

SUPPLEMENTARY INFORMATION

Organometallic Chemistry of New Carbon Material IV.

Structure and Dynamic Behavior of Group 6 metal Tricarbonyl Complexes of Graphene and Perforated Graphene: A DFT Study

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Cartesian coordinates of the computed stationary points

la-Cr

6	3.11879616	0.03028242	1.30743168
6	2.09273313	1.00516310	1.06205382
6	0.78552936	0.54708517	0.69017516
6	0.50229095	-0.86635330	0.62474233
6	1.52588295	-1.82304507	0.93115426
6	2.84348448	-1.34374496	1.24352793
1	4.12567128	0.37291569	1.54291698
1	3.63678051	-2.06672613	1.42962198
6	1.19962257	-3.21656319	0.87396594
6	2.32883721	2.41607391	1.13470626
6	1.32962402	3.31322664	0.87463801
6	0.01658318	2.88631042	0.50524637
6	-0.25415632	1.49718667	0.41239062
1	3.32650119	2.76062789	1.41085418
1	1.52813090	4.38454571	0.94150567
6	-1.02950634	3.80711682	0.22571402
6	-0.81787406	-1.31454739	0.28247961
6	-1.55713314	1.03942307	0.06821961
24	2.35174203	-0.43858217	-0.70920911
6	3.63081703	0.62613124	-1.46357962
6	3.14300691	-1.83849946	-1.57680393
6	1.32867226	-0.16762184	-2.21892424
8	4.45276111	1.29948414	-1.94540484
8	3.65553015	-2.72833081	-2.13061077
8	0.69260382	0.00154981	-3.17892525
1	1.98280516	-3.94151316	1.10067678
6	-0.06306403	-3.63337475	0.55319069
6	-1.10409391	-2.70323679	0.24677276
6	-1.83812083	-0.36215132	0.00344806

6	-2.28643187	3.37021558	-0.12147090
1	-0.81689846	4.87596998	0.28885912
1	-3.07815799	4.09035047	-0.33669259
6	-2.58690697	1.98317506	-0.20537501
6	-2.41870793	-3.12201689	-0.09490059
6	-3.14663774	-0.80883604	-0.33452626
6	-3.88407489	1.50464415	-0.55048614
1	-2.63474910	-4.19143963	-0.13087734
6	-3.40440051	-2.20623643	-0.37953473
6	-4.15354454	0.16044395	-0.61267992
1	-4.66868515	2.23294149	-0.76462995
1	-0.29306444	-4.69998328	0.52090997
1	-4.40822567	-2.54417406	-0.64388350
1	-5.15397244	-0.18788672	-0.87668712

Ib-Cr

6	-2.29599280	2.96447137	-0.55015561
6	-2.40927281	1.54918915	-0.52745099
6	-1.20232290	0.77416709	-0.48865118
6	0.07700244	1.43326209	-0.47250308
6	0.14712887	2.86628372	-0.49544095
6	-1.07044153	3.59587718	-0.53482359
6	1.28225436	0.65814110	-0.45420505
6	2.55735219	1.31616614	-0.45862316
6	2.58540322	2.72977280	-0.47801446
6	1.42195859	3.47801871	-0.49579789
6	1.21326335	-0.77941143	-0.45168044
6	2.41958356	-1.55645558	-0.45369126
6	3.66067189	-0.86652160	-0.45916065
6	3.72673478	0.51061887	-0.46152155
6	-0.06059655	-1.43576826	-0.46765246
6	-0.12790079	-2.86895963	-0.48546408

6	1.08255263	-3.59988084	-0.48351303
6	2.31224260	-2.96630669	-0.46818852
6	-1.27093136	-0.65728097	-0.48608589
6	-2.54654376	-1.31340532	-0.52241605
6	-2.56920805	-2.73309484	-0.54013137
6	-1.40971507	-3.47884529	-0.52241262
6	-3.64710386	0.86639140	-0.55921425
6	-3.71335339	-0.51541629	-0.55677949
1	-3.21194947	3.55752577	-0.57823459
1	-1.02122762	4.68619961	-0.55083702
1	3.55469444	3.23167240	-0.48089279
1	1.47679196	4.56804157	-0.51266656
1	4.58053914	-1.45416625	-0.45918288
1	4.69861810	1.00752750	-0.46341100
1	1.03284489	-4.69020006	-0.49654576
1	3.22907127	-3.55864586	-0.46918114
1	-3.53772077	-3.23587093	-0.56624059
1	-1.46506999	-4.56892206	-0.53456928
1	-4.56606176	1.45470322	-0.58824083
1	-4.68438979	-1.01320576	-0.58388999
24	-0.01845750	0.00315352	1.34499874
6	-0.82016084	-1.21203310	2.43963544
6	-0.69517629	1.29654275	2.43441369
6	1.41471094	-0.06664164	2.46693997
8	2.33049154	-0.11137349	3.18981128
8	-1.33248856	-1.98843522	3.14527015
8	-1.12782533	2.12311513	3.13640082

TS(la-b)-Cr

6	-2.57110399	2.72200664	-0.64665567
6	-2.62589737	1.29978803	-0.66442316
6	-1.40747610	0.56874623	-0.60604058

6	-0.16317841	1.27074214	-0.54004567
6	-0.13727399	2.69996754	-0.52824811
6	-1.37565794	3.39810537	-0.57870328
6	1.07419250	0.53835651	-0.50444565
6	2.32834005	1.23477886	-0.43329590
6	2.30568534	2.66455535	-0.43782578
6	1.12450185	3.36619925	-0.50246697
6	1.05053996	-0.89773937	-0.48165603
6	2.27847552	-1.62489478	-0.46466240
6	3.50564329	-0.90608475	-0.44420126
6	3.52996434	0.46865297	-0.41281392
6	-0.19961725	-1.58706486	-0.55238139
6	-0.21793451	-3.00972463	-0.56706697
6	1.01960374	-3.71040774	-0.51805181
6	2.22251689	-3.04501130	-0.47541273
6	-1.42355915	-0.85706433	-0.62490944
6	-2.66294271	-1.54980192	-0.69596521
6	-2.65184535	-2.97309949	-0.70022991
6	-1.47304532	-3.67692093	-0.63813068
6	-3.85130757	0.57959395	-0.73569602
6	-3.86864911	-0.79447753	-0.75168958
1	-3.50942460	3.27885952	-0.68428590
1	-1.36087044	4.48910820	-0.56438917
1	3.25710751	3.19700692	-0.39245434
1	1.13703135	4.45699765	-0.50246789
1	4.44020291	-1.46882212	-0.42932064
1	4.48209388	1.00056480	-0.37485921
1	1.00004918	-4.80199249	-0.52126752
1	3.15894926	-3.60476472	-0.44738089
1	-3.60487150	-3.50294836	-0.75117251
1	-1.48467174	-4.76848089	-0.64240408
1	-4.78638850	1.14136399	-0.77481982

1	-4.81835679	-1.33019959	-0.80265129
24	0.89308948	0.83060504	1.69490215
6	-0.43059283	0.24882584	2.77256925
6	1.06566771	2.26517736	2.77064986
6	2.04961055	-0.04775018	2.75735876
8	2.79996186	-0.62633920	3.44720554
8	-1.28101811	-0.13550391	3.48084643
8	1.18245614	3.19909092	3.46895938

TS(la-a)-Cr

6	2.78404780	-1.26753839	1.24407774
6	2.10035255	-0.00994313	1.13979304
6	0.71741377	-0.00507060	0.74079012
6	0.02520349	-1.24148621	0.55325030
6	0.71908507	-2.47987364	0.69574774
6	2.10547729	-2.45126187	1.00896181
1	3.82933674	-1.28052142	1.55132706
1	2.64110096	-3.39935641	1.08769979
6	0.00741701	-3.69204645	0.49829697
6	2.78943943	1.24365276	1.25605520
6	2.11596285	2.43246827	1.03225824
6	0.72971281	2.47001967	0.71935967
6	0.03052310	1.23603875	0.56506830
1	3.83476890	1.24921531	1.56339062
1	2.65565102	3.37745980	1.12002717
6	0.02326016	3.68706583	0.53349716
24	2.77878146	-0.00165111	-0.90579485
6	4.56367462	-0.00444670	-1.12805113
6	2.67888063	-1.26821606	-2.20058411
6	2.68436737	1.27762124	-2.18844691
8	5.72717651	-0.00626815	-1.27469596
8	2.62934689	-2.08285817	-3.03891749

8	2.63835933	2.10042462	-3.01897442
6	-1.35333688	1.23787446	0.23113659
6	-1.35864451	-1.23419379	0.21934416
1	0.54487538	-4.63686332	0.59707432
6	-1.33268968	-3.68642618	0.18414501
6	-2.05045707	-2.46794821	0.03612812
6	-2.04860956	0.00409465	0.06440366
6	-1.31685192	3.69019708	0.21933372
1	0.56476804	4.62858079	0.64127214
1	-1.84469790	4.63544085	0.08075395
6	-2.03984174	2.47627979	0.05971377
1	-1.86458648	-4.62802969	0.03656425
6	-3.43333714	-2.43078258	-0.29385967
6	-3.43288778	0.00866577	-0.27080430
6	-3.42286185	2.44820258	-0.27058483
6	-4.09390151	1.25811516	-0.42894766
1	-3.94851447	3.39590355	-0.40151075
1	-3.96305163	-3.37492544	-0.43381069
6	-4.09925720	-1.23636816	-0.44084750
1	-5.16039857	-1.22953140	-0.69775434
1	-5.15505728	1.25828616	-0.68588603

la-Mo

6	-2.54530583	2.59291012	-0.58799763
6	-2.63856072	1.16971747	-0.57233769
6	-1.44509074	0.40222459	-0.52531228
6	-0.17365427	1.06289079	-0.49126855
6	-0.11059857	2.49658768	-0.51108163
6	-1.33491834	3.23361004	-0.55155143
6	1.04323518	0.28007167	-0.48413951
6	2.32187214	0.93172262	-0.49652100
6	2.36284133	2.37184751	-0.45676858

6	1.18269178	3.13095022	-0.46326981
6	0.96938554	-1.15100049	-0.51080208
6	2.16291939	-1.91916532	-0.54331976
6	3.41949015	-1.24433049	-0.55178672
6	3.50050315	0.12288690	-0.52225579
6	-0.30123119	-1.79457875	-0.52830253
6	-0.37136956	-3.21558372	-0.54953061
6	0.83899198	-3.96304904	-0.56041415
6	2.06254739	-3.33756664	-0.56281383
6	-1.50386536	-1.02095365	-0.53555093
6	-2.76755260	-1.67400954	-0.56401540
6	-2.80544625	-3.09753393	-0.57205080
6	-1.65100233	-3.84024199	-0.56506123
6	-3.88751988	0.49015117	-0.59879600
6	-3.94941802	-0.88257188	-0.58935593
1	-3.46794145	3.17487293	-0.62131805
1	-1.28370998	4.32322859	-0.55811018
1	3.33098999	2.87078897	-0.44392006
1	1.23523097	4.21889931	-0.45574168
1	4.33182468	-1.84284355	-0.57383785
1	4.47085667	0.62121813	-0.52314709
1	0.77986137	-5.05290994	-0.57165916
1	2.98125336	-3.92663209	-0.57732051
1	-3.77769387	-3.59348178	-0.58750190
1	-1.69916799	-4.93067817	-0.57492153
1	-4.80431314	1.08180470	-0.62441351
1	-4.91654542	-1.38834911	-0.60607325
42	1.14929348	1.80075322	1.48515889
6	0.34606228	0.57547490	2.80612039
6	0.51217129	3.26280645	2.60240668
6	2.73495828	1.82060100	2.61533633
8	3.69862093	1.84016111	3.27406769

8 -0.13307358 -0.15505963 3.57570130
8 0.13237777 4.15435961 3.25347737

lb-Mo

6 -2.42988471 2.84900609 -0.63904916
6 -2.49433503 1.44027619 -0.47692044
6 -1.27162836 0.70007152 -0.48066713
6 -0.01409974 1.38224483 -0.62664812
6 0.00812924 2.80636408 -0.80521870
6 -1.22592037 3.50337558 -0.79786523
6 1.21463453 0.63676260 -0.67623416
6 2.45877486 1.31414702 -0.86649837
6 2.44115304 2.72494922 -1.02215511
6 1.26181244 3.44002222 -0.99352490
6 1.18647662 -0.79226958 -0.51776440
6 2.40875638 -1.54171542 -0.58749239
6 3.62098544 -0.83293543 -0.77955213
6 3.64758368 0.53983883 -0.91272926
6 -0.06696386 -1.48180385 -0.37142000
6 -0.09442270 -2.90644381 -0.25927872
6 1.13667351 -3.61081267 -0.31559683
6 2.33861931 -2.95275715 -0.47459218
6 -1.29138559 -0.72915469 -0.32284401
6 -2.54588191 -1.41551431 -0.19776045
6 -2.53042582 -2.82875414 -0.09158970
6 -1.35326025 -3.54739256 -0.11973446
6 -3.71339138 0.72731394 -0.33377413
6 -3.73579600 -0.64557929 -0.20090498
1 -3.36203171 3.41621621 -0.63700786
1 -1.20979625 4.58754909 -0.92276230
1 3.38966039 3.24426179 -1.16802316
1 1.28123996 4.52411107 -1.11868463

1	4.55231447	-1.40048827	-0.82199431
1	4.59856915	1.05466604	-1.05836227
1	1.11821936	-4.69850803	-0.23070068
1	3.26824281	-3.52312762	-0.51664894
1	-3.48285097	-3.35119551	0.01439540
1	-1.37682152	-4.63495769	-0.03443172
1	-4.64817323	1.29016825	-0.33111703
1	-4.68982438	-1.16511870	-0.09507507
42	0.12305429	0.14393268	1.51764966
6	-1.11540275	-0.47350035	2.87562212
6	0.24463487	1.77959211	2.55146952
6	1.52724190	-0.53831273	2.66732758
8	2.38350889	-0.95796131	3.34308982
8	-1.87474959	-0.85356641	3.67867969
8	0.31676099	2.77700016	3.15638915

TS(la-b)-Mo

6	-2.57872938	2.71860689	-0.70599991
6	-2.63373843	1.29668026	-0.71147774
6	-1.41535630	0.56517969	-0.64667441
6	-0.17172696	1.26688995	-0.58437712
6	-0.14511804	2.69570271	-0.58323091
6	-1.38298865	3.39410229	-0.64235646
6	1.06555869	0.53288076	-0.53690297
6	2.32149048	1.22882464	-0.48409925
6	2.29835700	2.65813943	-0.48579613
6	1.11690643	3.36033796	-0.55289062
6	1.04186056	-0.90332769	-0.52326156
6	2.26975891	-1.63078975	-0.51004860
6	3.49726876	-0.91302623	-0.49392830
6	3.52230621	0.46211251	-0.46366728
6	-0.20892648	-1.59169647	-0.58801229

6	-0.22812588	-3.01439291	-0.60089822
6	1.00918333	-3.71528752	-0.55694795
6	2.21253090	-3.05091678	-0.52011477
6	-1.43219540	-0.86107239	-0.65850066
6	-2.67200525	-1.55334143	-0.72494328
6	-2.66199668	-2.97639006	-0.72477639
6	-1.48357819	-3.68080250	-0.66557820
6	-3.85890182	0.57644939	-0.77719021
6	-3.87689667	-0.79767549	-0.78329678
1	-3.51646516	3.27553823	-0.74968245
1	-1.36743239	4.48502243	-0.63747964
1	3.24945882	3.19073958	-0.44071456
1	1.13075790	4.45094609	-0.55319484
1	4.43145689	-1.47599725	-0.48076512
1	4.47461692	0.99352812	-0.42881364
1	0.98920072	-4.80668485	-0.55938928
1	3.14842157	-3.61139369	-0.49617468
1	-3.61536085	-3.50563097	-0.77144281
1	-1.49598253	-4.77216686	-0.66778084
1	-4.79368498	1.13805656	-0.82050866
1	-4.82684217	-1.33284854	-0.83023412
42	0.91811331	0.84014718	1.84254723
6	-0.44277592	0.22196053	3.03858169
6	1.09293173	2.36065483	2.98550489
6	2.16067205	-0.04994007	2.98684140
8	2.92813201	-0.60933506	3.67518662
8	-1.27678733	-0.16771304	3.76445771
8	1.20663229	3.30792950	3.66803109

TS' (la-b)-Mo

6	-2.53898902	2.76279994	-0.81406723
6	-2.59982609	1.34526082	-0.73355234

6	-1.38120704	0.61316096	-0.64751646
6	-0.13524031	1.31487463	-0.64074926
6	-0.10338357	2.73910682	-0.72815853
6	-1.33805772	3.43554636	-0.81481999
6	1.09590028	0.57343850	-0.56621331
6	2.34935422	1.27082997	-0.52653519
6	2.33386397	2.69543315	-0.61655275
6	1.15950968	3.39938119	-0.73239594
6	1.07306491	-0.86434750	-0.50931518
6	2.29908330	-1.59383756	-0.46679113
6	3.52840100	-0.87299654	-0.47461435
6	3.55068560	0.50086144	-0.48410161
6	-0.18175279	-1.55009931	-0.51706319
6	-0.20527002	-2.97344615	-0.47312419
6	1.03012417	-3.67427792	-0.42586201
6	2.23691034	-3.01208776	-0.42592535
6	-1.40423865	-0.81469874	-0.59772658
6	-2.64536415	-1.50374772	-0.61263111
6	-2.64039741	-2.92662353	-0.55105984
6	-1.46534552	-3.63508468	-0.48512776
6	-3.82797471	0.62604323	-0.74206753
6	-3.84936103	-0.74618459	-0.68253504
1	-3.47505915	3.32084785	-0.87581119
1	-1.31989673	4.52469921	-0.87755426
1	3.28879648	3.22338376	-0.60245241
1	1.17902446	4.48761953	-0.80344918
1	4.46283834	-1.43487411	-0.44606922
1	4.50360514	1.03244169	-0.47017910
1	1.00820382	-4.76494643	-0.38818759
1	3.17097396	-3.57483212	-0.38900666
1	-3.59704895	-3.45191901	-0.55604460
1	-1.48327789	-4.72538497	-0.44058247

1	-4.76196471	1.18790610	-0.79714152
1	-4.80142036	-1.27976211	-0.68701460
42	0.79636801	0.54987701	1.79579594
6	-0.54945025	-0.12464006	2.98069974
6	0.81128834	2.13057328	2.87029298
6	2.08645580	-0.16885055	3.00924472
8	2.89214810	-0.60926905	3.73866747
8	-1.38109707	-0.54263363	3.69305714
8	0.82902321	3.11045861	3.51424069

