.141054 -0.318309 -2.484964
1 3.889379 -0.584938 -3.248305
1 2.204921 -0.835720 -2.726770
1 2.948234 0.760463 -2.587563
6 4.964055 0.113948 -0.880733
1 5.539986 -0.209082 -0.007015
1 5.617314 -0.037691 -1.755894
1 4.808771 1.198647 -0.797960
6 4.001121 -2.167117 -1.027935
1 3.109502 -2.806212 -1.090955
1 4.661039 -2.445516 -1.865705
1 4.539171 -2.429836 -0.104902
6 4.146440 -0.049823 2.208248
1 4.293658 -0.041362 3.300609
1 4.930355 -0.694690 1.791453
1 4.322728 0.976901 1.853550

6 2.657027 -2.051370 2.217296
 1 3.310763 -2.673404 1.590584
 1 2.953692 -2.219834 3.264855
 1 1.628121 -2.423208 2.106828
 6 1.735899 0.165465 2.774475
 1 1.777741 1.259768 2.674762
 1 0.712049 -0.152605 2.542578
 1 1.934817 -0.069751 3.832283
 6 -2.947911 -2.550577 -1.985485
 1 -2.109463 -3.248458 -1.869032
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 1 -2.640526 -1.775040 -2.703932
 6 -3.540590 -3.130231 0.344405
 1 -4.164412 -3.924238 -0.098010
 1 -2.570221 -3.585873 0.593827
 1 -4.024806 -2.835954 1.285370
 6 -4.764632 -1.313281 -0.860235
 1 -5.498930 -2.086319 -1.142050
 1 -5.162411 -0.805033 0.024615
 1 -4.749929 -0.588028 -1.685427
 6 -1.718219 1.080201 1.991592
 1 -1.717423 1.292314 3.072904
 1 -0.675795 1.089946 1.645919
 1 -2.235584 1.918387 1.501638
 6 -1.829541 -1.322416 2.666064
 1 -1.879483 -0.976851 3.711313
 1 -2.371491 -2.276437 2.614455
 1 -0.774505 -1.529412 2.434464
 6 -3.892598 -0.071068 2.062075
 1 -4.472159 -1.002755 2.022638
 1 -3.988622 0.316444 3.089637
 1 -4.378973 0.666606 1.406488

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27 0.163192 -1.054360 -0.597313
 15 2.179600 -0.251743 0.096716
 15 -2.010229 -0.761413 -0.080802
 7 -1.373963 1.559370 -1.080817
 7 0.850732 1.926758 -0.602350
 6 2.129207 1.624949 -0.035272
 1 2.247100 2.094355 0.959084
 1 2.966167 1.999968 -0.648527
 6 -2.571019 0.778510 -0.986065

1 -2.986741 0.506551 -1.974133
1 -3.372043 1.308768 -0.439879
6 0.168520 3.127825 -0.493873
6 -2.128165 3.938203 -0.704793
1 -3.184685 3.765470 -0.927254
6 -1.207177 2.899868 -0.790002
6 -1.671645 5.209476 -0.324341
1 -2.384073 6.034886 -0.255698
5 -0.100013 0.861529 -0.904367
6 -0.326212 5.432620 -0.036712
1 0.006666 6.431005 0.256386
6 0.610723 4.390934 -0.118087
1 1.664936 4.563903 0.114427
1 0.150611 -0.096334 -1.833876
6 2.749339 -0.576770 1.895430
6 3.666286 -0.591944 -1.090238
6 -3.374198 -2.008264 -0.611693
6 -2.364305 -0.283374 1.751212
1 0.229178 -2.365665 0.367927
6 0.390100 -3.164426 -0.551207
1 1.298076 -3.660819 -0.173772
1 -0.477586 -3.820249 -0.382509
6 0.492893 -2.559925 -1.875411
1 -0.305917 -2.764757 -2.593647
1 1.476837 -2.600691 -2.355278
6 3.129992 -0.217409 -2.476042
1 3.890009 -0.441761 -3.241520
1 2.212440 -0.758559 -2.734753
1 2.903899 0.857059 -2.553155
6 4.946763 0.215772 -0.868920
1 5.530966 -0.107941 -0.001280
1 5.600039 0.086319 -1.747677
1 4.775036 1.297062 -0.773540
6 4.017262 -2.077177 -1.050687
1 3.134991 -2.725673 -1.146932
1 4.697603 -2.329430 -1.880516
1 4.539681 -2.352179 -0.121842
6 4.178144 -0.146937 2.204360
1 4.348847 -0.191065 3.292676
1 4.921846 -0.809255 1.742682
1 4.391281 0.884776 1.887177
6 2.589394 -2.069046 2.187788
1 3.195380 -2.706126 1.528318
1 2.901969 -2.282061 3.222667