IM(la-b)-Mo

6	-2.55408817	2.75600076	-0.80355771
6	-2.61518196	1.33799341	-0.72478269
6	-1.39691411	0.60566991	-0.64124238
6	-0.15115121	1.30696623	-0.63472990
6	-0.11839136	2.73102543	-0.72505687
6	-1.35333159	3.42834543	-0.80752808
6	1.08077121	0.56587868	-0.56433911
6	2.33623935	1.26287572	-0.54026853
6	2.32008174	2.68726314	-0.63227621
6	1.14442817	3.39107597	-0.73994432
6	1.05618141	-0.87215914	-0.50673540
6	2.28228257	-1.60188463	-0.47023061
6	3.51238196	-0.88270260	-0.48873514
6	3.53673307	0.49142561	-0.50336757
6	-0.19860984	-1.55717568	-0.51428814
6	-0.22269797	-2.98018538	-0.47113967
6	1.01277429	-3.68174053	-0.42511675
6	2.21968502	-3.02051508	-0.42822513
6	-1.42055556	-0.82164590	-0.59197707
6	-2.66222782	-1.51041518	-0.60574266
6	-2.65788716	-2.93319373	-0.54565880

6	-1.48269957	-3.64179492	-0.48200649
6	-3.84376549	0.61969473	-0.73229905
6	-3.86600050	-0.75264497	-0.67370634
1	-3.49020644	3.31432285	-0.86250492
1	-1.33487070	4.51745835	-0.87082313
1	3.27509576	3.21522308	-0.62699051
1	1.16355860	4.47916008	-0.81304653
1	4.44625864	-1.44567082	-0.46475559
1	4.49049018	1.02165113	-0.49833324
1	0.99030184	-4.77241219	-0.38707705
1	3.15360418	-3.58367726	-0.39422811
1	-3.61465798	-3.45827327	-0.55007023
1	-1.50059692	-4.73215538	-0.43849723
1	-4.77746119	1.18222429	-0.78589871
1	-4.81831305	-1.28577199	-0.67762125
42	0.87026476	0.58704246	1.79931434
6	-0.46577131	-0.08695660	2.99549341
6	0.88874497	2.17068498	2.86983171
6	2.17012961	-0.12898909	3.00416407
8	2.98076626	-0.56981319	3.72778974
8	-1.29111036	-0.50460721	3.71530263
8	0.90571667	3.15240248	3.51090524

TS(la-a)-Mo

6	2.74390121	-1.26882285	1.27752184
6	2.06448496	-0.00992949	1.15109930
6	0.67776381	-0.00511735	0.76629502
6	-0.01389149	-1.24116278	0.57954348
6	0.68127410	-2.47906183	0.71851112
6	2.06739705	-2.45160091	1.03696737
1	3.78680154	-1.28015104	1.59345786
1	2.60107430	-3.39996574	1.12193078

6	-0.03034168	-3.69087004	0.52025940
6	2.74930257	1.24477154	1.28941443
6	2.07788170	2.43268804	1.06017776
6	0.69190514	2.46913417	0.74203366
6	-0.00856464	1.23560603	0.59130894
1	3.79224124	1.24861638	1.60540466
1	2.61563106	3.37789738	1.15415045
6	-0.01449738	3.68582163	0.55533119
42	2.86324448	-0.00118611	-1.04320105
6	4.76416024	-0.00479990	-1.17190674
6	2.87912857	-1.33346863	-2.43643637
6	2.88525243	1.34457140	-2.42332820
8	5.93584583	-0.00706868	-1.23827765
8	2.89503926	-2.15613595	-3.26913011
8	2.90499214	2.17529494	-3.24790323
6	-1.39335568	1.23743300	0.26017724
6	-1.39866769	-1.23389129	0.24843570
1	0.50716060	-4.63567558	0.61710647
6	-1.37106575	-3.68531413	0.20954003
6	-2.09018981	-2.46720102	0.06568365
6	-2.08919323	0.00401433	0.09569860
6	-1.35522204	3.68897772	0.24459622
1	0.52705682	4.62734507	0.66115071
1	-1.88283816	4.63423942	0.10650832
6	-2.07956842	2.47538372	0.08917562
1	-1.90273155	-4.62694679	0.06248130
6	-3.47410117	-2.43035724	-0.25974414
6	-3.47415825	0.00856417	-0.23550340
6	-3.46361699	2.44758266	-0.23655754
6	-4.13548080	1.25785973	-0.39180908
1	-3.98930596	3.39523381	-0.36626793
1	-4.00385388	-3.37446491	-0.39844848

6	-4.14084197	-1.23633718	-0.40366412
1	-5.20270013	-1.22976325	-0.65680442
1	-5.19735237	1.25825754	-0.64497870

la-W

6	-2.54291592	2.60038775	-0.57861987
6	-2.63572959	1.17571195	-0.56175682
6	-1.44331667	0.40769562	-0.51373710
6	-0.17017994	1.06939890	-0.48075954
6	-0.10726250	2.50522454	-0.50414279
6	-1.33425935	3.24167723	-0.54295121
6	1.04768982	0.28472604	-0.47441119
6	2.32929229	0.93534616	-0.49149153
6	2.37153798	2.37693935	-0.45073787
6	1.18764930	3.13972986	-0.45692264
6	0.97156506	-1.14821441	-0.50117481
6	2.16405423	-1.91678725	-0.53680934
6	3.42309586	-1.24351823	-0.54762047
6	3.50725992	0.12228450	-0.51779328
6	-0.29913955	-1.78962205	-0.51875276
6	-0.37032534	-3.21042306	-0.54237412
6	0.83899311	-3.95894824	-0.55532715
6	2.06350569	-3.33450426	-0.55815247
6	-1.50208582	-1.01456405	-0.52500924
6	-2.76624158	-1.66673237	-0.55483053
6	-2.80466608	-3.09076263	-0.56437818
6	-1.65106243	-3.83402954	-0.55838155
6	-3.88495697	0.49809480	-0.58907236
6	-3.94752071	-0.87499658	-0.58021011
1	-3.46591647	3.18169132	-0.61276388
1	-1.28312785	4.33122175	-0.55130823
1	3.33939750	2.87570765	-0.43455231

1	1.24170408	4.22726282	-0.44547819
1	4.33412197	-1.84387999	-0.57222944
1	4.47830071	0.61913393	-0.52137500
1	0.77871806	-5.04871672	-0.56805509
1	2.98170788	-3.92430938	-0.57448825
1	-3.77723580	-3.58602872	-0.58041628
1	-1.69998201	-4.92440525	-0.56961961
1	-4.80136957	1.09033759	-0.61494193
1	-4.91483296	-1.38036007	-0.59765468
74	1.15040857	1.79721495	1.45927218
6	0.33301876	0.53846511	2.74397521
6	0.48856220	3.24859520	2.58754933
6	2.73705482	1.80098954	2.59949610
8	3.70803570	1.80747156	3.25065960
8	-0.16112301	-0.22278597	3.47596060
8	0.08757662	4.13828065	3.23138678

Ib-W

6	-2.43054183	2.85102005	-0.63191813
6	-2.49713011	1.44356774	-0.46825151
6	-1.27300295	0.70275812	-0.46928309
6	-0.01272721	1.38521250	-0.61023291
6	0.00944488	2.81200282	-0.79161503
6	-1.22477906	3.50596361	-0.78764044
6	1.21776198	0.63918321	-0.66498020
6	2.46301657	1.31698752	-0.85789224
6	2.44322089	2.72658682	-1.01471719
6	1.26267587	3.44248353	-0.98300963
6	1.18869938	-0.79117083	-0.50075667
6	2.41327406	-1.54244768	-0.57278469
6	3.62279221	-0.83269336	-0.76826287
6	3.64965110	0.54122473	-0.90498251

6	-0.06625089	-1.48302627	-0.35920427
6	-0.09400385	-2.90937470	-0.24919851
6	1.13708323	-3.61152790	-0.30688880
6	2.34045597	-2.95218136	-0.46299742
6	-1.29123991	-0.72784277	-0.30590598
6	-2.54856075	-1.41573578	-0.18295029
6	-2.53104119	-2.82783032	-0.08028070
6	-1.35308534	-3.54794118	-0.11125947
6	-3.71434684	0.72922606	-0.32654624
6	-3.73618709	-0.64485604	-0.19017792
1	-3.36215374	3.41902057	-0.63375653
1	-1.20972873	4.58993004	-0.91444223
1	3.39073476	3.24660633	-1.16412985
1	1.28301405	4.52631510	-1.11022008
1	4.55442577	-1.39960224	-0.81258700
1	4.60092584	1.05441164	-1.05411864
1	1.11962241	-4.69946252	-0.22553219
1	3.26933784	-3.52363068	-0.50674040
1	-3.48313377	-3.35126927	0.02374774
1	-1.37834266	-4.63567602	-0.02927168
1	-4.64997566	1.29058424	-0.32753737
1	-4.69085743	-1.16362865	-0.08639601
74	0.11983989	0.14116409	1.48105596
6	-1.12962667	-0.48751222	2.83571443
6	0.23997157	1.79016700	2.50966687
6	1.53714594	-0.54903558	2.62391661
8	2.40681781	-0.97974114	3.27789180
8	-1.90340782	-0.88018766	3.62097752
8	0.31021147	2.80195846	3.09349774

TS(la-b)-W

6	-2.58052343	2.71055939	-0.66565361
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6	-2.63369904	1.28794471	-0.68780529
6	-1.41561440	0.55807920	-0.62685641
6	-0.17226336	1.26261648	-0.55466456
6	-0.14643177	2.69315495	-0.53904062
6	-1.38716715	3.38847269	-0.59065646
6	1.07069202	0.53168180	-0.51820913
6	2.32865970	1.23014147	-0.45959737
6	2.30014633	2.66111326	-0.46203310
6	1.11622138	3.36033797	-0.52422573
6	1.04775206	-0.90753796	-0.50063828
6	2.27736598	-1.63268057	-0.49544510
6	3.50398582	-0.91357574	-0.48231773
6	3.52847989	0.46183089	-0.44503975
6	-0.20327704	-1.59591300	-0.57375693
6	-0.22005470	-3.01825598	-0.59351305
6	1.01823358	-3.71764368	-0.54909639
6	2.22120536	-3.05248663	-0.51028516
6	-1.42861987	-0.86754501	-0.65009529
6	-2.66616243	-1.56131448	-0.72564962
6	-2.65352760	-2.98461030	-0.73155833
6	-1.47417113	-3.68672488	-0.66805298
6	-3.85757019	0.56617623	-0.76460155
6	-3.87288301	-0.80769117	-0.78326932
1	-3.51917125	3.26622656	-0.70510097
1	-1.37445078	4.47921439	-0.57431414
1	3.24987982	3.19616349	-0.42027119
1	1.12764858	4.45077820	-0.52383196
1	4.43873210	-1.47542866	-0.47400155
1	4.48077752	0.99312555	-0.40934761
1	0.99944862	-4.80903081	-0.55518462
1	3.15749177	-3.61227659	-0.48896759
1	-3.60555765	-3.51549754	-0.78533207

1	-1.48428420	-4.77807610	-0.67475958
1	-4.79320557	1.12650128	-0.80516631
1	-4.82146995	-1.34457602	-0.83755980
74	0.90016942	0.86006757	1.78611917
6	-0.50616153	0.29473061	2.96854576
6	1.14143660	2.40082468	2.90258498
6	2.11543935	-0.09500505	2.91994449
8	2.87491974	-0.70772678	3.57519237
8	-1.38033395	-0.07141731	3.66243226
8	1.29791435	3.37527288	3.54108013

TS'(la-b)-W

6	-2.53066000	2.76896766	-0.79773638
6	-2.59251118	1.35295821	-0.70815252
6	-1.37349997	0.62040862	-0.62366310
6	-0.12715286	1.32427373	-0.62848895
6	-0.09454090	2.74901483	-0.72163460
6	-1.32911106	3.44297292	-0.80763843
6	1.10499508	0.57895691	-0.56050686
6	2.35946032	1.27830474	-0.49943726
6	2.34196872	2.70346929	-0.59561455
6	1.16965384	3.40784866	-0.72708296
6	1.08479896	-0.86112843	-0.49669695
6	2.31205578	-1.59064678	-0.46018417
6	3.54078184	-0.86788587	-0.46950647
6	3.56061025	0.50592612	-0.46316332
6	-0.17254766	-1.54516748	-0.49293503
6	-0.19574199	-2.96895891	-0.44733583
6	1.03944571	-3.66880511	-0.40949509
6	2.24800852	-3.00743024	-0.41889024
6	-1.39599679	-0.80887037	-0.57514931
6	-2.63583035	-1.49693120	-0.58346574

6	-2.63106866	-2.92039969	-0.51670365
6	-1.45695125	-3.62969169	-0.45222400
6	-3.82075618	0.63277978	-0.70952719
6	-3.84081832	-0.73895723	-0.64842102
1	-3.46670536	3.32710150	-0.85865732
1	-1.31242037	4.53175081	-0.87556336
1	3.29678530	3.23140924	-0.57551661
1	1.19093210	4.49547810	-0.80399225
1	4.47603823	-1.42833281	-0.44713309
1	4.51308146	1.03809556	-0.44327399
1	1.01772087	-4.75942246	-0.37096197
1	3.18132696	-3.57156675	-0.38729489
1	-3.58817063	-3.44481375	-0.51564794
1	-1.47562048	-4.71975984	-0.40394073
1	-4.75521375	1.19409700	-0.76090501
1	-4.79259331	-1.27297601	-0.64680853
74	0.75348425	0.52188397	1.72785717
6	-0.62207642	-0.16835821	2.88342301
6	0.76792409	2.12104455	2.78832151
6	2.05717994	-0.21188181	2.92959884
8	2.88695404	-0.66677952	3.62634336
8	-1.48412202	-0.60419089	3.55118753
8	0.79090324	3.12621285	3.39661788

IM(la-b)-W

6	-2.56190989	2.74485275	-0.80543049
6	-2.62118892	1.32739435	-0.71917056
6	-1.40208677	0.59812558	-0.62507457
6	-0.15860056	1.30471517	-0.61518758
6	-0.12658214	2.72863925	-0.71643581
6	-1.36282368	3.42125280	-0.80888699
6	1.07727367	0.56432878	-0.53998282

6	2.33442125	1.26662467	-0.50394229
6	2.31217296	2.69105755	-0.60832743
6	1.13575879	3.39110059	-0.73434219
6	1.05602563	-0.87672077	-0.47544229
6	2.28505166	-1.60278889	-0.44016714
6	3.51400603	-0.88053958	-0.46112626
6	3.53528529	0.49407338	-0.46716163
6	-0.19889870	-1.56265257	-0.48670496
6	-0.21980971	-2.98565126	-0.44373197
6	1.01734775	-3.68363826	-0.39587365
6	2.22404875	-3.02085393	-0.39863631
6	-1.42235635	-0.82974402	-0.57517124
6	-2.66143261	-1.52083331	-0.59498836
6	-2.65454655	-2.94397215	-0.53184747
6	-1.47863518	-3.65008449	-0.46015371
6	-3.84835512	0.60602007	-0.73159916
6	-3.86721080	-0.76599928	-0.67073893
1	-3.49895904	3.30082134	-0.87167436
1	-1.34765112	4.50988284	-0.87932784
1	3.26553489	3.22192170	-0.59994225
1	1.15329922	4.47823548	-0.81784669
1	4.44910198	-1.44114302	-0.43935414
1	4.48823674	1.02567756	-0.45834393
1	0.99722551	-4.77436962	-0.35773707
1	3.15843537	-3.58305505	-0.36451766
1	-3.61023148	-3.47087437	-0.54046531
1	-1.49447026	-4.74038917	-0.41522273
1	-4.78306533	1.16614580	-0.79158348
1	-4.81801491	-1.30166916	-0.67857781
74	0.88362160	0.60529200	1.74971697
6	-0.48260166	-0.06711764	2.92677110
6	0.90877252	2.21987177	2.78687803

6	2.19861423	-0.12441018	2.94235240
8	3.03274669	-0.58342030	3.63105465
8	-1.33868611	-0.49113005	3.60965204
8	0.93113635	3.23502366	3.37829188

TS(la-a)-W

6	2.76871924	-1.27108071	1.31191270
6	2.08513097	-0.01015463	1.19384333
6	0.70558753	-0.00517117	0.77051083
6	0.01505944	-1.24292509	0.57594068
6	0.70792850	-2.48100040	0.72351951
6	2.09371952	-2.45147034	1.04763084
1	3.80630790	-1.28505736	1.64378029
1	2.62996525	-3.39928765	1.12291112
6	-0.00000271	-3.69193974	0.51717320
6	2.77412551	1.24664055	1.32392270
6	2.10420557	2.43238174	1.07092347
6	0.71855346	2.47095594	0.74715084
6	0.02036599	1.23733766	0.58778048
1	3.81175869	1.25299412	1.65588554
1	2.64451550	3.37712632	1.15522602
6	0.01583065	3.68683619	0.55240653
74	2.80478028	-0.00143117	-0.96213312
6	4.70244506	-0.00427607	-1.22643853
6	2.68852516	-1.35723802	-2.33720104
6	2.69437034	1.36777966	-2.32434859
8	5.87179611	-0.00623121	-1.34815098
8	2.60235509	-2.20462514	-3.14361873
8	2.61184827	2.22308874	-3.12274389
6	-1.36000994	1.23807994	0.24292804
6	-1.36532234	-1.23447524	0.23110605
1	0.53695720	-4.63664746	0.61742039

6	-1.33837606	-3.68645527	0.19258189
6	-2.05510092	-2.46861759	0.04129527
6	-2.05388277	0.00406120	0.07174365
6	-1.32255404	3.69018545	0.22782648
1	0.55683671	4.62823138	0.66165527
1	-1.84824856	4.63541904	0.08319098
6	-2.04448819	2.47693204	0.06493518
1	-1.86811101	-4.62800228	0.03892462
6	-3.43548141	-2.43075588	-0.29893970
6	-3.43486839	0.00868850	-0.27417806
6	-3.42501439	2.44824333	-0.27560938
6	-4.09441030	1.25812462	-0.43786646
1	-3.94970279	3.39552568	-0.41151960
1	-3.96422501	-3.37443564	-0.44389271
6	-4.09976440	-1.23627921	-0.44979805
1	-5.15873142	-1.22927314	-0.71479491
1	-5.15339328	1.25819830	-0.70289215

Ila-Cr

6	-4.16025915	5.10640055	0.42872727
6	-4.16957239	3.66871507	0.35809635
6	-2.91398324	2.98162055	0.31484876
6	-1.67006963	3.74034916	0.34744964
6	-1.70978370	5.16957321	0.43124450
6	-2.99462293	5.81776842	0.46497559
6	-0.42519075	3.11228821	0.30926688
6	0.78547154	3.80274750	0.36286358
6	0.75101952	5.23132580	0.45765707
6	-0.49675850	5.87746922	0.48288468
6	2.06670800	3.10915906	0.34065526
6	3.28360769	3.85787880	0.43840019

6	3.20058229	5.29217812	0.52680432
6	1.99976914	5.94291228	0.53144546
6	2.14934329	1.71929267	0.23757065
6	3.35818459	1.02599204	0.24207552
6	4.57685496	1.76491843	0.37391356
6	4.50697338	3.16523878	0.45551517
6	3.39964312	-0.42783830	0.17180762
6	4.65388848	-1.11158301	0.27396171
6	5.85776776	-0.32481814	0.38451991
6	5.81696782	1.03826772	0.43368263
6	2.21692890	-1.20511670	-0.00279846
6	2.19960763	-2.61489643	0.08400870
6	3.46082033	-3.31220497	0.18542080
6	4.66055038	-2.54695721	0.21587792
6	0.94875083	-3.37432751	0.07853992
6	0.98858537	-4.80233091	0.11942661
6	2.27524073	-5.45680455	0.17476495
6	3.44337651	-4.75866178	0.20677816
6	-0.28557868	-2.73607624	0.08701412
6	-1.50257049	-3.42555821	0.10531949
6	-1.47246862	-4.85470819	0.11215434
6	-0.22361238	-5.50662536	0.12443262
6	-2.77886565	-2.72662118	0.12955413
6	-4.00044371	-3.47463544	0.14213476
6	-3.92210444	-4.91077567	0.13119654
6	-2.72289800	-5.56614880	0.12025445
6	-2.85320676	-1.33356447	0.15219994
6	-4.05573596	-0.62955843	0.19256083
6	-5.28073451	-1.37245149	0.19726624
6	-5.22025666	-2.77600547	0.17037213
6	-4.09048814	0.82690235	0.23864325
6	-5.34887141	1.50878242	0.28142955

6	-6.55401942	0.72124872	0.27247586
6	-6.52185606	-0.64384533	0.23393110
6	-2.92241614	1.58839874	0.25405389
6	-5.35473901	2.91319567	0.33707663
1	-3.02201085	6.90792003	0.52294772
1	-5.11904288	5.62847477	0.45740539
1	-6.31419408	3.43595241	0.37059235
1	-7.51264635	1.24359982	0.30118275
1	-7.45458969	-1.21180298	0.23204548
1	-6.15372893	-3.34475845	0.17627376
1	-4.85429559	-5.47958059	0.13664330
1	-2.69704587	-6.65776399	0.11791938
1	-0.19961930	-6.59907224	0.14592303
1	2.29597802	-6.54809886	0.19676764
1	4.39963344	-5.28200683	0.25356403
1	5.61735381	-3.06889839	0.24736376
1	6.81257678	-0.85028575	0.43751316
1	6.74536732	1.60537441	0.52541478
1	5.43517450	3.73547683	0.54394834
1	4.13060287	5.86062147	0.59177421
1	1.97015757	7.03248861	0.59893908
1	-0.52467650	6.96809352	0.55095104
1	-0.39770304	2.02950220	0.24187872
1	-1.96983758	1.06948799	0.22477420
1	-1.92682248	-0.76853704	0.14373329
1	-0.30685678	-1.65091423	0.08868188
1	1.27961940	-0.68725321	-0.16520360
1	1.22763340	1.15173279	0.16003973
24	3.56206689	-1.92131060	-1.58664985
6	5.11452035	-1.96307527	-2.57405977
6	2.91545426	-3.19495221	-2.73169317
6	2.90563488	-0.66238451	-2.75956204

8	2.48772806	0.13173905	-3.50107707
8	6.09747012	-1.99435823	-3.19828791
8	2.50656231	-4.00592019	-3.46219841

IIb-Cr

6	-3.99174895	5.14674933	0.18372421
6	-4.07971163	3.71137803	0.23619613
6	-2.86422926	2.95446195	0.20670480
6	-1.58295544	3.64272111	0.12709293
6	-1.54364641	5.07271755	0.08799855
6	-2.78939873	5.79253957	0.11523541
6	-0.37445390	2.94438581	0.09447802
6	0.87038052	3.56712950	0.03777712
6	0.91572483	4.99721402	0.00669258
6	-0.29216634	5.71270481	0.02808177
6	2.11364514	2.80096195	0.01988770
6	3.37734183	3.49108581	-0.01472175
6	3.36846086	4.93159392	-0.05012553
6	2.20378066	5.64230865	-0.04232774
6	2.11710958	1.41488338	0.04009991
6	3.29211465	0.64151330	0.05872529
6	4.55972169	1.32836021	0.03344696
6	4.55750853	2.74499447	-0.01707195
6	3.24959308	-0.82146004	0.13463599
6	4.47521094	-1.57956842	0.18459366
6	5.72335910	-0.86570811	0.05870825
6	5.76406570	0.53429698	-0.01353355
6	2.03165244	-1.52325078	0.19300536
6	1.94788772	-2.90140319	0.31644470
6	3.16934746	-3.66345732	0.35738740
6	4.39072770	-2.99123372	0.28113616
6	0.66239817	-3.58838010	0.40980935

6	0.62477786	-5.01420311	0.52707793
6	1.87315124	-5.73442269	0.54925315
6	3.07699416	-5.09694235	0.47151100
6	-0.54404960	-2.89203769	0.39816995
6	-1.79089309	-3.51205638	0.49907652
6	-1.83460012	-4.93829156	0.60814257
6	-0.62247230	-5.65245188	0.61871203
6	-3.02990342	-2.74620530	0.50301701
6	-4.28710936	-3.42433661	0.60675724
6	-4.28260241	-4.86011971	0.70313052
6	-3.11988914	-5.57808177	0.70560752
6	-3.03235855	-1.35420930	0.41734044
6	-4.19541939	-0.58560246	0.43164292
6	-5.45579669	-1.25828778	0.53189597
6	-5.46794736	-2.66129830	0.61507189
6	-4.15313934	0.86924194	0.35606153
6	-5.37212511	1.62056407	0.38245045
6	-6.61572893	0.90139351	0.47668347
6	-6.65536314	-0.46240780	0.54743406
6	-2.94755590	1.56357733	0.26581951
6	-5.30272379	3.02299232	0.32013159
1	-2.75709354	6.88349742	0.08035297
1	-4.91949918	5.72250137	0.20326257
1	-6.23163798	3.59881345	0.34176767
1	-7.54455615	1.47549850	0.49306291
1	-7.61583254	-0.97698248	0.62019039
1	-6.42861720	-3.17703638	0.69283428
1	-5.24210589	-5.37607968	0.77884019
1	-3.15095067	-6.66684348	0.78359168
1	-0.65276577	-6.74172576	0.70445345
1	1.83823023	-6.82265199	0.63335963
1	4.00401143	-5.67320390	0.49240385

1	5.31850750	-3.56715115	0.30803833
1	6.65238466	-1.43421871	0.03353269
1	6.72436199	1.04241923	-0.09455556
1	5.51723708	3.26565286	-0.04752358
1	4.32731831	5.45229396	-0.08663153
1	2.23218799	6.73358062	-0.07167043
1	-0.25905044	6.80492001	0.00056709
1	-0.40810474	1.85987629	0.11850212
1	-2.02551293	0.99192562	0.24580777
1	-2.07884648	-0.84209815	0.34051819
1	-0.51468309	-1.81072599	0.31001206
1	1.11263240	-0.94829352	0.15817334
1	1.16624602	0.89359973	0.06207238
24	4.58929954	-0.22309392	-1.72059033
6	5.38258463	-1.54281523	-2.69759159
6	3.17692621	-0.25095682	-2.91362305
6	5.44445444	0.94741137	-2.82730702
8	6.00244674	1.68277575	-3.54131873
8	5.90183231	-2.37510842	-3.32980440
8	2.30162957	-0.27013378	-3.67979635

TS(IIa-b)-Cr

6	-4.12972837	5.14588066	0.39974319
6	-4.17002479	3.70782502	0.35138965
6	-2.92847023	2.99540674	0.31598963
6	-1.66878616	3.72652645	0.33711679
6	-1.67762212	5.15833956	0.39045272
6	-2.94880651	5.83307552	0.41817245
6	-0.44041519	3.06907342	0.30921832
6	0.78658590	3.73286996	0.33537838
6	0.78382178	5.16597863	0.38594134
6	-0.44979358	5.84009237	0.41215079

6	2.04721339	3.01008277	0.30411358
6	3.27795444	3.73648269	0.32102099
6	3.23147830	5.17179531	0.37254236
6	2.04597726	5.85178625	0.40387180
6	2.09922139	1.60775280	0.26003694
6	3.29249965	0.90080078	0.20237013
6	4.52773447	1.62196111	0.24157097
6	4.49198038	3.01903916	0.29667362
6	3.32345847	-0.56012923	0.11837944
6	4.56471867	-1.27799308	0.31230879
6	5.78451143	-0.50210574	0.27461281
6	5.75650539	0.86807647	0.21995335
6	2.17733042	-1.33413321	-0.15476192
6	2.09740660	-2.72336138	0.11627786
6	3.32295377	-3.43144339	0.30192852
6	4.54377547	-2.69584709	0.26620653
6	0.83990241	-3.43215036	0.16154406
6	0.83916255	-4.86058513	0.31608976
6	2.09549455	-5.53573254	0.44318650
6	3.28390053	-4.85221637	0.45119281
6	-0.39156597	-2.76810627	0.11275636
6	-1.61781403	-3.42767877	0.19198883
6	-1.61961746	-4.85984278	0.29089844
6	-0.39183795	-5.53608102	0.35571650
6	-2.88639468	-2.70725070	0.20400608
6	-4.12029166	-3.43375173	0.26114107
6	-4.06922397	-4.87057350	0.31497354
6	-2.88269003	-5.54616656	0.33899961
6	-2.93983044	-1.31486817	0.19102741
6	-4.13238342	-0.59116172	0.23531877
6	-5.36845027	-1.31243194	0.26928903
6	-5.32867273	-2.71727472	0.27996203

6	-4.14431509	0.86426528	0.26410359
6	-5.38992004	1.56952840	0.30542437
6	-6.60756162	0.80267799	0.31597846
6	-6.59716847	-0.56371774	0.30230227
6	-2.96280778	1.60351386	0.26974435
6	-5.36944039	2.97487958	0.34336201
1	-2.95346652	6.92443295	0.45583861
1	-5.07683303	5.68906445	0.42330440
1	-6.31885519	3.51582442	0.37343097
1	-7.55755053	1.34063758	0.34242555
1	-7.53871221	-1.11663836	0.31903695
1	-6.26977241	-3.27214660	0.31577301
1	-5.01199200	-5.42038850	0.35123426
1	-2.87509350	-6.63650287	0.39729979
1	-0.39260609	-6.62444126	0.45588148
1	2.09206978	-6.62235220	0.54993211
1	4.22642607	-5.39107302	0.56190161
1	5.48988507	-3.23487691	0.33470160
1	6.73633111	-1.03394890	0.29576366
1	6.69808723	1.42000179	0.18775518
1	5.43329701	3.57364298	0.32258293
1	4.17611643	5.71926174	0.38519303
1	2.04273595	6.94306524	0.44142134
1	-0.45242971	6.93251767	0.44942664
1	-0.43608915	1.98504515	0.26204952
1	-2.02064170	1.06631190	0.24556679
1	-2.00423729	-0.76565650	0.16017354
1	-0.38679342	-1.68440786	0.03699206
1	1.27606217	-0.80952229	-0.46329987
1	1.17009912	1.04477434	0.28455076
24	4.24275826	-1.37922146	-1.81989289
6	5.70325626	-1.80798309	-2.81693896

6	3.30688216	-2.59224159	-2.78926390
6	3.82026508	-0.11598724	-3.05676088
8	3.55007658	0.69878713	-3.85034726
8	6.63137155	-2.08517571	-3.47208376
8	2.71939865	-3.38391058	-3.41531314

TS'(IIa-b)-Cr

6	1.00851196	-3.44958535	-0.35929304
6	2.23027456	-2.81996106	0.13041048
6	3.49211170	-3.48843199	-0.05581793
6	3.47752429	-4.84389829	-0.53817469
6	2.31528147	-5.47614346	-0.88615902
6	1.04911560	-4.80210080	-0.84798379
6	-0.21336019	-2.76027274	-0.37185368
6	-0.14704304	-5.38722508	-1.28659688
1	-0.12822149	-6.42005281	-1.64315765
6	-1.36722671	-4.68610856	-1.30418251
6	-1.39412828	-3.32394140	-0.85982891
1	-0.24027820	-1.74671074	0.01356851
6	-2.63535139	-2.56560731	-0.92507430
6	-2.59527757	-5.28408949	-1.75230484
6	-3.77010505	-4.58566656	-1.76717655
1	-2.57342034	-6.32439129	-2.08290600
6	-3.83884036	-3.20729071	-1.36332215
6	-2.68802498	-1.21342567	-0.58941838
6	-5.02951145	-2.46181928	-1.39730975
1	-5.94986297	-2.95200577	-1.72514490
6	-5.07566124	-1.10634679	-1.02899713
6	-3.86251313	-0.46098840	-0.62444890
1	-1.76669303	-0.71769449	-0.30117843
6	-6.28956782	-0.33321136	-1.04502140
6	-3.88122185	0.94693958	-0.25169109

6	-6.30896975	0.98287844	-0.67852193
1	-7.21246956	-0.82669503	-1.35687565
6	-5.11560258	1.67294878	-0.26502909
6	-2.72119916	1.61624338	0.13502042
6	-5.10971551	3.02359434	0.12426969
1	-6.05057094	3.58005113	0.11386128
6	-3.93621448	3.68118118	0.53256301
6	-2.70453264	2.95087182	0.53717021
1	-1.78311596	1.07181283	0.11984156
6	-3.91440408	5.05846569	0.94983196
6	-1.47625498	3.60101983	0.97340670
6	-2.76162458	5.66982228	1.35581918
1	-4.85288091	5.61686373	0.93877065
6	-1.50399841	4.97076548	1.39082955
6	-0.26158846	2.91769074	1.01257110
1	-2.78018104	6.71611153	1.66819426
6	-0.30628270	5.57191445	1.81491981
1	-0.32191393	6.62018248	2.12444783
6	0.91083691	4.87010275	1.85600015
6	0.92841808	3.49602224	1.45171076
1	-0.23882749	1.88676487	0.67585867
6	2.14657521	5.47257700	2.27973538
6	2.17142040	2.73997981	1.50594863
6	3.31972944	4.77191713	2.30201935
1	2.13295570	6.52195212	2.58199646
6	3.38087139	3.38666160	1.91857163
6	2.22649265	1.38835418	1.15990897
6	4.57877883	2.64938342	1.91804301
1	4.24270283	5.26207489	2.61856485
6	3.40380660	0.64283417	1.18344546
1	1.31808145	0.90102068	0.82008697
1	5.50677775	3.15013600	2.20552737

6	4.62557217	1.29661595	1.54553091
6	3.41780297	-0.76367086	0.80980732
6	5.84987973	0.54393932	1.48779042
6	4.67430595	-1.46542328	0.72845108
6	2.21810355	-1.48164559	0.60721824
6	5.87418107	-0.76127141	1.08215667
1	6.78018154	1.04799849	1.75695518
6	4.67773352	-2.80095098	0.29916841
1	1.27874381	-1.03221575	0.91259081
1	4.43183999	-5.36676434	-0.62444076
1	2.34310162	-6.50604751	-1.24653136
1	5.63103540	-3.32887867	0.22097176
1	6.82252485	-1.29850074	1.02198126
1	-4.68771734	-5.07085589	-2.10662311
1	-7.24821388	1.53984045	-0.69616345
24	2.40437704	-1.61169462	-1.67623195
6	1.90999896	-2.23946964	-3.30898390
6	3.76595837	-0.69319988	-2.45340798
6	1.34273538	-0.18972050	-1.98318259
8	4.63539134	-0.09663290	-2.95632419
8	0.65316563	0.74036808	-2.16979463
8	1.56568773	-2.62729386	-4.35638338

TS''(IIa-b)-Cr

6	1.01419556	-3.36558579	-0.30516499
6	2.25468723	-2.71147563	0.11514136
6	3.51494381	-3.39516127	-0.02763735
6	3.49885102	-4.72499610	-0.59226906
6	2.33932167	-5.33712932	-0.98297857
6	1.05081327	-4.69515278	-0.85956773
6	-0.20047511	-2.66386637	-0.36603922
6	-0.15167024	-5.29194296	-1.27332972

1	-0.12408806	-6.31153654	-1.66410941
6	-1.37986064	-4.60445243	-1.24252215
6	-1.39663284	-3.23922999	-0.81697484
1	-0.22913583	-1.65277719	0.02446079
6	-2.63415647	-2.47978817	-0.85694055
6	-2.61815366	-5.20616063	-1.65624151
6	-3.79168529	-4.50488875	-1.65289371
1	-2.60500889	-6.24908865	-1.97853820
6	-3.84921904	-3.12274367	-1.26161244
6	-2.67789347	-1.12484592	-0.52471790
6	-5.03799684	-2.37348349	-1.27597210
1	-5.96631987	-2.86271069	-1.58195633
6	-5.07292034	-1.01548961	-0.91591770
6	-3.85073649	-0.37122517	-0.53507906
1	-1.75015315	-0.62829232	-0.25949752
6	-6.28382856	-0.23783496	-0.91928066
6	-3.85971237	1.03832486	-0.16390622
6	-6.29227921	1.08168615	-0.56504412
1	-7.21312206	-0.72991900	-1.21378322
6	-5.09091778	1.76968558	-0.17130104
6	-2.69494844	1.70382922	0.21541395
6	-5.07547690	3.12309421	0.20758238
1	-6.01405715	3.68342254	0.20167804
6	-3.89574607	3.77923545	0.59977730
6	-2.66749180	3.04307242	0.60372920
1	-1.76138116	1.15101754	0.21028832
6	-3.86560370	5.16055488	1.00344097
6	-1.43295109	3.69381790	1.02201462
6	-2.70772693	5.77098383	1.39523191
1	-4.80207579	5.72228795	0.99384113
6	-1.45246919	5.06726607	1.42679931
6	-0.21839797	3.00911336	1.05533842