1 1.540287 -2.388420 2.095259
 6 1.797095 0.179659 2.820120
 1 1.913415 1.271368 2.762590
 1 0.749556 -0.057244 2.597416
 1 1.991608 -0.109329 3.865394
 6 -2.952437 -2.554611 -1.976060
 1 -2.085522 -3.221855 -1.899330
 1 -3.776919 -3.142581 -2.411366
 1 -2.699267 -1.761951 -2.696623
 6 -3.453295 -3.180056 0.364085
 1 -4.083791 -3.977952 -0.061644
 1 -2.465866 -3.623763 0.564388
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 6 -4.757962 -1.375614 -0.773164
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 6 -1.699784 1.074843 1.990103
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 1 -2.229650 -2.301514 2.613746
 1 -0.663323 -1.515463 2.339019
 6 -3.834468 -0.142449 2.131335
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 1 -3.907066 0.228365 3.167194
 1 -4.365357 0.588614 1.502979

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 15 -1.997837 -0.747410 -0.067389
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 7 0.845985 1.937457 -0.390552
 6 2.089850 1.595466 0.229853
 1 2.127692 1.944947 1.278550
 1 2.960249 2.047994 -0.276055
 6 -2.571621 0.845148 -0.866152
 1 -3.021986 0.643969 -1.856426
 1 -3.346205 1.353274 -0.262398
 6 0.192716 3.159531 -0.341371

6 -2.075262 4.011501 -0.667605
 1 -3.126274 3.853381 -0.924103
 6 -1.175410 2.951514 -0.683324
 6 -1.604946 5.283617 -0.310215
 1 -2.300413 6.126009 -0.292851
 5 -0.108354 0.889601 -0.710272
 6 -0.265875 5.487327 0.021477
 1 0.077049 6.487040 0.298242
 6 0.649156 4.424475 0.010464
 1 1.696310 4.581432 0.282781
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 6 3.621451 -0.455708 -1.109132
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 6 -2.324326 -0.385663 1.798133
 1 0.242982 -2.552150 0.051022
 6 0.386112 -3.068225 -1.020220
 1 1.326564 -3.615423 -0.854115
 1 -0.442475 -3.792152 -1.014501
 6 0.400723 -2.161122 -2.199613
 1 -0.406464 -2.326754 -2.921279
 1 1.357396 -2.127491 -2.735867
 6 3.110966 0.157608 -2.416215
 1 3.841442 -0.023749 -3.220922
 1 2.146441 -0.255381 -2.731072
 1 2.985625 1.247671 -2.337138
 6 4.925571 0.268212 -0.761822
 1 5.524419 -0.240830 -0.000036
 1 5.553598 0.317165 -1.666828
 1 4.778781 1.307733 -0.435523
 6 3.926345 -1.936976 -1.308376
 1 3.028591 -2.522304 -1.549951
 1 4.639713 -2.075541 -2.137571
 1 4.387879 -2.383992 -0.415052
 6 4.198433 -0.569605 2.180170
 1 4.386605 -0.780901 3.245971
 1 4.885275 -1.206396 1.607932
 1 4.475353 0.480690 2.007152
 6 2.480754 -2.358159 1.960111
 1 3.008426 -2.939046 1.189132
 1 2.819804 -2.733116 2.939364
 1 1.407449 -2.585847 1.875844
 6 1.869470 -0.157685 2.905413
 1 2.128267 0.902772 3.034851

1 0.801571 -0.216919 2.659841
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 1 -1.577003 -1.217183 3.664901
 1 -2.162035 -2.451151 2.535387
 6 -3.785303 -0.285194 2.221839
 1 -4.326001 -1.238029 2.144673
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 1 -4.341960 0.476535 1.655112
 6 -3.382453 -3.212795 0.206159
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 1 -3.817556 -2.921089 -2.547926
 1 -2.782308 -1.492496 -2.732462
 6 -4.767079 -1.340890 -0.716624
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 1 -4.822630 -0.495945 -1.417554

1-B-TS₁

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 7 1.137998 1.846414 -0.346470
 6 2.457360 1.306976 -0.388852
 1 3.143274 1.764583 0.347260
 1 2.932217 1.439259 -1.378896
 6 -2.457299 1.307143 -0.388620
 1 -2.932236 1.439572 -1.378604
 1 -3.143118 1.764715 0.347601
 6 0.713463 3.163460 -0.335100
 6 -1.420009 4.361214 -0.320551
 1 -2.513086 4.363519 -0.326545
 6 -0.713270 3.163509 -0.335005

6 -0.697471 5.561918 -0.303034
 1 -1.237869 6.511344 -0.292445
 5 0.000020 0.952174 -0.365765
 6 0.697846 5.561868 -0.303120
 1 1.238314 6.511255 -0.292597
 6 1.420293 4.361112 -0.320729
 1 2.513369 4.363333 -0.326864
 1 -0.000032 -1.158953 -1.780123
 6 2.805473 -0.639151 1.774886
 6 3.478386 -1.278425 -1.219994
 6 -3.478415 -1.278125 -1.220115
 6 -2.805574 -0.639240 1.774872
 1 -0.000062 -0.869964 1.236729
 6 -0.000090 -3.015201 -0.000523
 1 0.913691 -3.409301 0.455838
 1 -0.913921 -3.409258 0.455775
 6 -0.000047 -2.707316 -1.392239
 1 -0.898620 -2.940975 -1.974529
 1 0.898542 -2.940991 -1.974499
 6 2.924119 -1.078114 -2.634728
 1 3.589106 -1.572575 -3.360545
 1 1.915383 -1.482572 -2.770953
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 6 4.860489 -0.618926 -1.191164
 1 5.456488 -0.885694 -0.313053
 1 5.432356 -0.956984 -2.070846
 1 4.818957 0.477741 -1.251425
 6 3.628793 -2.767550 -0.918269
 1 2.666256 -3.297745 -0.892335
 1 4.249738 -3.251555 -1.689455
 1 4.128082 -2.939615 0.046605
 6 4.310522 -0.447725 1.937074
 1 4.546221 -0.348845 3.009176
 1 4.886651 -1.307679 1.569855
 1 4.689085 0.460317 1.444110
 6 2.409002 -1.990526 2.366102
 1 2.863687 -2.838724 1.833684
 1 2.748683 -2.046557 3.412844
 1 1.320028 -2.131163 2.354191
 6 2.098939 0.463937 2.567697
 1 2.445087 1.472860 2.301966
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 1 -2.305962 0.325641 3.640745