1	-2.71979234	6.82006579	1.69837848
6	-0.25024730	5.66687124	1.84060818
1	-0.26201157	6.71592861	2.14765145
6	0.96535381	4.96234053	1.87891908
6	0.97805011	3.58836620	1.47538127
1	-0.20475028	1.97120884	0.73953163
6	2.20211001	5.55981123	2.30914047
6	2.22165193	2.82957421	1.52289286
6	3.36977694	4.85140862	2.34699587
1	2.19131501	6.60936349	2.61079007
6	3.42829572	3.46602443	1.96184983
6	2.27505173	1.48548059	1.15648376
6	4.61651111	2.71610434	1.99105470
1	4.29127899	5.33521520	2.67749691
6	3.44360129	0.72377457	1.20367350
1	1.36492837	1.01284420	0.80166650
1	5.54117054	3.20398487	2.31001188
6	4.65789218	1.36189920	1.61801570
6	3.45921103	-0.67986598	0.82983902
6	5.87002995	0.58884551	1.61443490
6	4.69330512	-1.40263296	0.81150010
6	2.28239091	-1.35595904	0.48019467
6	5.89073009	-0.71988203	1.21985552
1	6.79589101	1.07835267	1.92383935
6	4.69300076	-2.73698403	0.36317649
1	1.33907872	-0.82806190	0.56510944
1	4.45403378	-5.23426123	-0.73130753
1	2.37562049	-6.33138368	-1.43153233
1	5.64305983	-3.26985701	0.28270991
1	6.83179163	-1.27308205	1.20869844
1	-4.71705547	-4.99166713	-1.96800596
1	-7.22907293	1.64291155	-0.57567864

24	2.03419914	-2.50127041	-2.12625993
6	1.35413610	-3.07649101	-3.70866482
6	3.53560512	-1.94783738	-2.98527902
6	1.31615406	-0.88708820	-2.48109071
8	4.49804366	-1.57748603	-3.53602606
8	0.85560152	0.16132405	-2.73068219
8	0.90553904	-3.43550438	-4.72683518

IM(IIa-b)-Cr

6	1.12062274	-3.37259258	-0.45689972
6	2.34123320	-2.71253198	-0.03340359
6	3.58972481	-3.43282274	-0.02614239
6	3.56349525	-4.81747166	-0.41820946
6	2.41318701	-5.43952079	-0.81754219
6	1.14970286	-4.75237783	-0.87300213
6	-0.09873339	-2.65950302	-0.54998070
6	-0.04429561	-5.34815235	-1.28191503
1	-0.03189104	-6.40009592	-1.57805720
6	-1.27879784	-4.64833434	-1.32512087
6	-1.31124332	-3.27721180	-0.95405097
1	-0.18989541	-1.70118343	-0.03313835
6	-2.55777323	-2.54696476	-0.96924267
6	-2.50984333	-5.27829561	-1.71503664
6	-3.69719013	-4.59725719	-1.71695160
1	-2.48321631	-6.32979499	-2.00777178
6	-3.77145281	-3.21392974	-1.34225630
6	-2.61878630	-1.19041471	-0.63528273
6	-4.97212214	-2.48110741	-1.33518605
1	-5.89851828	-2.98447327	-1.62352226
6	-5.02197378	-1.12533855	-0.97140318
6	-3.80359761	-0.46131885	-0.60682503
1	-1.69373503	-0.67441209	-0.39921232

6	-6.24374855	-0.36488907	-0.95533092
6	-3.83088486	0.94323539	-0.21401614
6	-6.26673937	0.95327812	-0.59643902
1	-7.16957963	-0.86864934	-1.24079414
6	-5.07225866	1.65655413	-0.20743169
6	-2.67603822	1.61807983	0.17824678
6	-5.07402354	3.00594266	0.18550231
1	-6.02037839	3.55304509	0.18936695
6	-3.90234078	3.67453285	0.58165782
6	-2.66476086	2.95425876	0.58014294
1	-1.73712391	1.07393350	0.17930883
6	-3.89074725	5.05217175	0.99849721
6	-1.43906118	3.61725737	1.00508349
6	-2.74128932	5.67390738	1.39713232
1	-4.83458915	5.60148148	0.99378314
6	-1.47698482	4.98640306	1.42270244
6	-0.21390948	2.94992963	1.03158573
1	-2.76731949	6.71965511	1.71071470
6	-0.28360642	5.59706869	1.84664932
1	-0.31112597	6.64114480	2.16925004
6	0.94179875	4.90956829	1.87790594
6	0.97533513	3.54298485	1.45223124
1	-0.18796099	1.91204536	0.71570270
6	2.16768014	5.51543879	2.32828755
6	2.23230310	2.80357203	1.48577822
6	3.34360494	4.82087390	2.36928467
1	2.14034806	6.55949374	2.64744133
6	3.42600253	3.44416137	1.95800790
6	2.31213625	1.47681474	1.07404943
6	4.62185526	2.70815167	1.99213721
1	4.25420523	5.31039022	2.72086137
6	3.48933280	0.72393091	1.12747748

1	1.41662234	1.00818124	0.67890028
1	5.53374547	3.19899379	2.34178557
6	4.68739754	1.36133786	1.59152501
6	3.52298463	-0.66245689	0.72228612
6	5.89946712	0.59324043	1.61249427
6	4.74125515	-1.39245947	0.76378649
6	2.34816007	-1.33610506	0.29708984
6	5.92650208	-0.71552343	1.21249247
1	6.81605460	1.07794107	1.95478417
6	4.74281716	-2.75913747	0.37941167
1	1.39827306	-0.84111636	0.51331494
1	4.50341050	-5.37258196	-0.40506572
1	2.44114584	-6.48779894	-1.12101087
1	5.68844528	-3.30636396	0.40725779
1	6.86412735	-1.27438928	1.23651800
1	-4.61717859	-5.10587952	-2.01216863
1	-7.21147370	1.50112194	-0.59545903
24	1.48319389	-1.58634751	-1.80197233
6	0.24384507	-1.26391222	-3.11339496
6	2.40633453	-2.50969936	-3.04443778
6	2.40133252	-0.10571131	-2.37177470
8	3.00225752	-3.09500892	-3.86293187
8	2.99502986	0.82184302	-2.75389103
8	-0.52878096	-1.06882914	-3.96416367

Ila-Mo

6	-4.16634827	5.10323148	0.48605601
6	-4.17452407	3.66655330	0.40224331
6	-2.91868144	2.98103922	0.34754670
6	-1.67554034	3.74040317	0.38292795
6	-1.71639182	5.16812886	0.48406154
6	-3.00133230	5.81497573	0.52699764

6	-0.43018143	3.11396863	0.33429545
6	0.77938503	3.80483662	0.39642851
6	0.74358855	5.23138016	0.51406669
6	-0.50417802	5.87629114	0.54599065
6	2.06162259	3.11275523	0.36717432
6	3.27719970	3.86072599	0.49259656
6	3.19219471	5.29322676	0.60375313
6	1.99117199	5.94271441	0.60716635
6	2.14669675	1.72676891	0.23315537
6	3.35625823	1.03293267	0.24488057
6	4.57268508	1.77043200	0.40952705
6	4.50005118	3.16967181	0.51276523
6	3.40053715	-0.41788863	0.15010385
6	4.65523672	-1.10123440	0.26087215
6	5.85480966	-0.31710136	0.40381576
6	5.81149076	1.04605853	0.47626183
6	2.21531638	-1.19733004	-0.03083063
6	2.19811770	-2.60830682	0.05270019
6	3.46305548	-3.30743546	0.16216498
6	4.66308309	-2.54056182	0.19781510
6	0.94764710	-3.36919923	0.06560250
6	0.98933473	-4.79639080	0.13164650
6	2.27535309	-5.45021793	0.19136929
6	3.44447966	-4.75250588	0.20521100
6	-0.28742679	-2.73264361	0.06694206
6	-1.50301136	-3.42271169	0.10861959
6	-1.47132936	-4.85149298	0.13599958
6	-0.22206802	-5.50160154	0.15167249
6	-2.77958141	-2.72497468	0.13929990
6	-3.99999024	-3.47411562	0.16717614
6	-3.92021637	-4.90998494	0.16858881
6	-2.72050680	-5.56410517	0.15941165

6	-2.85494786	-1.33223435	0.16033827
6	-4.05766880	-0.62969086	0.21153197
6	-5.28167269	-1.37364665	0.22566603
6	-5.22015133	-2.77696146	0.20179844
6	-4.09339581	0.82634076	0.26308995
6	-5.35197449	1.50667313	0.31720488
6	-6.55628769	0.71824641	0.31277608
6	-6.52309913	-0.64651739	0.27137530
6	-2.92602771	1.58850344	0.27642641
6	-5.35903647	2.91040994	0.38138113
1	-3.02923835	6.90423222	0.59660890
1	-5.12534245	5.62401100	0.52238917
1	-6.31863315	3.43193692	0.42375270
1	-7.51495671	1.23964301	0.34884830
1	-7.45503087	-1.21539972	0.27475633
1	-6.15279116	-3.34658574	0.21785049
1	-4.85161370	-5.47951936	0.18501839
1	-2.69330666	-6.65543461	0.16983109
1	-0.19662513	-6.59341760	0.18911681
1	2.29590396	-6.54085862	0.22892832
1	4.40071055	-5.27533088	0.25385700
1	5.61898225	-3.06167795	0.25860818
1	6.80900319	-0.84264751	0.46287159
1	6.73749267	1.61232760	0.59119638
1	5.42643170	3.73881458	0.62260606
1	4.12099670	5.86090030	0.68689244
1	1.95986336	7.03087334	0.69145910
1	-0.53300583	6.96560737	0.63020325
1	-0.40170334	2.03209606	0.25522605
1	-1.97327687	1.07069641	0.23973391
1	-1.92933534	-0.76635495	0.14566516
1	-0.31076494	-1.64793315	0.04227774

1	1.27505044	-0.67796253	-0.16873368
1	1.22683889	1.16176630	0.12338528
42	3.58377035	-1.93211677	-1.80321770
6	2.90542159	-0.59854786	-3.08338309
8	2.49466448	0.20613094	-3.81795373
6	2.89000018	-3.27788221	-3.03521321
8	2.47216833	-4.09627985	-3.75371950
6	5.22843068	-2.01331381	-2.88023509
8	6.21614985	-2.06518792	-3.49629087

Ilb-Mo

6	-4.21330273	4.96861569	0.34163952
6	-4.24368218	3.53016487	0.31667526
6	-2.99819604	2.82443171	0.28378287
6	-1.74432398	3.56590086	0.27762380
6	-1.76285663	4.99655021	0.31614884
6	-3.03739102	5.66399040	0.34363439
6	-0.50841226	2.91877147	0.24383734
6	0.71106993	3.59287168	0.25808466
6	0.69817406	5.02325964	0.30849877
6	-0.53859760	5.68799138	0.33050343
6	1.98381137	2.88006572	0.23813932
6	3.21590512	3.61816841	0.29027036
6	3.15080832	5.05589636	0.33484946
6	1.95832349	5.71978358	0.33997549
6	2.04422796	1.49374630	0.17294910
6	3.24623514	0.76891262	0.19461078
6	4.48551904	1.50560552	0.25754701
6	4.42748170	2.91850937	0.28711390
6	3.26139595	-0.70127643	0.19631440
6	4.51558879	-1.41214007	0.26075312
6	5.74146149	-0.64158534	0.22496200

6	5.72701073	0.76040765	0.22351838
6	2.07456825	-1.45076914	0.17650203
6	2.04273063	-2.83788612	0.24477105
6	3.28978485	-3.55032484	0.29838723
6	4.48668270	-2.82586883	0.29353864
6	0.78494226	-3.57673644	0.26647193
6	0.80152520	-5.00696977	0.32006982
6	2.07578089	-5.67727865	0.35293947
6	3.25433008	-4.98898298	0.34618308
6	-0.44817064	-2.92794451	0.25081395
6	-1.67048316	-3.60032750	0.28615386
6	-1.65952705	-5.03096184	0.32799680
6	-0.42127670	-5.69699435	0.34380897
6	-2.93936784	-2.88484923	0.29061991
6	-4.17004727	-3.61601904	0.32524100
6	-4.11003062	-5.05347518	0.35359877
6	-2.92003770	-5.72446248	0.35714227
6	-2.99594003	-1.49182422	0.27293611
6	-4.18927364	-0.77139745	0.29135778
6	-5.42318441	-1.49714657	0.32189107
6	-5.38056445	-2.90179331	0.33621544
6	-4.20428745	0.68568388	0.28960332
6	-5.45289131	1.38591991	0.31841061
6	-6.66808011	0.61478909	0.34033353
6	-6.65400654	-0.75117021	0.34198695
6	-3.02604747	1.43049807	0.26944369
6	-5.43922632	2.79117640	0.32936313
1	-3.04881624	6.75547778	0.36731975
1	-5.16399328	5.50518180	0.36331093
1	-6.39096197	3.32804273	0.35317028
1	-7.61943588	1.15030435	0.35825738
1	-7.59412745	-1.30612734	0.36123068

1	-6.32103712	-3.45809649	0.36134150
1	-5.04946367	-5.60946323	0.37659073
1	-2.90895188	-6.81589505	0.38337333
1	-0.41004299	-6.78923973	0.38030393
1	2.08336435	-6.76853008	0.38799017
1	4.20309123	-5.52793255	0.37480652
1	5.43572250	-3.36540761	0.32587272
1	6.69324454	-1.17144149	0.23603677
1	6.66766308	1.30980415	0.23333926
1	5.36519890	3.47756296	0.31825853
1	4.08826166	5.61434095	0.36233814
1	1.94340885	6.81103501	0.37258617
1	-0.54987885	6.78031717	0.36450240
1	-0.49797195	1.83415097	0.21140883
1	-2.08138958	0.89741484	0.24754835
1	-2.06246218	-0.93945020	0.24968842
1	-0.46009772	-1.84341514	0.21592390
1	1.13465901	-0.91216442	0.12486484
1	1.11563174	0.93576775	0.12231996
42	4.68262043	0.04632184	-1.76430247
6	5.66528734	-1.25910588	-2.81259804
6	3.29769003	0.02937658	-3.17681999
6	5.63822850	1.36863632	-2.81651535
8	6.23142008	2.16174523	-3.43535402
8	6.27463313	-2.04181587	-3.42897995
8	2.48035260	0.01907834	-4.00502629

TS(IIa-b)-Mo

6	-4.12428539	5.14133863	0.36278175
6	-4.16241246	3.70350546	0.31400170
6	-2.92000386	2.99257570	0.28791699
6	-1.66184443	3.72575574	0.31773741

6	-1.67282918	5.15696379	0.37546310
6	-2.94475120	5.83011216	0.39269673
6	-0.43222657	3.07037016	0.29722437
6	0.79290451	3.73562537	0.34029324
6	0.78799093	5.16768676	0.40007235
6	-0.44618481	5.84024612	0.41354791
6	2.05547031	3.01448290	0.32470638
6	3.28570594	3.74173155	0.37518960
6	3.23606493	5.17683724	0.43279041
6	2.04941480	5.85458090	0.44344871
6	2.10845134	1.61502119	0.26963983
6	3.30299137	0.90626220	0.24330804
6	4.53673208	1.62718439	0.32203184
6	4.49882131	3.02501673	0.37940820
6	3.33143586	-0.55428962	0.16631314
6	4.57400965	-1.27188331	0.36867549
6	5.79420034	-0.49375722	0.38040110
6	5.76615971	0.87555830	0.33989294
6	2.18149261	-1.32914408	-0.09270461
6	2.10852251	-2.71837815	0.17290114
6	3.33492605	-3.42462552	0.37177978
6	4.55339350	-2.68904216	0.36952841
6	0.85228215	-3.43144197	0.20571743
6	0.85252858	-4.85896063	0.36172017
6	2.10960572	-5.53192341	0.50281295
6	3.29541362	-4.84706579	0.52271070
6	-0.37897155	-2.76979886	0.14199625
6	-1.60482323	-3.43051083	0.20934270
6	-1.60565053	-4.86177137	0.31148715
6	-0.37725197	-5.53614272	0.38989584
6	-2.87335726	-2.71065124	0.20471860
6	-4.10694916	-3.43767439	0.25166822

6	-4.05500296	-4.87405980	0.31051464
6	-2.86837549	-5.54885404	0.34831915
6	-2.92718911	-1.31850775	0.18482301
6	-4.12016250	-0.59537754	0.21335374
6	-5.35583927	-1.31735237	0.23904929
6	-5.31576354	-2.72187108	0.25572809
6	-4.13310085	0.86022464	0.23477651
6	-5.37946467	1.56438922	0.26407005
6	-6.59651630	0.79675240	0.26727548
6	-6.58515550	-0.56938457	0.25828463
6	-2.95242628	1.60054132	0.24546298
6	-5.36087597	2.96954383	0.29847961
1	-2.95118112	6.92119995	0.43207661
1	-5.07215275	5.68310997	0.37858461
1	-6.31090024	3.50949344	0.32052241
1	-7.54683946	1.33413214	0.28391366
1	-7.52628401	-1.12280148	0.26873874
1	-6.25684580	-3.27688954	0.28442749
1	-4.99745156	-5.42456879	0.33861479
1	-2.86083125	-6.63885382	0.40926721
1	-0.37760199	-6.62422752	0.49131460
1	2.10688925	-6.61814543	0.61155661
1	4.23743549	-5.38380662	0.64593539
1	5.49836130	-3.22580781	0.46756556
1	6.74513435	-1.02531854	0.43105517
1	6.70705714	1.42927963	0.34841591
1	5.43912629	3.57906960	0.43311962
1	4.17919517	5.72551529	0.46784427
1	2.04400658	6.94547925	0.48639168
1	-0.45076769	6.93230328	0.45626121
1	-0.42663113	1.98671882	0.24565413
1	-2.00970064	1.06423367	0.22983017

1	-1.99188010	-0.76879640	0.16130437
1	-0.37634136	-1.68674460	0.06245258
1	1.27446612	-0.80584346	-0.38262908
1	1.17838176	1.05415330	0.26158317
42	4.21072244	-1.40095505	-1.95221585
6	5.67663509	-1.88276364	-3.12292980
6	3.11155460	-2.61085313	-2.95874993
6	3.77640958	-0.05761914	-3.26271587
8	3.51838918	0.77304989	-4.04617417
8	6.56298644	-2.16900209	-3.83077187
8	2.44155458	-3.36457948	-3.55149655