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 7 1.137222 1.843638 -0.439263
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 1 3.111207 1.791863 0.332516
 1 2.974308 1.422573 -1.390094
 6 -2.459260 1.309443 -0.418550
 1 -2.974261 1.422121 -1.390536
 1 -3.111391 1.791654 0.332007
 6 0.713301 3.158649 -0.396528
 6 -1.420516 4.355982 -0.353739
 1 -2.513669 4.357972 -0.359507
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 6 -0.698107 5.555876 -0.308216
 1 -1.238359 6.504936 -0.275849
 5 0.000003 0.942433 -0.472625

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 1 1.237642 6.505091 -0.275600
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6 -2.082273 0.515931 2.558044
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 6 -3.628135 -2.778871 -0.869484
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 1 -2.667021 -3.311225 -0.841662
 6 -2.913516 -1.122258 -2.608393
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 6 -4.856988 -0.635792 -1.176979
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 1 -4.818228 0.459213 -1.261447

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 7 1.136018 1.858618 -0.325969
 6 2.454168 1.322663 -0.361485
 1 3.134082 1.772370 0.385530
 1 2.939327 1.465110 -1.345217
 6 -2.454209 1.322534 -0.361720
 1 -2.939261 1.464836 -1.345525
 1 -3.134249 1.772256 0.385173
 6 0.713559 3.172934 -0.323958
 6 -1.420512 4.371382 -0.320784
 1 -2.513653 4.373576 -0.327452
 6 -0.713690 3.172907 -0.324042
 6 -0.697744 5.572541 -0.314676
 1 -1.238150 6.522121 -0.313801
 5 -0.000019 0.948153 -0.339304
 6 0.697528 5.572566 -0.314598
 1 1.237900 6.522165 -0.313664
 6 1.420339 4.371433 -0.320624

1 2.513480 4.373664 -0.327166
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 6 2.803295 -0.645984 1.776170
 6 3.472446 -1.248744 -1.220892
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 6 0.000111 -2.991081 0.007023
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 1 -0.893137 -3.494302 0.400436
 6 0.000088 -2.810011 -1.474923
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 1 0.887073 -3.223656 -1.975667
 6 2.889505 -1.073372 -2.626297
 1 3.583696 -1.494211 -3.371217
 1 1.922642 -1.572693 -2.752221
 1 2.741934 -0.014432 -2.885525
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 1 4.265754 -3.207917 -1.712507
 1 4.200321 -2.893738 0.025372
 6 2.487764 -2.026127 2.349499
 1 2.957490 -2.846078 1.787875
 1 2.863390 -2.086539 3.383678
 1 1.406601 -2.215390 2.382688
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 1 4.915402 -1.202576 1.574702
 1 4.628605 0.552718 1.456746
 6 2.020418 0.392828 2.581219
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 6 -4.294985 -0.375466 1.944701
 1 -4.915202 -1.203183 1.574509
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 6 -3.663155 -2.733093 -0.920605
 1 -4.199902 -2.893857 0.025788
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27 0.000001 -0.989865 -0.006516
 15 2.197116 -0.666497 0.032505
 15 -2.197115 -0.666499 0.032502
 7 -1.167425 1.787796 -0.451820
 7 1.167426 1.787797 -0.451823
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 6 0.715762 3.090421 -0.267021
 6 -1.417399 4.274293 -0.078276
 1 -2.510513 4.273900 -0.068197
 6 -0.715762 3.090420 -0.267018
 6 -0.696240 5.463515 0.111121
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 5 0.000001 0.920056 -0.406327
 6 0.696239 5.463516 0.111117
 1 1.238270 6.399623 0.264181
 6 1.417399 4.274295 -0.078283
 1 2.510514 4.273903 -0.068208
 1 0.000001 0.253900 0.930143
 1 0.000002 -0.084922 -1.300219