TS'(IIa-b)-Mo

6	1.00491218	-3.47158155	-0.32895554
6	2.23013129	-2.83769426	0.14875915
6	3.48830536	-3.52216210	0.00045384
6	3.46756690	-4.88385346	-0.46131404
6	2.30390413	-5.51213887	-0.81353561
6	1.04139641	-4.83073221	-0.79650076
6	-0.21226572	-2.77610322	-0.35777573
6	-0.15592671	-5.41566940	-1.23386646
1	-0.14090051	-6.45323707	-1.57616585
6	-1.37231580	-4.70948680	-1.26520257
6	-1.39520791	-3.34196976	-0.83790201
1	-0.23498170	-1.75529002	0.00859395
6	-2.63332837	-2.58010015	-0.91210716
6	-2.60141391	-5.30717016	-1.71131295
6	-3.77263746	-4.60378453	-1.73809618
1	-2.58299466	-6.35092602	-2.03039447
6	-3.83757258	-3.22142601	-1.34758301
6	-2.68305788	-1.22571184	-0.58512818
6	-5.02578540	-2.47309304	-1.38992088

1	-5.94675101	-2.96303585	-1.71589071
6	-5.06896630	-1.11532484	-1.03053866
6	-3.85534686	-0.47063472	-0.62710349
1	-1.76202119	-0.73055898	-0.29553924
6	-6.28104481	-0.33991329	-1.05288219
6	-3.87190749	0.93877655	-0.26012680
6	-6.29857966	0.97733773	-0.69132037
1	-7.20401423	-0.83276788	-1.36482692
6	-5.10504779	1.66638861	-0.27741702
6	-2.71160325	1.60743052	0.12608699
6	-5.09828804	3.01766492	0.10873337
1	-6.03816340	3.57539889	0.09492276
6	-3.92499819	3.67388843	0.51885942
6	-2.69440415	2.94222762	0.52718952
1	-1.77377113	1.06289772	0.111109461
6	-3.90260821	5.05148450	0.93447863
6	-1.46697082	3.59106421	0.96719429
6	-2.75052635	5.66166034	1.34340455
1	-4.84016476	5.61098962	0.91976562
6	-1.49420520	4.96088073	1.38359441
6	-0.25384690	2.90594165	1.01204871
1	-2.76860239	6.70816153	1.65446434
6	-0.29760524	5.56076079	1.81188501
1	-0.31290332	6.60926938	2.12007495
6	0.91794647	4.85705941	1.85862872
6	0.93476401	3.48279099	1.45618745
1	-0.23137542	1.87529662	0.67518165
6	2.15300111	5.45802088	2.28592456
6	2.17607427	2.72481660	1.51668685
6	3.32490324	4.75596452	2.31266268
1	2.13990964	6.50761996	2.58676238
6	3.38535611	3.37015901	1.93131248

6	2.22926440	1.37260955	1.17381906
6	4.58183522	2.63114233	1.93440325
1	4.24746511	5.24525061	2.63119675
6	3.40486574	0.62592225	1.20132267
1	1.32090125	0.88640047	0.83238917
1	5.51013143	3.13059537	2.22259977
6	4.62642966	1.27768055	1.56423628
6	3.41786479	-0.78222327	0.82941473
6	5.84888005	0.52187467	1.50863647
6	4.67200356	-1.48997762	0.75693092
6	2.21758044	-1.49864172	0.62764633
6	5.87214392	-0.78494137	1.10836357
1	6.77982270	1.02461534	1.77753710
6	4.67371351	-2.83381090	0.35103402
1	1.27701445	-1.04864560	0.92866430
1	4.41805410	-5.41609183	-0.52861572
1	2.32857320	-6.54748227	-1.15777300
1	5.62549469	-3.36632727	0.29050116
1	6.81972668	-1.32376630	1.05396026
1	-4.69093654	-5.08848866	-2.07581882
1	-7.23648966	1.53604831	-0.71302413
42	2.42756349	-1.51628353	-1.79863814
6	1.87284358	-2.09603713	-3.55819017
6	3.81334639	-0.46993609	-2.63777814
6	1.26750442	-0.02632496	-2.07534840
8	4.66206239	0.16668215	-3.12984501
8	0.54744822	0.88893548	-2.22235436
8	1.49882643	-2.44836427	-4.60881400

TS''(IIa-b)-Mo

6	1.00985677	-3.36773321	-0.29541657
6	2.25344904	-2.71223823	0.12510300

6	3.51120087	-3.40651187	0.01019733
6	3.49141793	-4.74003413	-0.54734121
6	2.33106333	-5.35210386	-0.93838747
6	1.04180069	-4.70869775	-0.82277416
6	-0.20218807	-2.66456929	-0.36249999
6	-0.16229200	-5.30863550	-1.22423229
1	-0.13835907	-6.33446257	-1.59837873
6	-1.39017097	-4.61837619	-1.19952970
6	-1.40282157	-3.24768422	-0.79523045
1	-0.22703599	-1.64718793	0.01098829
6	-2.63964770	-2.48864847	-0.83577297
6	-2.63039920	-5.22387063	-1.60037356
6	-3.80279740	-4.52071002	-1.60377924
1	-2.62002801	-6.27111725	-1.90786843
6	-3.85682010	-3.13425300	-1.22902130
6	-2.68075471	-1.13139788	-0.51288700
6	-5.04438812	-2.38329632	-1.24659799
1	-5.97436457	-2.87369030	-1.54505235
6	-5.07606560	-1.02251884	-0.89793922
6	-3.85243878	-0.37700876	-0.52422437
1	-1.75235517	-0.63409920	-0.25237935
6	-6.28563947	-0.24314525	-0.90491201
6	-3.85893870	1.03430085	-0.15995897
6	-6.29138203	1.07850802	-0.55952698
1	-7.21595691	-0.73559213	-1.19487655
6	-5.08897857	1.76701076	-0.17061525
6	-2.69354237	1.69963089	0.21702297
6	-5.07202988	3.12196267	0.20160346
1	-6.00975474	3.68338655	0.19294341
6	-3.89177383	3.77793139	0.59155736
6	-2.66464752	3.04030475	0.59984068
1	-1.76086344	1.14554550	0.21566519

6	-3.86065112	5.16058037	0.98978195
6	-1.43008828	3.69098500	1.01787434
6	-2.70299752	5.77074457	1.38170896
1	-4.79626298	5.72329593	0.97622040
6	-1.44902784	5.06542533	1.41857929
6	-0.21638283	3.00522391	1.05587020
1	-2.71416068	6.82071365	1.68111180
6	-0.24777523	5.66470446	1.83476786
1	-0.25939449	6.71428177	2.13948429
6	0.96641750	4.95866418	1.87927474
6	0.97916505	3.58429671	1.47810490
1	-0.20320812	1.96649608	0.74318280
6	2.20155151	5.55502108	2.31499218
6	2.22195087	2.82464803	1.53217702
6	3.36770502	4.84509494	2.36180267
1	2.19043339	6.60498653	2.61450976
6	3.42653303	3.45917121	1.97931592
6	2.27619342	1.48116324	1.16579172
6	4.61271830	2.70708635	2.02022355
1	4.28759063	5.32796319	2.69754407
6	3.44304027	0.71748667	1.22284482
1	1.36771561	1.01009042	0.80543165
1	5.53513792	3.19325581	2.34763714
6	4.65450268	1.35224305	1.64982149
6	3.45832532	-0.68545333	0.84970321
6	5.86323358	0.57472918	1.66354611
6	4.68768873	-1.41436699	0.85393339
6	2.28233279	-1.35547796	0.48045213
6	5.88251321	-0.73602559	1.27560635
1	6.78716178	1.06116987	1.98263386
6	4.68644372	-2.75210484	0.41237887
1	1.34101455	-0.82185168	0.54667289

1	4.44449345	-5.25587073	-0.67496740
1	2.36733248	-6.35154912	-1.37486673
1	5.63464814	-3.29042283	0.34926357
1	6.82072893	-1.29380396	1.28005865
1	-4.72962619	-5.00997012	-1.90987126
1	-7.22708483	1.64112899	-0.57291424
42	2.06307419	-2.46292254	-2.26951967
6	1.35303428	-3.04724564	-3.96788860
6	3.64127959	-1.85405729	-3.20182726
6	1.29948580	-0.75353715	-2.65264084
8	4.60933628	-1.47974843	-3.74143429
8	0.83135168	0.29520635	-2.88894597
8	0.90017225	-3.41244729	-4.98277185

IM(IIa-b)-Mo

6	1.10794838	-3.37136263	-0.43247994
6	2.33298512	-2.70883530	-0.00768679
6	3.57976242	-3.42878533	-0.00151408
6	3.55323808	-4.81295757	-0.39811549
6	2.40335659	-5.43483886	-0.79684787
6	1.13785759	-4.74942115	-0.84826713
6	-0.11477094	-2.66232834	-0.50460617
6	-0.05693089	-5.34583252	-1.25752523
1	-0.04327833	-6.39665431	-1.55692411
6	-1.28949181	-4.64592916	-1.30278979
6	-1.32288806	-3.27629163	-0.92267054
1	-0.20434622	-1.71480655	0.02984333
6	-2.57002549	-2.54542416	-0.93965320
6	-2.51980998	-5.27254689	-1.70097168
6	-3.70643513	-4.59124027	-1.70349687
1	-2.49259514	-6.32209450	-1.99988110
6	-3.78162707	-3.20952739	-1.32164564

6	-2.63092579	-1.19050757	-0.60191512
6	-4.98135397	-2.47563366	-1.31784883
1	-5.90656393	-2.97654112	-1.61360321
6	-5.03148198	-1.12099732	-0.95008918
6	-3.81474566	-0.45964867	-0.57712258
1	-1.70625027	-0.67651625	-0.36035079
6	-6.25189687	-0.35855543	-0.94056028
6	-3.84167885	0.94441183	-0.18375725
6	-6.27445498	0.95954064	-0.58221652
1	-7.17677521	-0.86047594	-1.23164238
6	-5.08111664	1.66065521	-0.18665292
6	-2.68809384	1.61691075	0.21546537
6	-5.08213405	3.01084242	0.20278957
1	-6.02700230	3.56021234	0.19937896
6	-3.91110277	3.67786210	0.60264950
6	-2.67557330	2.95454211	0.61133310
1	-1.75109654	1.06981165	0.22642582
6	-3.89804338	5.05745880	1.01226796
6	-1.44999185	3.61736348	1.03631239
6	-2.74871225	5.67904254	1.41080577
1	-4.84048499	5.60867060	1.00102499
6	-1.48592337	4.98945279	1.44359635
6	-0.22630827	2.94829809	1.06910949
1	-2.77345076	6.72656856	1.71778180
6	-0.29213498	5.60138002	1.86375318
1	-0.31829954	6.64760544	2.17890832
6	0.93238018	4.91288716	1.89856822
6	0.96410986	3.54348807	1.48268577
1	-0.20231688	1.90742457	0.76348197
6	2.15943720	5.52077606	2.34229213
6	2.22102497	2.80462857	1.51582755
6	3.33516093	4.82633695	2.38381890

1	2.13338662	6.56655066	2.65519846
6	3.41626890	3.44773204	1.97923140
6	2.30065748	1.47660045	1.10815259
6	4.61313064	2.71327394	2.00911255
1	4.24681731	5.31765533	2.72956711
6	3.47851809	0.72576015	1.15773087
1	1.40415209	1.00565752	0.71820897
1	5.52644306	3.20667963	2.35087804
6	4.67816706	1.36571417	1.61185716
6	3.51132877	-0.66184211	0.75363780
6	5.89225847	0.59994283	1.62493058
6	4.73269920	-1.38899725	0.78545960
6	2.33380969	-1.33808311	0.34446432
6	5.91937545	-0.70845158	1.22538965
1	6.81010022	1.08690588	1.95991475
6	4.73397858	-2.75480444	0.40376705
1	1.38322145	-0.85621446	0.58035008
1	4.49350899	-5.36706978	-0.38873944
1	2.43213572	-6.48190581	-1.10354013
1	5.67983177	-3.30147212	0.42761750
1	6.85837492	-1.26488645	1.24264999
1	-4.62526563	-5.09759030	-2.00539276
1	-7.21792167	1.50915588	-0.58742774
42	1.51330054	-1.54039118	-1.96166820
6	0.26070359	-1.28861549	-3.44110201
6	2.51552233	-2.60505137	-3.19136602
6	2.56747491	-0.04103279	-2.64119469
8	3.12818872	-3.25034217	-3.95173736
8	3.21310779	0.84485339	-3.03948959
8	-0.49042405	-1.15814969	-4.32374633

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6	-4.16633113	5.10263830	0.48624167
6	-4.17465879	3.66590925	0.40318450
6	-2.91904128	2.98019156	0.34678585
6	-1.67572327	3.73950674	0.37960956
6	-1.71646307	5.16733670	0.48056048
6	-3.00128748	5.81434280	0.52519507
6	-0.43046020	3.11313863	0.32880674
6	0.77922179	3.80418188	0.38953253
6	0.74346340	5.23077696	0.50733398
6	-0.50433542	5.87559748	0.54070931
6	2.06131558	3.11235852	0.35923697
6	3.27651646	3.86028910	0.48414842
6	3.19188634	5.29272034	0.59511964
6	1.99087797	5.94228293	0.59926523
6	2.14662232	1.72581800	0.22508609
6	3.35626591	1.03326831	0.23595143
6	4.57253978	1.77034395	0.40137039
6	4.49975080	3.16913212	0.50452192
6	3.40014658	-0.41825486	0.14310945
6	4.65544650	-1.10211882	0.25742464
6	5.85555756	-0.31692395	0.39913563
6	5.81171359	1.04572003	0.47007238
6	2.21285938	-1.19893703	-0.04485395
6	2.19501039	-2.61328140	0.04671045
6	3.46018284	-3.31336351	0.15862189
6	4.66386780	-2.54451122	0.18933989
6	0.94384271	-3.37380715	0.06059937
6	0.98514865	-4.80099676	0.12397054
6	2.27135946	-5.45580311	0.18268003
6	3.44059500	-4.75910705	0.19917184
6	-0.28980366	-2.73569874	0.06775582
6	-1.50637174	-3.42514976	0.10878694

6	-1.47563395	-4.85370562	0.13236893
6	-0.22642555	-5.50497409	0.14490584
6	-2.78217312	-2.72656869	0.14175106
6	-4.00307430	-3.47502196	0.17020360
6	-3.92441329	-4.91075262	0.16904166
6	-2.72509621	-5.56559415	0.15624844
6	-2.85676739	-1.33365714	0.16299870
6	-4.05907097	-0.63056695	0.21546136
6	-5.28347820	-1.37397569	0.23139180
6	-5.22280164	-2.77719388	0.20688545
6	-4.09428315	0.82557783	0.26601416
6	-5.35257821	1.50623600	0.32163925
6	-6.55723390	0.71828614	0.31974188
6	-6.52460619	-0.64643624	0.27883055
6	-2.92673970	1.58758196	0.27685072
6	-5.35931526	2.90999141	0.38483301
1	-3.02899307	6.90363133	0.59453858
1	-5.12527842	5.62341630	0.52386286
1	-6.31875069	3.43169841	0.42856426
1	-7.51561621	1.24010899	0.35718636
1	-7.45668801	-1.21505507	0.28395222
1	-6.15572770	-3.34632769	0.22356408
1	-4.85615947	-5.47969042	0.18581539
1	-2.69853261	-6.65695883	0.16419350
1	-0.20193761	-6.59686168	0.18060821
1	2.29148784	-6.54645412	0.21826426
1	4.39667260	-5.28204448	0.24786508
1	5.61966462	-3.06531516	0.24723378
1	6.80947278	-0.84265187	0.45937332
1	6.73757622	1.61207921	0.58539871
1	5.42598419	3.73844371	0.61464169
1	4.12081791	5.86027438	0.67753809

1	1.95958671	7.03046305	0.68335324
1	-0.53313495	6.96491578	0.62486741
1	-0.40202127	2.03128194	0.24935191
1	-1.97413249	1.06955150	0.23908841
1	-1.93089661	-0.76820880	0.14658805
1	-0.31184104	-1.65081858	0.04857621
1	1.27378155	-0.68033242	-0.19110700
1	1.22687552	1.16032615	0.11662231
74	3.58574247	-1.93265262	-1.78354023
6	2.92291435	-0.57506272	-3.05304838
8	2.51865083	0.25228875	-3.76823614
6	2.89350480	-3.27853552	-3.02497250
8	2.47081495	-4.10236566	-3.73726340
6	5.24714900	-1.99860268	-2.84346609
8	6.25299008	-2.03736774	-3.43376531

IIb-W

6	-4.20920486	4.96852216	0.33814107
6	-4.23947025	3.53017217	0.31214462
6	-2.99394182	2.82447702	0.27843122
6	-1.74022664	3.56591340	0.27278428
6	-1.75888548	4.99626052	0.31290333
6	-3.03323416	5.66384951	0.34077042
6	-0.50395494	2.91879801	0.23811384
6	0.71517236	3.59280416	0.25389210
6	0.70208735	5.02298013	0.30616379
6	-0.53435950	5.68765594	0.32842991
6	1.98874834	2.87995808	0.23327068
6	3.22170497	3.61975052	0.28793190
6	3.15509879	5.05754287	0.33423951
6	1.96226992	5.72022767	0.33919806
6	2.04976432	1.49567570	0.16542771

6	3.25401980	0.76932301	0.18883203
6	4.49414129	1.50807215	0.25676655
6	4.43291069	2.92290527	0.28580036
6	3.26919132	-0.70160476	0.19057091
6	4.52426667	-1.41449535	0.26028607
6	5.75097229	-0.64444467	0.22155147
6	5.73645286	0.76338281	0.21989896
6	2.08016410	-1.45266947	0.16886932
6	2.04770244	-2.83774026	0.24008468
6	3.29560624	-3.55186789	0.29661548
6	4.49220084	-2.83021858	0.29280223
6	0.78911773	-3.57665896	0.26216825
6	0.80536407	-5.00667478	0.31787535
6	2.07964244	-5.67772141	0.35274939
6	3.25858026	-4.99062053	0.34637191
6	-0.44363367	-2.92792567	0.24476222
6	-1.66635413	-3.60026484	0.28096201
6	-1.65558845	-5.03059900	0.32443496
6	-0.41711901	-5.69661505	0.34163888
6	-2.93508677	-2.88480211	0.28491566
6	-4.16581770	-3.61593461	0.32027326
6	-4.10594404	-5.05328875	0.34959164
6	-2.91590469	-5.72423447	0.35384162
6	-2.99165466	-1.49172792	0.26646615
6	-4.18495995	-0.77137529	0.28510664
6	-5.41889539	-1.49709284	0.31630101
6	-5.37633954	-2.90166020	0.33109905
6	-4.19998302	0.68574304	0.28345966
6	-5.44861391	1.38594651	0.31304215
6	-6.66383505	0.61479766	0.33512090
6	-6.64975479	-0.75111087	0.33666177
6	-3.02178340	1.43049302	0.26314486

6	-5.43501647	2.79112501	0.32464059
1	-3.04451185	6.75531340	0.36537895
1	-5.15991155	5.50503794	0.36013975
1	-6.38675336	3.32796084	0.34896771
1	-7.61516007	1.15035246	0.35339499
1	-7.58983766	-1.30612052	0.35616730
1	-6.31680898	-3.45794314	0.35667359
1	-5.04539746	-5.60922365	0.37283137
1	-2.90469667	-6.81563890	0.38099445
1	-0.40585201	-6.78881329	0.37940059
1	2.08632837	-6.76893594	0.38897598
1	4.20689189	-5.53025922	0.37631030
1	5.44060146	-3.37050479	0.32808817
1	6.70280080	-1.17364193	0.22895217
1	6.67716650	1.31211126	0.22611151
1	5.36997684	3.48270288	0.31971694
1	4.09210091	5.61666444	0.36272145
1	1.94648523	6.81143166	0.37281200
1	-0.54557149	6.77994193	0.36359564
1	-0.49373803	1.83421416	0.20340851
1	-2.07714158	0.89742301	0.24044899
1	-2.05819582	-0.93935578	0.24257445
1	-0.45573915	-1.84343712	0.20750319
1	1.14106373	-0.91297960	0.11488663
1	1.12198263	0.93661199	0.11288027
74	4.67484172	0.04612559	-1.73452205
6	5.62960709	-1.27321716	-2.80300609
6	3.23878889	0.02915159	-3.09649552
6	5.60218392	1.38202994	-2.80659745
8	6.17688054	2.19254122	-3.42373392
8	6.22088359	-2.07341091	-3.41794198
8	2.37511476	0.01883959	-3.87918632

TS(Ila-b)-W

6	-4.12014523	5.14189253	0.35789473
6	-4.15965011	3.70441782	0.30057126
6	-2.91776449	2.99299036	0.27090487
6	-1.65883667	3.72401672	0.30700820
6	-1.66860432	5.15473148	0.37778302
6	-2.93987210	5.82909084	0.39599511
6	-0.43072774	3.06668889	0.28290483
6	0.79540212	3.72956578	0.33809942
6	0.79177702	5.16147956	0.41494453
6	-0.44156520	5.83572267	0.42854786
6	2.05568777	3.00634767	0.32059485
6	3.28439046	3.73260878	0.39104606
6	3.23764614	5.16652343	0.46713149
6	2.05247601	5.84680121	0.47604543
6	2.10884235	1.60487302	0.24363455
6	3.30418936	0.90085414	0.21499585
6	4.53687640	1.62149749	0.31332435
6	4.49881412	3.01645909	0.39300408
6	3.34254769	-0.55796653	0.10313786
6	4.58008387	-1.28039375	0.34082596
6	5.80039753	-0.49914658	0.35162050
6	5.76745321	0.87077638	0.32062209
6	2.21067526	-1.35229735	-0.22700084
6	2.11693350	-2.73295303	0.12398197
6	3.33713619	-3.43676107	0.34803757
6	4.56228324	-2.70066567	0.31544216
6	0.86076642	-3.43513614	0.18731055
6	0.85641238	-4.85901954	0.38923906
6	2.10803779	-5.53300981	0.55011530
6	3.29681198	-4.85056133	0.54691240

6	-0.37085260	-2.77071769	0.10945338
6	-1.59748952	-3.42646420	0.20424038
6	-1.60097601	-4.85590183	0.34141547
6	-0.37534730	-5.53103554	0.43688509
6	-2.86715003	-2.70710461	0.19609333
6	-4.10065704	-3.43372579	0.25988346
6	-4.04984870	-4.86867135	0.34376012
6	-2.86324382	-5.54201693	0.39485341
6	-2.92224754	-1.31559636	0.16353161
6	-4.11632371	-0.59333396	0.19435262
6	-5.35143825	-1.31528208	0.23030995
6	-5.30998442	-2.71934275	0.26027075
6	-4.13085305	0.86172912	0.21316668
6	-5.37715773	1.56583030	0.24597385
6	-6.59387378	0.79784422	0.25335659
6	-6.58132399	-0.56828416	0.24954005
6	-2.95023989	1.60159840	0.22343641
6	-5.35839019	2.97096852	0.28314473
1	-2.94517984	6.91986107	0.44348678
1	-5.06741896	5.68467022	0.37518369
1	-6.30827793	3.51101963	0.30838727
1	-7.54449703	1.33465512	0.27103837
1	-7.52186559	-1.12257357	0.26540911
1	-6.25020560	-3.27513652	0.30006197
1	-4.99256555	-5.41794651	0.38387772
1	-2.85479479	-6.63046107	0.47915282
1	-0.37866967	-6.61586210	0.56861716
1	2.10105029	-6.61508840	0.69374643
1	4.23775888	-5.38475074	0.68788791
1	5.50751235	-3.23541875	0.41704469
1	6.75243843	-1.02869389	0.40071603
1	6.70742833	1.42607680	0.33348558

1	5.43825239	3.57030184	0.46200082
1	4.18190401	5.71212254	0.51681875
1	2.04808642	6.93706457	0.53217297
1	-0.44456501	6.92726774	0.48282812
1	-0.42556560	1.98364593	0.22032599
1	-2.00780327	1.06503013	0.20736222
1	-1.98675561	-0.76635801	0.13212798
1	-0.36285067	-1.69009284	-0.00295466
1	1.31412951	-0.83590701	-0.56057828
1	1.18117294	1.03975456	0.21631452
74	4.19275605	-1.40696817	-1.92370404
6	5.65639797	-1.88414593	-3.12933457
6	3.03646631	-2.58918341	-2.92099594
6	3.74066820	-0.00797986	-3.18212388
8	3.46897436	0.87335628	-3.90628367
8	6.54527496	-2.16445046	-3.83732712
8	2.32966634	-3.33372957	-3.48308765

TS'(IIa-b)-W

6	1.00789232	-3.46931135	-0.32641026
6	2.23099763	-2.84388169	0.17083155
6	3.49522507	-3.50944661	-0.02502667
6	3.47655712	-4.86322831	-0.50995910
6	2.31283687	-5.49610908	-0.85475714
6	1.04817261	-4.82173990	-0.81897401
6	-0.21196877	-2.77313809	-0.34089515
6	-0.14726825	-5.40002973	-1.26499863
1	-0.13117026	-6.43214319	-1.62314752
6	-1.36435114	-4.69343387	-1.28946923
6	-1.39104763	-3.33242539	-0.84304985
1	-0.24224016	-1.76727502	0.06425181
6	-2.62944190	-2.57204520	-0.91635700

6	-2.59019239	-5.28953656	-1.74502697
6	-3.76395596	-4.59014592	-1.76362327
1	-2.56726740	-6.32910639	-2.07709784
6	-3.83199758	-3.21249205	-1.35916800
6	-2.68093247	-1.21839147	-0.58637289
6	-5.02161173	-2.46635341	-1.39814234
1	-5.94115659	-2.95617769	-1.72823799
6	-5.06742721	-1.11067070	-1.03210102
6	-3.85457736	-0.46509272	-0.62759759
1	-1.75942610	-0.72273040	-0.29862341
6	-6.28123946	-0.33788887	-1.05066172
6	-3.87371790	0.94380609	-0.25955147
6	-6.30131014	0.97820613	-0.68515391
1	-7.20344441	-0.83199865	-1.36285682
6	-5.10841671	1.66886590	-0.27221614
6	-2.71367106	1.61427383	0.12323912
6	-5.10355384	3.01939115	0.11662823
1	-6.04469025	3.57507643	0.10660887
6	-3.93040970	3.67722548	0.52475151
6	-2.69838206	2.94810717	0.52708466
1	-1.77462282	1.07213132	0.10270132
6	-3.90916980	5.05371377	0.94410528
6	-1.47088915	3.59753047	0.96502993
6	-2.75683510	5.66463636	1.35140586
1	-4.84770232	5.61168307	0.93388980
6	-1.49922486	4.96588291	1.38594805
6	-0.25710914	2.91345353	1.00440790
1	-2.77580700	6.71017463	1.66565129
6	-0.30233055	5.56585004	1.81309862
1	-0.31792808	6.61337259	2.12461433
6	0.91401310	4.86320232	1.85501592
6	0.93157801	3.48997417	1.44833048

1	-0.23358106	1.88426573	0.66328716
6	2.14902958	5.46434653	2.28155323
6	2.17280460	2.73225340	1.50519846
6	3.32134507	4.76277365	2.30419094
1	2.13567249	6.51315506	2.58509425
6	3.38161390	3.37805079	1.91971282
6	2.22709820	1.38012968	1.15912092
6	4.57927580	2.64068190	1.91989536
1	4.24438250	5.25155028	2.62207287
6	3.40386095	0.63549736	1.18538018
1	1.32108508	0.89222643	0.81298817
1	5.50717264	3.14098190	2.20787331
6	4.62523976	1.28821353	1.54820624
6	3.41697584	-0.77388945	0.81706675
6	5.84885871	0.53450026	1.49311507
6	4.67550359	-1.48049585	0.74532896
6	2.20968319	-1.50013780	0.65818010
6	5.87364492	-0.77263235	1.09392705
1	6.77917999	1.03928677	1.76008946
6	4.68224342	-2.81911564	0.32999885
1	1.27928836	-1.07081877	1.01738969
1	4.43033015	-5.38595512	-0.60032233
1	2.34111692	-6.52531794	-1.21620448
1	5.63546858	-3.34714497	0.25780833
1	6.82201707	-1.30972906	1.03686761
1	-4.68068302	-5.07352907	-2.10738012
1	-7.24054209	1.53480739	-0.70360537
74	2.38440513	-1.54570658	-1.71279478
6	1.82355846	-2.19347480	-3.45747755
6	3.84056025	-0.57533779	-2.54603514
6	1.25565777	-0.02898838	-2.04664188
8	4.74739975	-0.00126313	-3.01446483

8 0.54759297 0.89631723 -2.20298295
8 1.44195506 -2.60726626 -4.48455495

TS''(IIa-b)-W

6 1.00737004 -3.38139542 -0.27017611
6 2.25212543 -2.72513862 0.15022938
6 3.51792049 -3.40113516 -0.00847582
6 3.50055511 -4.71453685 -0.61453251
6 2.34008395 -5.32637644 -1.00647378
6 1.04347602 -4.70563537 -0.84427013
6 -0.20490397 -2.67346645 -0.33981864
6 -0.15972146 -5.30465511 -1.24900101
1 -0.13113758 -6.31964771 -1.65066969
6 -1.39034938 -4.61917352 -1.20584663
6 -1.40470613 -3.25321183 -0.78749541
1 -0.23643023 -1.66797483 0.06400513
6 -2.63923512 -2.49296410 -0.82989869
6 -2.62947747 -5.22305932 -1.61036228
6 -3.80295307 -4.52129969 -1.60695731
1 -2.61783903 -6.26761153 -1.92673273
6 -3.85679464 -3.13705672 -1.22621340
6 -2.67867647 -1.13410195 -0.51151496
6 -5.04361003 -2.38521357 -1.24482930
1 -5.97359399 -2.87479442 -1.54457438
6 -5.07419493 -1.02420561 -0.89769579
6 -3.84966570 -0.37868504 -0.52616929
1 -1.74883037 -0.63633239 -0.25667104
6 -6.28338098 -0.24445273 -0.90628377
6 -3.85544076 1.03419514 -0.16771482
6 -6.28856346 1.07804027 -0.56431535
1 -7.21390644 -0.73745985 -1.19457342
6 -5.08547578 1.76702921 -0.17856059

6	-2.68934750	1.70058046	0.20477870
6	-5.06807565	3.12280891	0.19033252
1	-6.00581318	3.68421038	0.18151199
6	-3.88742894	3.77942415	0.57785536
6	-2.66030988	3.04188292	0.58554622
1	-1.75636672	1.14702405	0.20134732
6	-3.85608026	5.16245436	0.97458630
6	-1.42577687	3.69254443	1.00307202
6	-2.69835358	5.77260362	1.36630990
1	-4.79160226	5.72531090	0.96061360
6	-1.44474120	5.06679382	1.40423881
6	-0.21246206	3.00606995	1.04221547
1	-2.70930506	6.82272597	1.66518676
6	-0.24386044	5.66529569	1.82248261
1	-0.25528526	6.71484136	2.12731740
6	0.96953981	4.95822043	1.86973338
6	0.98220560	3.58389213	1.46822238
1	-0.19897265	1.96794203	0.72758052
6	2.20382495	5.55372076	2.30888075
6	2.22368490	2.82233361	1.52731918
6	3.36905589	4.84262051	2.35920009
1	2.19276475	6.60378951	2.60801045
6	3.42747359	3.45649877	1.97779122
6	2.27744357	1.47824274	1.16315193
6	4.61331995	2.70438587	2.02119924
1	4.28859533	5.32457371	2.69715406
6	3.44375625	0.71327943	1.22601257
1	1.37097170	1.00826731	0.79597955
1	5.53560329	3.19094552	2.34839862
6	4.65548028	1.34938491	1.65196673
6	3.45975562	-0.68913990	0.85610433
6	5.86507087	0.57426768	1.66197179

6	4.69100033	-1.41374739	0.84920987
6	2.27928568	-1.36390477	0.49943656
6	5.88579458	-0.73490928	1.26808608
1	6.78899037	1.06148145	1.97985706
6	4.69358866	-2.74636845	0.39070955
1	1.33556415	-0.83920847	0.59516969
1	4.45709099	-5.21027400	-0.78690693
1	2.38147629	-6.30458622	-1.48795318
1	5.64474860	-3.27512905	0.30085326
1	6.82532733	-1.29041758	1.26543438
1	-4.72964809	-5.00934143	-1.91535230
1	-7.22404449	1.64099855	-0.57839242
74	2.03056689	-2.44898508	-2.19140147
6	1.31809505	-3.07689515	-3.88102147
6	3.63636262	-1.85450875	-3.09970382
6	1.25453756	-0.73602702	-2.56749658
8	4.63239568	-1.50014255	-3.60538614
8	0.77227479	0.31442371	-2.77851534
8	0.85918410	-3.48993493	-4.87710623

IM(IIa-b)-W

6	1.11165569	-3.37260903	-0.43767285
6	2.33493472	-2.71103601	-0.01347927
6	3.58253121	-3.43176171	-0.00016767
6	3.55268412	-4.81848826	-0.38741000
6	2.40255389	-5.44050282	-0.78623203
6	1.13831453	-4.75364477	-0.84772936
6	-0.10672964	-2.64636858	-0.53524509
6	-0.05638722	-5.34645749	-1.25679785
1	-0.04699279	-6.39959613	-1.54794313
6	-1.28880165	-4.64152389	-1.30926137
6	-1.32064777	-3.26981125	-0.94494404

1	-0.20974993	-1.72141802	0.03847637
6	-2.56576696	-2.54071986	-0.96196109
6	-2.51959930	-5.27243046	-1.69775635
6	-3.70744708	-4.59260830	-1.69980508
1	-2.49251426	-6.32460023	-1.98731478
6	-3.78076463	-3.20905799	-1.32795566
6	-2.62487544	-1.18215728	-0.63451801
6	-4.98129459	-2.47645584	-1.31696544
1	-5.90874310	-2.98007666	-1.60087082
6	-5.02983784	-1.12079214	-0.95382855
6	-3.81008535	-0.45490932	-0.59720364
1	-1.69741539	-0.66466114	-0.41138966
6	-6.25211043	-0.36173050	-0.93213999
6	-3.83755169	0.94896320	-0.20225641
6	-6.27480862	0.95631891	-0.57380234
1	-7.17855093	-0.86664991	-1.21283183
6	-5.07961571	1.66052875	-0.18944075
6	-2.68277612	1.62357623	0.18944804
6	-5.08199960	3.00862401	0.20682606
1	-6.02897520	3.55428785	0.21562504
6	-3.91009565	3.67727973	0.60135685
6	-2.67196319	2.95849443	0.59498151
1	-1.74386418	1.07961357	0.18924495
6	-3.89941048	5.05332639	1.02273644
6	-1.44649624	3.62124999	1.01994171
6	-2.75012046	5.67488379	1.42128153
1	-4.84379851	5.60130848	1.02173180
6	-1.48526788	4.98867091	1.44222428
6	-0.22085766	2.95502956	1.04316971
1	-2.77660562	6.71928440	1.73858211
6	-0.29248401	5.59888143	1.86769236
1	-0.32092894	6.64130546	2.19500525

6	0.93321003	4.91237687	1.89562398
6	0.96797841	3.54788262	1.46416199
1	-0.19458157	1.91750258	0.72647051
6	2.15791046	5.51689704	2.35037286
6	2.22530459	2.80914445	1.49567468
6	3.33354388	4.82238572	2.39178738
1	2.12965177	6.55949664	2.67350179
6	3.41726090	3.44757263	1.97528212
6	2.30772606	1.48548306	1.07599453
6	4.61330542	2.71250811	2.00999857
1	4.24304922	5.31038714	2.74770585
6	3.48407941	0.73115796	1.13590157
1	1.41638629	1.01936107	0.66854706
1	5.52382031	3.20289661	2.36338003
6	4.68054478	1.36700315	1.60602421
6	3.51635509	-0.65386617	0.73235303
6	5.89193069	0.59896111	1.62872957
6	4.73221604	-1.38522753	0.77854179
6	2.33326975	-1.32677339	0.31089111
6	5.91763974	-0.70937295	1.22780086
1	6.80816162	1.08226361	1.97318935
6	4.73387164	-2.75579014	0.40425450
1	1.38627488	-0.85827005	0.59197047
1	4.49153162	-5.37486666	-0.37248950
1	2.43093616	-6.48927942	-1.08702469
1	5.67921721	-3.30275550	0.43765243
1	6.85412197	-1.26971071	1.25352437
1	-4.62746542	-5.10240598	-1.99201355
1	-7.21994140	1.50305658	-0.56861994
74	1.51524362	-1.55886049	-1.93844209
6	0.24258613	-1.28494589	-3.40713751
6	2.51859563	-2.61398235	-3.18609378

6	2.55552533	-0.03398220	-2.60501194
8	3.13366558	-3.26714507	-3.94100425
8	3.19509277	0.86561436	-2.98642284
8	-0.52475870	-1.14627633	-4.27647546