6 3.105653 -1.082188 1.641525
6 3.125180 -1.307085 -1.493752
6 -3.125160 -1.307078 -1.493767
6 -3.105672 -1.082201 1.641512
1 0.000000 -2.239101 -0.856137
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6 2.464496 -0.619650 -2.693286
1 2.964702 -0.946483 -3.618322
1 1.403434 -0.893951 -2.774814
1 2.527761 0.477844 -2.658764
6 2.906305 -2.812647 -1.636786
1 1.837567 -3.065540 -1.581995
1 3.286907 -3.146748 -2.615105
1 3.433319 -3.395145 -0.870451
6 4.619725 -1.000859 -1.492726
1 5.170847 -1.616972 -0.769181
1 5.040969 -1.230337 -2.484680
1 4.847051 0.056156 -1.287042
6 4.474185 -0.417278 1.785967
1 4.881609 -0.650499 2.782667
1 5.209210 -0.768123 1.053033
1 4.426971 0.679171 1.718657
6 3.245859 -2.598216 1.755539
1 4.010928 -2.998498 1.075362
1 3.553391 -2.868067 2.778129
1 2.293736 -3.109985 1.547674
6 2.201691 -0.585096 2.773023
1 2.013985 0.498523 2.719884
1 1.225630 -1.088189 2.758169
1 2.686009 -0.785917 3.741894
6 -2.464600 -0.619473 -2.693270
1 -2.527985 0.478012 -2.658648
1 -1.403511 -0.893648 -2.774868
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6 -2.906109 -2.812602 -1.636918
1 -3.286693 -3.146674 -2.615254
1 -1.837339 -3.065370 -1.582169
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6 -4.619742 -1.001035 -1.492667
1 -5.040975 -1.230423 -2.484647
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 15 2.240633 -0.337368 0.268654
 15 -2.126000 -0.676494 0.178761
 7 -1.276196 1.372992 -1.286727
 7 1.011028 1.679395 -1.054271
 6 2.291364 1.394721 -0.455528
 1 2.470336 2.105827 0.368289
 1 3.140132 1.515376 -1.151555
 6 -2.520098 0.678533 -1.070576
 1 -2.907970 0.241095 -2.004425
 1 -3.293261 1.366619 -0.695518
 6 0.374257 2.908800 -0.954635
 6 -1.900036 3.805299 -1.006260
 1 -2.978485 3.668974 -1.122310
 6 -1.030479 2.721739 -1.103564
 6 -1.363055 5.073238 -0.752857
 1 -2.033705 5.932177 -0.678337
 5 -0.012540 0.669865 -1.243152
 6 0.012407 5.254566 -0.597616
 1 0.407777 6.253749 -0.402090
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 1 1.973052 4.316484 -0.581184
 1 0.055433 0.271362 0.926944
 1 0.130416 -0.483337 -1.697593
 6 2.905834 -0.050241 2.032365
 6 3.516246 -1.322752 -0.740149
 6 -3.144478 -2.231253 -0.260971
 6 -2.785144 0.090490 1.801953
 1 0.200779 -2.273738 -1.362893
 1 0.097881 -1.484681 1.523387
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1 3.513490 -3.110467 0.541816
1 2.180034 -3.049587 -0.622470
6 4.989346 -1.026082 -0.487636
1 5.332479 -1.357614 0.502270
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1 5.233756 0.040602 -0.601209
6 4.165011 0.817741 2.083953
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1 5.031427 0.370912 1.586238
1 4.010720 1.819992 1.658718
6 3.182846 -1.406777 2.675783
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1 3.384427 -1.277719 3.751057
1 2.318563 -2.082228 2.580886
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1 -2.627073 -2.863648 -1.080915
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 1 -0.372117 -1.583849 -1.212130