Illa-Cr

6	1.02916421	-0.36185890	0.93077136
6	1.25160213	0.69965897	0.00005203
6	0.19908762	1.11083524	-0.88538223
6	-1.07062169	0.45654610	-0.83778475
6	-1.29447806	-0.60979939	0.09690149
6	-0.24634712	-1.01888441	0.97815037
6	-0.47243871	-2.07504911	1.91651412
6	2.07464083	-0.76415002	1.82035749
6	2.51954456	1.36135616	-0.04024541
6	0.41833537	2.18083558	-1.80909250
6	-2.12294229	0.87304760	-1.71314513
6	-2.56890998	-1.25712455	0.15203151
6	1.83850004	-1.81108044	2.74952902
6	3.32618645	-0.10242366	1.77434514
6	2.72494615	2.42448806	-0.95811463
6	3.54805299	0.95799872	0.84611236
6	-0.62974923	2.58752772	-2.67077406
6	1.67918081	2.83242911	-1.83853287
6	-1.73826445	-2.70863437	1.96559166
6	0.57071253	-2.46343366	2.79737366
6	-2.78420817	-2.30068072	1.08530606
6	-3.60687466	-0.83391503	-0.71900494
6	-3.38487199	0.22642881	-1.64720328
6	-1.89753957	1.93504327	-2.62282230
6	2.87904846	-2.20961550	3.63860638

6	4.36759208	-0.50071165	2.66454257
6	4.81136840	1.62010713	0.80833208
6	3.98723613	3.08580900	-0.99649296
6	-4.05659458	-2.94355338	1.14320550
6	-4.87802847	-1.47649387	-0.66176853
6	-4.43439406	0.64318787	-2.51726424
6	-2.94803863	2.35288534	-3.49325839
6	2.64953517	-3.26164444	4.57028617
6	4.14121635	-1.55432905	3.59185936
6	5.02726823	2.67996127	-0.11432440
6	-4.27609129	-3.99428490	2.07755803
6	-5.09821548	-2.53088327	0.26798865
6	-5.70122831	-0.00422398	-2.45873259
6	-4.21184584	1.70399988	-3.43908613
6	-5.92199386	-1.05903617	-1.53546025
6	-1.96495534	-3.75944404	2.90378284
6	0.34470978	-3.51372066	3.73440463
6	-3.23444457	-4.40055991	2.95434920
6	-0.92208362	-4.15981725	3.78316967
6	3.70625211	-3.65933680	5.46203308
6	1.38840730	-3.91055670	4.61795589
6	-5.56024388	-4.63907600	2.12711242
6	-6.37912625	-3.17960794	0.32464646
6	-7.20095232	-1.71506662	-1.47291864
6	-7.39922756	-2.74765839	-0.55713496
6	-6.57141624	-4.22352551	1.25981563
6	-5.26934290	2.12320912	-4.31705712
6	-6.75394379	0.42091433	-3.34253444
6	-8.02147232	-0.25576859	-3.25840571
6	-6.51845150	1.46092348	-4.24093458
6	3.44127035	-4.72700688	6.39018568
6	-8.23362310	-1.26951858	-2.37107952

1	-8.82281774	0.06444062	-3.93095029
6	1.15250771	-4.97340362	5.55856992
6	-1.14945783	-5.21946339	4.72673806
6	-3.45348645	-5.46079595	3.90050140
6	-5.74826549	-5.69848897	3.08280221
6	4.20071270	4.15036767	-1.91768009
6	1.89664552	3.90117205	-2.75641946
6	-0.41254287	3.65763802	-3.58907748
6	-2.72480695	3.41770725	-4.41060182
6	-5.02164216	3.18180119	-5.22217262
6	-3.78773681	3.83041582	-5.28645904
6	-1.46212816	4.06748834	-4.45834294
6	0.85046007	4.30908983	-3.63036199
6	5.47876443	4.81027441	-1.95165700
6	3.16041268	4.55613924	-2.79342298
6	-4.74824519	-6.08853797	3.92458081
6	-0.09418300	-5.59699902	5.59191220
6	-2.41884703	-5.84321708	4.75525811
6	2.22924732	-5.35067141	6.43600552
1	-7.32423015	1.77885887	-4.91070338
1	-5.82661481	3.50103349	-5.89226815
6	4.93755855	-3.00781474	5.40173850
6	5.19055746	-1.95699782	4.48714196
6	5.62735010	0.15975173	2.61959995
6	5.84833459	1.21591959	1.69519784
6	6.30018748	3.34550979	-0.15408419
6	6.48756082	4.39889077	-1.08142517
6	7.31589246	2.92322400	0.73543272
6	7.11949826	1.88615405	1.64826553
6	6.67251508	-0.24997768	3.51793845
6	6.43484666	-1.28721197	4.42071289
6	7.93444020	0.43802247	3.44545919

6	8.14661293	1.45198691	2.55797518
6	5.66145492	5.88124967	-2.89571357
6	3.37213966	5.63197103	-3.72497571
6	1.07012156	5.38552781	-4.55655066
6	-1.23389732	5.14462441	-5.38297515
6	-3.52828170	4.90953157	-6.20254854
6	-2.31604039	5.53335341	-6.24836179
6	2.33678370	6.01794217	-4.57543096
6	0.01215071	5.77221478	-5.41237610
6	4.66163737	6.27123556	-3.73733208
1	-2.14401319	6.35151002	-6.95409501
1	0.17915058	6.59164012	-6.11917643
1	2.50532182	6.83727746	-5.28199455
1	4.82561171	7.08820672	-4.44632859
1	-4.33509542	5.22396834	-6.87128904
1	-4.91652651	-6.89687388	4.64242991
1	-2.59244603	-6.65153900	5.47317007
1	-0.26628884	-6.40535760	6.31016591
1	2.05279880	-6.16000144	7.15074677
1	8.73183978	0.12656773	4.12676885
1	7.23530334	-1.59432096	5.10179030
1	5.73718948	-3.31613508	6.08326313
1	4.24399791	-5.03248675	7.06791411
24	0.55303943	-1.16261549	-1.19559296
6	1.36743994	-2.77518884	-0.86302372
6	1.80492810	-0.87453782	-2.50863215
6	-0.47728002	-2.01558903	-2.45459990
8	-1.14021390	-2.55072168	-3.24884360
8	2.60003570	-0.68071952	-3.33743226
8	1.88315324	-3.79555876	-0.64039479
1	-6.72405823	-6.19185031	3.12095461
1	-7.54686641	-4.71906792	1.30279359

1	-8.37510370	-3.24250732	-0.51545986
1	-9.20638725	-1.76828349	-2.32671410
1	9.11532292	1.95932026	2.52267960
1	8.28647727	3.42914005	0.70492246
1	7.45773993	4.90553922	-1.11322541
1	6.63316661	6.38318432	-2.92472912

IIIb-Cr

6	1.106592540	-0.221397520	0.889198650
6	1.313847130	0.853738690	-0.013878310
6	0.266952470	1.273291970	-0.892625890
6	-0.992834180	0.619821690	-0.873402280
6	-1.213285270	-0.463873590	0.036232890
6	-0.161926810	-0.884825500	0.919315910
6	-0.385328150	-1.957721530	1.835213020
6	2.132938540	-0.633142520	1.771917000
6	2.570233510	1.515255150	-0.040703540
6	0.484558610	2.351250800	-1.791247540
6	-2.038423060	1.038601620	-1.729773290
6	-2.482812070	-1.117150980	0.074254840
6	1.908608700	-1.708001120	2.688438440
6	3.392256710	0.029389500	1.745287380
6	2.787172390	2.593995270	-0.946452660
6	3.610410540	1.099958010	0.838932610
6	-0.560864530	2.771991750	-2.662008300
6	1.747709920	3.010709730	-1.818795590
6	-1.660809700	-2.617401140	1.870439670
6	0.660739900	-2.369797950	2.722550690
6	-2.705619760	-2.198803190	0.992733820
6	-3.533913660	-0.688973160	-0.799108960
6	-3.309039580	0.382995510	-1.691747710
6	-1.820903840	2.118930260	-2.630424030

6	2.949658640	-2.115562710	3.574941950
6	4.432824000	-0.383861340	2.630851540
6	4.873783470	1.764245700	0.810884500
6	4.050645390	3.255566590	-0.973455440
6	-3.984852730	-2.849052740	1.037304610
6	-4.798798360	-1.339306570	-0.744914940
6	-4.357382560	0.813033010	-2.558723780
6	-2.870863640	2.543795810	-3.499248490
6	2.721625990	-3.181923890	4.487547640
6	4.208987380	-1.454113740	3.541998700
6	5.090472850	2.838468060	-0.095718180
6	-4.198831510	-3.904053140	1.957175000
6	-5.019943970	-2.414260830	0.170689670
6	-5.620546790	0.161488240	-2.515112030
6	-4.134672240	1.890273870	-3.461231160
6	-5.841537640	-0.910739820	-1.609360420
6	-1.887938950	-3.689018620	2.798304770
6	0.423842130	-3.431969250	3.639778630
6	-3.153522220	-4.322924100	2.835046010
6	-0.846247100	-4.086404730	3.674983320
6	3.776616990	-3.589843560	5.377393950
6	1.461464900	-3.837379810	4.521417800
6	-5.482666330	-4.549619170	1.997988380
6	-6.299211380	-3.062773140	0.216096360
6	-7.120975120	-1.570512050	-1.559001390
6	-7.319692140	-2.616404790	-0.661280590
6	-6.491993140	-4.121960380	1.135362710
6	-5.189311650	2.319640480	-4.334590850
6	-6.673132480	0.598573480	-3.393859360
6	-7.939897740	-0.082994390	-3.322587800
6	-6.438196770	1.652966760	-4.273474350
6	3.511057850	-4.672646020	6.289155040

6	-8.152474140	-1.110927960	-2.452609160
1	-8.740520260	0.246589900	-3.991484100
6	1.225023830	-4.915163800	5.447276440
6	-1.073427300	-5.156599810	4.603560760
6	-3.375041320	-5.394118720	3.767749060
6	-5.669408530	-5.622498360	2.940761590
6	4.266036410	4.331879460	-1.878454700
6	1.964967680	4.091741660	-2.723741400
6	-0.341559720	3.855017930	-3.565984790
6	-2.649112480	3.621473320	-4.399325120
6	-4.942108170	3.393439870	-5.223223980
6	-3.710629130	4.045004130	-5.273376320
6	-1.387532780	4.274973130	-4.433087390
6	0.920411030	4.510294990	-3.595109710
6	5.543800420	4.994104370	-1.901581990
6	3.226578030	4.748647940	-2.750700060
6	-4.671090580	-6.022524340	3.779043600
6	-0.018156970	-5.542294360	5.468468610
6	-2.341997920	-5.784766070	4.619778670
6	2.301470700	-5.300703190	6.322699670
1	-7.242544920	1.980679910	-4.940213990
1	-5.746023200	3.720559790	-5.890787490
6	5.004646740	-2.933811340	5.330786700
6	5.255967280	-1.867388850	4.432184220
6	5.690280200	0.278346310	2.599528630
6	5.910426990	1.349192400	1.691453150
6	6.361641280	3.505092170	-0.124160780
6	6.550771930	4.572180800	-1.036148360
6	7.377685530	3.071608450	0.760624150
6	7.181316780	2.021825550	1.656887700
6	6.735870600	-0.142981630	3.493604130
6	6.499621850	-1.193362440	4.379314670

6	7.996935480	0.548761100	3.433564520
6	8.208262440	1.575819830	2.561895360
6	5.727026540	6.078713380	-2.830530300
6	3.439570040	5.837812440	-3.667265940
6	1.140531820	5.598442400	-4.505356130
6	-1.159362820	5.365879750	-5.342315890
6	-3.450624850	5.138375380	-6.173012810
6	-2.239984470	5.764942580	-6.205770960
6	2.406339920	6.233920340	-4.513741210
6	0.084292300	5.995871230	-5.359458560
6	4.728652620	6.479036990	-3.668255970
1	-2.067079590	6.593752530	-6.898763610
1	0.252377400	6.825437750	-6.054097430
1	2.574343370	7.063168480	-5.208792490
1	4.892472350	7.306235970	-4.365377310
1	-4.256243570	5.460734560	-6.839415580
1	-4.841099640	-6.840141140	4.485808970
1	-2.515104460	-6.602731230	5.326620800
1	-0.190346430	-6.360703850	6.175104130
1	2.125892020	-6.120850830	7.025180400
1	8.793626170	0.228603340	4.111660750
1	7.299292650	-1.509259560	5.057300750
1	5.803870090	-3.249021580	6.009612150
1	4.312705420	-4.985462940	6.964840560
1	-6.644601300	-6.117448930	2.971469230
1	-7.467146610	-4.618567890	1.168962150
1	-8.295013230	-3.112866040	-0.628764380
1	-9.124527390	-1.611842410	-2.418730470
1	9.175868510	2.085820880	2.535466620
1	8.347420000	3.579616890	0.738515890
1	7.520683670	5.079870290	-1.058378030
1	6.698207900	6.582195420	-2.850200090

24	-0.862853010	-2.728813350	-0.293547660
6	-0.020821600	-4.332375780	0.024450610
6	0.367462820	-2.421294080	-1.627199970
6	-1.900479590	-3.599618870	-1.537344310
8	-2.566334080	-4.147536000	-2.319671720
8	1.147180780	-2.217278320	-2.467144940
8	0.510620770	-5.346527340	0.235819830

TS(III)-Cr

6	1.08387010	-0.24504669	0.99672190
6	1.29634161	0.82692234	0.07893163
6	0.25500786	1.22108091	-0.81374566
6	-1.01854045	0.57624842	-0.76343519
6	-1.24149138	-0.47394277	0.18736162
6	-0.18452167	-0.89897870	1.05844502
6	-0.40907058	-1.95690446	1.98644542
6	2.12405780	-0.64881696	1.87707314
6	2.55418971	1.47511489	0.02801515
6	0.46879053	2.27895650	-1.73848233
6	-2.06860745	0.97845521	-1.63886668
6	-2.48990960	-1.17305298	0.19278544
6	1.89802875	-1.70044331	2.80881229
6	3.38550137	0.00935390	1.82750263
6	2.77282573	2.53117721	-0.90435009
6	3.60113826	1.06608268	0.90491507
6	-0.58172133	2.68572043	-2.60805010
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6	-1.07300131	-5.12295728	4.78361408
6	-3.37002927	-5.38527744	3.94515715
6	-5.65387095	-5.64960854	3.10495135
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6	5.53519064	4.89634042	-1.92465946
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8	-1.48768618	-2.21209456	-3.96643435
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TS'(III)-Cr

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IM(IIIa-b)-Cr

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Ild-Cr

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6	-1.510645690	-0.766569950	0.242317860
6	-0.449448970	-1.162564830	1.105316790
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6	1.863096270	-0.888186280	1.908096120
6	2.260386280	1.225427310	0.041435550
6	0.133844820	2.026720050	-1.672617900
6	-2.378189550	0.697347020	-1.539036340
6	-2.765820000	-1.430774490	0.308106240
6	1.663722080	-1.946237730	2.839862190
6	3.119542330	-0.218236090	1.847368640
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6	3.320838960	0.833731520	0.915973380
6	-0.933267490	2.430895440	-2.525891750
6	1.392300370	2.689237330	-1.740289180
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6	0.411828280	-2.613285760	2.900843460
6	-2.960999930	-2.494020780	1.235526800

6	-3.828101910	-1.031680790	-0.551867020
6	-3.634997210	0.031454050	-1.472716790
6	-2.185478610	1.766665380	-2.460288800
6	2.722452470	-2.335828580	3.714751560
6	4.175557570	-0.605723050	2.727066540
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6	-4.220845480	-3.161433610	1.299818140
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6	2.521388810	-3.394174460	4.643537950
6	3.973968000	-1.663645040	3.657461890
6	4.783504910	2.560675620	-0.076396040
6	-4.413551320	-4.223071610	2.226936740
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6	-6.148117790	-1.298194120	-1.344997740
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6	-7.026212040	0.176948970	-3.134087620
6	-8.281179460	-0.521681900	-3.040634920

6	-6.819381670	1.225574610	-4.028373500
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TS(IIIId-e)-Cr

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Ile-Cr

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6 6.49288456 4.38774362 -1.06983666
6 7.30351922 2.94240206 0.76318627
6 7.10267449 1.91721831 1.67968258

6	6.65407819	-0.20712241	3.55924753
6	6.41945568	-1.23926277	4.46299062
6	7.91763853	0.47948262	3.48379935
6	8.13056253	1.48755391	2.59224396
6	5.69980207	5.79969438	-2.97652617
6	3.35057839	5.62195958	-3.75064103
6	1.03830712	5.38038367	-4.54898643
6	-1.27037818	5.14223054	-5.35699247
6	-3.56676334	4.90329539	-6.16672524
6	-2.35651920	5.52685855	-6.22086864
6	2.29571561	6.00378216	-4.59801453
6	-0.02948606	5.76643255	-5.39999523
6	4.67226736	6.19472087	-3.84080320
1	-2.18576037	6.34048614	-6.93197334
1	0.13687378	6.57945736	-6.11394268
1	2.46388927	6.81140800	-5.31702945
1	4.86197161	6.96100893	-4.59658371
1	-4.37687589	5.21226480	-6.83403049
1	-4.90961433	-6.88019486	4.70088752
1	-2.58797651	-6.62523954	5.52892569
1	-0.26491380	-6.37149160	6.36275516
1	2.05398532	-6.11980682	7.20039415
1	8.71429895	0.16948684	4.16664328
1	7.22073397	-1.54536401	5.14357572
1	5.72959261	-3.26587751	6.12701156
1	4.24286790	-4.98580763	7.11424159
1	-6.72093741	-6.18200749	3.17963706
1	-7.54808595	-4.71329180	1.36322427
1	-8.38107267	-3.24300797	-0.45356414
1	-9.21794397	-1.77505875	-2.26657944
1	9.09940532	1.99407721	2.55227645
1	8.27504356	3.44557832	0.72639328

1	7.46651182	4.88562335	-1.11106016
1	6.68815359	6.25837779	-3.06104015
24	5.05388330	4.02727005	-4.15349348
6	4.57699008	2.24746904	-4.40708395
6	6.80783268	3.56456240	-4.40400210
6	4.95370899	4.28168421	-5.96406197
8	4.88862985	4.45797578	-7.11504849
8	7.92917307	3.28305847	-4.55701619
8	4.28399526	1.13545812	-4.57244885