6 -0.634896 -2.825183 0.849987
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 6 -2.465100 -1.438210 2.579287
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 6 -2.387599 0.830125 -2.429490
 6 3.465473 -1.603836 -1.087569
 6 3.070008 -1.534174 -2.568448
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 6 3.459635 -3.079011 -0.686692
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 6 3.589997 0.816267 1.922900
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1 -4.937979 0.158196 -2.542315
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1 2.479573 -3.547533 -0.850857
1 3.742608 -3.251345 0.357800
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1 3.676451 -2.248844 -3.147042
1 2.012002 -1.793131 -2.726235
1 3.239006 -0.544122 -3.012043
1 5.581378 -1.545290 -1.552852
1 4.909956 0.049093 -1.184166
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1 0.542876 -0.825918 2.176024
1 1.463257 -0.088562 3.508371
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1 3.840274 0.871933 2.995140
1 4.538377 0.705673 1.376480
1 3.149782 1.787144 1.653541
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6 -0.512891 3.114911 0.123402
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6 -1.094967 4.340294 0.438503
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1 -0.770838 6.470704 0.523685
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15 -2.116037 -0.645580 -0.051084
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7 1.132780 1.742072 0.146918
6 2.430314 1.183009 0.353780
1 2.803809 1.341608 1.383240
1 3.203462 1.589966 -0.326033
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1 -2.805094 1.340036 -1.384157
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6 5.009461 -0.296837 -1.066714
6 3.362482 -0.852538 -2.744154
6 6.021986 -0.486482 -2.006144
1 5.267589 -0.004547 -0.044794
6 4.375421 -1.050077 -3.678721
1 2.314196 -0.983263 -3.031978
6 5.707539 -0.863193 -3.311366
1 7.065009 -0.341109 -1.714814

1 4.123272 -1.344130 -4.700094
1 6.503438 -1.009861 -4.045207
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6 2.183534 0.795100 2.272148
6 3.588088 2.014747 0.732199
6 2.396742 1.771057 3.241163
1 1.545308 -0.063213 2.500409
6 3.808394 2.984699 1.709430
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6 3.207711 2.871582 2.962301
1 1.925517 1.667289 4.221554
1 4.454471 3.837124 1.485273
1 3.376326 3.637303 3.723183
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6 -3.435312 0.431916 -2.344910
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1 -3.923512 -0.471485 0.910090
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1 0.083031 3.190019 0.414146
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1 -2.302688 6.744669 -0.107726
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6 0.691958 1.787149 -2.145596
1 0.693009 1.115165 -3.033105
1 -0.175604 2.458101 -2.257365
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1 2.029355 3.291024 -2.952488

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6 0.868931 -2.362443 1.015613
6 -0.913506 -0.511436 1.707436
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6 -0.878952 -0.849957 3.073570
1 -0.554091 -1.855335 3.363460
6 -1.342212 0.791395 1.391505
6 -1.648858 1.344640 3.728196
6 -4.177169 -3.208437 0.529759
1 -5.185451 -2.914628 0.835562
6 -1.711677 1.706988 2.386544
1 -2.033964 2.716121 2.111224
6 -3.970908 -4.424324 -0.119292
6 -2.677165 -4.783052 -0.503847
1 -2.501684 -5.736444 -1.010191
6 0.908771 -3.551947 1.766205
1 -0.031196 -4.069234 1.986516
6 -1.231333 0.057030 4.069347
1 -1.179073 -0.239787 5.120447
6 3.309842 -2.268392 1.235398
1 4.257603 -1.766806 1.015542
6 2.103794 -4.089094 2.241863
1 2.092741 -5.017635 2.819313
6 3.312067 -3.444349 1.980928
28 0.054448 -0.290565 -1.229511
15 -1.390138 1.146606 -0.395497
15 2.073784 -0.218826 -0.281084
5 -0.547374 -1.683538 0.657173
1 -0.563346 -1.621911 -0.879511
1 0.304074 0.386720 -2.814730
6 3.642985 -0.367551 -1.231110
6 4.874728 0.147095 -0.801711
6 3.603231 -1.081303 -2.437664
6 6.027835 -0.042334 -1.561294
1 4.937089 0.699248 0.140004
6 4.755922 -1.276684 -3.194714
1 2.652179 -1.500259 -2.778880

6 5.972711 -0.752021 -2.760204
 1 6.979211 0.364489 -1.209463
 1 4.703945 -1.840075 -4.129603
 1 6.877480 -0.898181 -3.354879
 6 2.438286 1.154310 0.873655
 6 2.138239 1.060244 2.239345
 6 2.901663 2.380619 0.368525
 6 2.288999 2.166887 3.075103
 1 1.778097 0.113080 2.650886
 6 3.081550 3.474302 1.209944
 1 3.125497 2.478384 -0.698940
 6 2.767088 3.374268 2.566694
 1 2.038821 2.077583 4.135278
 1 3.455377 4.416496 0.800461
 1 2.895268 4.235871 3.226503
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 6 -0.097624 5.018241 0.064962
 1 0.281329 3.114665 0.998386
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 1 4.253940 -3.859728 2.347852
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 1 -1.923410 2.062993 4.504742
 6 -0.137199 -1.789560 -2.478470
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1 -0.807794 -0.356269 -3.983588
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6 -1.616854 -2.635975 0.448345
6 -2.929469 -2.354639 0.871252
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6 1.027842 -2.324434 1.054366
6 -0.756334 -0.470678 1.787782
6 -1.433991 -3.831037 -0.277347
1 -0.425064 -4.099359 -0.613080
6 -0.610511 -0.736728 3.160179
1 -0.197954 -1.701622 3.475992
6 -1.306690 0.778070 1.437569
6 -1.476578 1.438194 3.759953
6 -3.999144 -3.197277 0.569955
1 -5.005829 -2.939350 0.910910
6 -1.661244 1.722257 2.408491
1 -2.066651 2.693045 2.106069
6 -3.787122 -4.360348 -0.167961
6 -2.493959 -4.679711 -0.586378
1 -2.313404 -5.596674 -1.154244
6 1.101813 -3.527510 1.779655
1 0.176151 -4.061308 2.020470
6 -0.955514 0.199907 4.133539
1 -0.808291 -0.034330 5.191507
6 3.474335 -2.201572 1.191141
1 4.406623 -1.683861 0.942976
6 2.320643 -4.055266 2.204331
1 2.341700 -4.994976 2.763027
6 3.512440 -3.390729 1.915642
28 0.179836 -0.125953 -1.273951
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15 2.115261 -0.166065 -0.250857
5 -0.394985 -1.648734 0.750565
1 -0.279844 -1.601092 -1.041611
1 0.687846 1.119333 -1.877977
6 3.634107 -0.236501 -1.280924
6 4.821526 0.442512 -0.977999
6 3.600217 -1.052901 -2.421156
6 5.940517 0.314546 -1.800127
1 4.878916 1.075364 -0.088608

6 4.720178 -1.188296 -3.236757
 1 2.681941 -1.596448 -2.663411
 6 5.893419 -0.497799 -2.931686
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 1 4.675753 -1.832071 -4.118415
 1 6.770666 -0.594842 -3.575507
 6 2.437293 1.231636 0.880929
 6 2.309923 1.095014 2.269179
 6 2.701768 2.503635 0.347367
 6 2.434679 2.205776 3.103198
 1 2.106113 0.111756 2.702145
 6 2.855902 3.605039 1.184239
 1 2.780497 2.632892 -0.737200
 6 2.712829 3.461342 2.565927
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 1 4.469999 -3.804110 2.241778
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 1 0.596310 -2.538770 -2.468655

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1 -0.751002 -0.061690 -3.737456
1 1.042994 -0.441621 -3.729281

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1 -0.641115 0.362450 -5.217817
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6 4.302544 0.037482 4.420690
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1 3.992010 -2.102600 4.446757
1 4.751559 0.065100 5.416205
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1 3.747465 -1.676696 -4.176676
1 6.334648 -2.876231 -0.946239
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2-PC'

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2-PC

6 2.529223 -1.243237 0.945048
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