Ligand III

6	1.05651210	-0.25868402	0.98912589
6	1.27796436	0.79932375	0.06294572
6	0.23439475	1.20640976	-0.81539653
6	-1.03057183	0.55539971	-0.76764883
6	-1.25201809	-0.50261116	0.15853556
6	-0.20845137	-0.90969634	1.03687599
6	-0.42973665	-1.96630322	1.96217026
6	2.09877874	-0.66510634	1.86663273
6	2.54137907	1.44974560	0.01545901
6	0.45549769	2.26337538	-1.74031364
6	-2.07301044	0.96220394	-1.64478939
6	-2.51560614	-1.15269102	0.20642687
6	1.87640745	-1.72328345	2.79299213
6	3.36374607	-0.01326753	1.81851934
6	2.76203422	2.50817988	-0.91101077
6	3.58463465	1.04221261	0.89457788
6	-0.58891177	2.67021704	-2.61836602
6	1.72099099	2.91425674	-1.78724743
6	-1.69540091	-2.61677982	2.00956309
6	0.61449259	-2.37270839	2.84064934
6	-2.73643416	-2.21069407	1.13332284

6 -3.55904095 -0.74471815 -0.67227429
6 -3.33814150 0.31075394 -1.59619750
6 -1.85083316 2.02079108 -2.57070719
6 2.92287634 -2.13064237 3.67376349
6 4.40944708 -0.42147932 2.69976662
6 4.85252116 1.69562422 0.84661323
6 4.03033384 3.16086740 -0.95808473
6 -4.00507640 -2.86266046 1.18111989
6 -4.82726631 -1.39741666 -0.62357282
6 -4.38421052 0.71967074 -2.47671818
6 -2.89765005 2.42885467 -3.45073919
6 2.69826673 -3.18813301 4.59865575
6 4.18619118 -1.47878323 3.62472425
6 5.07182744 2.75285279 -0.07938449
6 -4.22342628 -3.91948860 2.10825837
6 -5.04671908 -2.45432588 0.30275303
6 -5.64757281 0.06735160 -2.42619119
6 -4.16111243 1.77729861 -3.40135159
6 -5.86842214 -0.98791211 -1.50247276
6 -1.91701549 -3.67714707 2.93870898
6 0.39173849 -3.43319315 3.76938541
6 -3.18261314 -4.32548382 2.98432522
6 -0.87307463 -4.08235024 3.81580456
6 3.75797858 -3.59335762 5.48371311
6 1.43661063 -3.83740916 4.64630950
6 -5.50513917 -4.57211092 2.15087732
6 -6.32321773 -3.11065712 0.35143398
6 -7.14454582 -1.65049774 -1.44758190
6 -7.34217823 -2.68423155 -0.53379435
6 -6.51451392 -4.15922450 1.28291024
6 -5.21421188 2.18847381 -4.28707746
6 -6.69761471 0.48509928 -3.31693980

6	-7.96287481	-0.19678630	-3.23837373
6	-6.46165839	1.52313147	-4.21665843
6	3.49575124	-4.66648454	6.40656881
6	-8.17499414	-1.21034360	-2.35116821
1	-8.76218915	0.11986950	-3.91512608
6	1.20469770	-4.90730181	5.58015134
6	-1.09671924	-5.14936204	4.75070929
6	-3.39882034	-5.39372425	3.92382063
6	-5.69096259	-5.63716893	3.10121495
6	4.24836285	4.21834222	-1.88456301
6	1.94225658	3.97532581	-2.71566915
6	-0.36649453	3.73140733	-3.54637191
6	-2.67334724	3.48699108	-4.37496141
6	-4.96520216	3.24369304	-5.19716218
6	-3.73349269	3.89311598	-5.25907931
6	-1.41168337	4.13626770	-4.42261996
6	0.89817383	4.38086010	-3.59244688
6	5.52965423	4.87186255	-1.92624252
6	3.20754582	4.62432067	-2.76062839
6	-4.69128984	-6.02711753	3.94265639
6	-0.04068895	-5.53235887	5.61202988
6	-2.36479641	-5.77792085	4.77580710
6	2.28395469	-5.29008977	6.45233423
1	-7.26462594	1.83663749	-4.89195139
1	-5.76813271	3.55724740	-5.87247611
6	4.98957014	-2.94370829	5.42204536
6	5.23883700	-1.88901643	4.51142226
6	5.67250559	0.23149252	2.64991063
6	5.89335954	1.28675732	1.72618967
6	6.34787903	3.41012229	-0.12708568
6	6.53891913	4.45922024	-1.05802925
6	7.36658140	2.98421737	0.75868782

6	7.16905458	1.95024268	1.67223454
6	6.72211194	-0.18535755	3.54158857
6	6.48603235	-1.22315734	4.44155014
6	7.98699296	0.49732059	3.46384715
6	8.19911703	1.51088104	2.57664267
6	5.71508610	5.93771471	-2.87576610
6	3.42332110	5.69345504	-3.69919929
6	1.12136731	5.44881098	-4.52639249
6	-1.18020169	5.20705887	-5.35553676
6	-3.47164220	4.96704063	-6.18110726
6	-2.25984520	5.59064783	-6.22688484
6	2.38920496	6.07788422	-4.55095500
6	0.06508463	5.83232427	-5.38716683
6	4.71541261	6.32764676	-3.71721324
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1	0.23521550	6.64660727	-6.09924845
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1	4.88082464	7.14075751	-4.43041478
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1	-6.66509747	-6.13426731	3.13467953
1	-7.48779101	-4.65964071	1.32006602
1	-8.31547086	-3.18461924	-0.49667540
1	-9.14583454	-1.71331312	-2.31047561
1	9.16963055	2.01453953	2.53667049

1	8.33951459	3.48536281	0.72236908
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1	6.68888852	6.43551387	-2.90851826

IIIa-Mo

6	1.02097183	-0.34249056	0.95238009
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6	-1.08140306	0.47729974	-0.81778419
6	-1.30547186	-0.59097876	0.11820524
6	-0.25655739	-1.00061198	0.99979329
6	-0.48705887	-2.04427290	1.94695176
6	2.05934704	-0.73356183	1.85099697
6	2.50390533	1.39087914	-0.00817919
6	0.40291346	2.21068391	-1.77609447
6	-2.13660866	0.90339316	-1.68062271
6	-2.58229618	-1.22661565	0.18374263
6	1.82102006	-1.77713750	2.78536200
6	3.30897799	-0.06632064	1.81089065
6	2.70737242	2.45934666	-0.92229757
6	3.53056363	0.99288951	0.88385433
6	-0.64787365	2.62314034	-2.63288567
6	1.66290800	2.86697493	-1.80139593
6	-1.75598560	-2.67280272	2.00202364
6	0.55488891	-2.42870188	2.83310519
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6	-3.40164875	0.26038947	-1.61039125
6	-1.91409898	1.97134975	-2.58513188
6	2.85858666	-2.16890142	3.67984306
6	4.34684633	-0.45931820	2.70680492
6	4.79049655	1.66068531	0.85125763

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6 -4.07551878 -2.90170676 1.18609762
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6 -2.96718046 2.39400442 -3.44931684
6 2.62719622 -3.21618079 4.61555179
6 4.11945582 -1.51109010 3.63551699
6 5.00530274 2.72189337 -0.06964546
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6 -5.72122254 0.04052285 -2.41147702
6 -4.23135735 1.74662285 -3.39338878
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6 -3.25571544 -4.35344149 3.00138711
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6 -6.59443549 -4.17021118 1.31344145
6 -5.29073994 2.17090917 -4.26528969
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6 -8.04502160 -0.20221529 -3.20200365
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6 3.41449630 -4.67230724 6.44412016
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6 -5.77329739 -5.64156877 3.13937816
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6 -3.81095938 3.87990381 -5.23246601
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6 5.45367261 4.85818711 -1.89980640
6 3.13815309 4.59945356 -2.74608809
6 -4.77361442 -6.03149371 3.98089723
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6 -2.44321314 -5.78941435 4.80781402
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6 4.91132071 -2.95605908 5.45325633
6 5.16546557 -1.90799704 4.53595174
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6 6.27486586 3.39239240 -0.10388097
6 6.46119042 4.44819507 -1.02853525
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6 6.64629620 -0.19941363 3.56966652
6 6.40803914 -1.23527766 4.47304935
6 7.90597680 0.49247645 3.50131859
6 8.11812621 1.50604472 2.61405431
6 5.63454731 5.93250762 -2.83995049

6	3.34755178	5.67977177	-3.67263169
6	1.04656472	5.43194563	-4.50471616
6	-1.25771928	5.19372408	-5.32896058
6	-3.55331373	4.96259259	-6.14437204
6	-2.34144775	5.58616958	-6.19018013
6	2.31193317	6.06680663	-4.52116978
6	-0.01249632	5.82181576	-5.35729781
6	4.63507913	6.32238950	-3.68125888
1	-2.17083734	6.40721967	-6.89254345
1	0.15297517	6.64471890	-6.06005809
1	2.47844266	6.88960451	-5.22384836
1	4.79748566	7.14217940	-4.38701424
1	-4.36144449	5.28001562	-6.80973809
1	-4.94345372	-6.83615162	4.70216360
1	-2.61848276	-6.59344214	5.52978850
1	-0.29294887	-6.34822483	6.36560876
1	2.02482942	-6.10158263	7.20785051
1	8.70155117	0.18438212	4.18592384
1	7.20626224	-1.53854895	5.15809542
1	5.70905254	-3.26019057	6.13853524
1	4.21558420	-4.97442931	7.12493108
42	0.61032364	-1.28097373	-1.31931315
6	1.48119832	-2.99137696	-1.00030576
6	1.93059325	-0.99804017	-2.71980741
6	-0.45403308	-2.20183791	-2.66277316
8	-1.11287000	-2.74168123	-3.45961672
8	2.72574858	-0.80120142	-3.55015656
8	2.00209905	-4.01234593	-0.78410083
1	-6.75052067	-6.13131064	3.18100656
1	-7.57162029	-4.66146820	1.36032946
1	-8.39908580	-3.18634006	-0.45798382
1	-9.23115695	-1.71104702	-2.26718131

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1	8.25742300	3.48328180	0.76185930
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IIIb-Mo

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6	1.307938680	0.840504870	0.004908190
6	0.260855240	1.261724110	-0.870395020
6	-0.997915380	0.603840520	-0.854595960
6	-1.212191430	-0.488749200	0.041100410
6	-0.156844440	-0.914982290	0.921161110
6	-0.379286230	-1.988367770	1.837983680
6	2.129697830	-0.649695260	1.788547280
6	2.560878360	1.507422700	-0.015477030
6	0.473508600	2.346542740	-1.760674830
6	-2.047704640	1.029995110	-1.703701490
6	-2.481346130	-1.144527630	0.078403680
6	1.907153610	-1.724792130	2.702296170
6	3.385540380	0.019109610	1.767102290
6	2.774225640	2.591894470	-0.914250960
6	3.601047870	1.092866150	0.864617130
6	-0.574465010	2.771420890	-2.626564390
6	1.733898600	3.010088680	-1.784186210
6	-1.656693990	-2.650332260	1.871915820
6	0.660899460	-2.391998510	2.731269040
6	-2.704824150	-2.227914940	0.998923540
6	-3.537653410	-0.704275090	-0.779163930
6	-3.316567410	0.375191890	-1.664865320
6	-1.833389930	2.117082860	-2.596270250
6	2.945808800	-2.128801630	3.592368390
6	4.424520910	-0.391021490	2.654940630

6	4.860770900	1.762795170	0.842206060
6	4.034832660	3.258532740	-0.936208210
6	-3.986474160	-2.866303510	1.054819280
6	-4.805454600	-1.350298150	-0.719065600
6	-4.368973670	0.811982710	-2.522988360
6	-2.886274720	2.547776650	-3.457616950
6	2.718025010	-3.195091720	4.504635510
6	4.202215670	-1.462959640	3.563892280
6	5.074644130	2.841482480	-0.059356490
6	-4.202103590	-3.918276430	1.978909520
6	-5.025520540	-2.425350770	0.194257720
6	-5.632571960	0.162229600	-2.476366080
6	-4.149767600	1.894569100	-3.418854970
6	-5.851463760	-0.913794330	-1.574666930
6	-1.887400810	-3.710944180	2.808521770
6	0.423131970	-3.452568510	3.651829390
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6	-7.132427440	-1.568555100	-1.518852180
6	-7.329939230	-2.615928600	-0.622736650
6	-6.499286850	-4.126240350	1.167844530
6	-5.207791200	2.330223550	-4.284553340
6	-6.688598860	0.606155180	-3.346321210
6	-7.956354750	-0.072179900	-3.271386760
6	-6.456359080	1.664980700	-4.221263870
6	3.505606980	-4.680711850	6.309969140
6	-8.167213710	-1.102630880	-2.404541560
1	-8.759509170	0.262442660	-3.934350250

6	1.222179780	-4.927952510	5.464788100
6	-1.074855670	-5.171464280	4.620231540
6	-3.378660920	-5.405754790	3.789699100
6	-5.676263990	-5.626925670	2.971817400
6	4.246833790	4.340187880	-1.834882450
6	1.947293710	4.097571970	-2.681844810
6	-0.359100940	3.860896780	-3.522458070
6	-2.668015680	3.631484950	-4.350869510
6	-4.963453610	3.409103980	-5.167448300
6	-3.732512530	4.060398330	-5.218219160
6	-1.407594330	4.285551050	-4.383900880
6	0.901260500	4.518905570	-3.549206690
6	5.521666760	5.006939230	-1.853651020
6	3.206416180	4.758350790	-2.704942000
6	-4.676741910	-6.028798530	3.807226840
6	-0.021018980	-5.554785600	5.486536460
6	-2.345112360	-5.796561870	4.639734740
6	2.297221300	-5.310357210	6.342548750
1	-7.263573750	1.997488360	-4.881799970
1	-5.769682170	3.740554090	-5.829721370
6	4.997193060	-2.939551230	5.354120300
6	5.247723640	-1.872851560	4.456964530
6	5.679075540	0.276353700	2.628548550
6	5.896839210	1.349612060	1.723976850
6	6.342695060	3.513300930	-0.082654390
6	6.529033200	4.584609260	-0.989235860
6	7.358560430	3.080663120	0.802432930
6	7.164733670	2.027728220	1.694509060
6	6.723539650	-0.142317940	3.524740100
6	6.488855800	-1.194287470	4.408052060
6	7.981705900	0.554327490	3.469326290
6	8.191005230	1.583773670	2.600701280

6	5.701855340	6.096543040	-2.776601020
6	3.415972160	5.853194820	-3.614607290
6	1.117608900	5.613267810	-4.452181520
6	-1.182901600	5.382702620	-5.286094660
6	-3.475733580	5.159177110	-6.111581100
6	-2.265881930	5.786316470	-6.143875650
6	2.381310600	6.251542550	-4.457910520
6	0.059281440	6.014230560	-5.301744200
6	4.702695400	6.498086040	-3.612188980
1	-2.095422480	6.619440220	-6.831917750
1	0.224651540	6.848528380	-5.991015320
1	2.546602950	7.085393060	-5.147753390
1	4.864008330	7.329331880	-4.304685660
1	-4.283320760	5.485255300	-6.773392990
1	-4.847435970	-6.843600090	4.516708010
1	-2.519274520	-6.611393580	5.349594240
1	-0.194161990	-6.370326080	6.195917710
1	2.121548200	-6.129119120	7.046260310
1	8.777752850	0.235992240	4.148656250
1	7.287609000	-1.507852740	5.087856600
1	5.795011320	-3.252287870	6.035389080
1	4.306288770	-4.990953200	6.987619790
1	-6.653188970	-6.117587770	3.007448470
1	-7.476437590	-4.617988770	1.206469660
1	-8.306970780	-3.108171220	-0.585432250
1	-9.140423300	-1.600527550	-2.367111350
1	9.156372750	2.097674630	2.577819260
1	8.326001650	3.592746310	0.784118100
1	7.496855200	5.095967210	-1.007873610
1	6.671247550	6.603043670	-2.793286430
42	-0.798642110	-2.891848410	-0.435293090
6	0.029179940	-4.629062360	-0.130923230

6	0.548063370	-2.616678880	-1.818692940
6	-1.870272530	-3.770825300	-1.804500890
8	-2.535014700	-4.282794200	-2.614219820
8	1.357589510	-2.427992740	-2.635904270
8	0.520941470	-5.665526300	0.077121780

TS(III)-Mo

6	1.05076594	-0.26635959	0.99224953
6	1.26335215	0.80389286	0.07257799
6	0.22171012	1.20003749	-0.81875791
6	-1.05014247	0.55350723	-0.77090855
6	-1.26782363	-0.50966334	0.16771226
6	-0.21574438	-0.92234040	1.05176688
6	-0.44301477	-1.97387374	1.98440036
6	2.08830785	-0.66445736	1.87810599
6	2.51929743	1.45625231	0.02584674
6	0.43303503	2.26331485	-1.73772416
6	-2.10208765	0.96062172	-1.63972706
6	-2.52499103	-1.19082619	0.19168135
6	1.86103284	-1.71280065	2.81267605
6	3.34811046	-0.00447463	1.83000930
6	2.73623272	2.51497084	-0.90308237
6	3.56426846	1.05037817	0.90570913
6	-0.61859650	2.67305471	-2.60391328
6	1.69567297	2.91828281	-1.77963487
6	-1.71161020	-2.61985682	2.03481708
6	0.59966441	-2.36535355	2.86622271
6	-2.74347135	-2.23582919	1.13888421
6	-3.57467894	-0.76562563	-0.67683307
6	-3.36711285	0.30832404	-1.58151989
6	-1.88217166	2.02440316	-2.55518090
6	2.90529440	-2.11004704	3.69956527
6	4.39108438	-0.40435969	2.71653888

6	4.82782675	1.70851446	0.85781721
6	4.00094739	3.17106174	-0.94845197
6	-4.01117214	-2.88407065	1.18799541
6	-4.83926918	-1.41936892	-0.62093028
6	-4.41513848	0.72107221	-2.45247016
6	-2.93507041	2.43752949	-3.42435451
6	2.67888899	-3.15881576	4.63318672
6	4.16715469	-1.45602167	3.64709549
6	5.04318713	2.76616568	-0.06890143
6	-4.23106898	-3.93008426	2.12691760
6	-5.05164862	-2.47858907	0.30563243
6	-5.67469487	0.06225579	-2.40307470
6	-4.19732532	1.78536827	-3.37074290
6	-5.88639040	-1.00222445	-1.48903249
6	-1.93255838	-3.67000601	2.97057342
6	0.37421380	-3.41578789	3.80457757
6	-3.19517901	-4.32340281	3.01328024
6	-0.88992235	-4.06462014	3.85408057
6	3.73694434	-3.55502459	5.52282100
6	1.41772247	-3.80933178	4.68578369
6	-5.51114844	-4.58450212	2.16940356
6	-6.32691209	-3.13374321	0.35894368
6	-7.15978047	-1.66847425	-1.43193689
6	-7.34921062	-2.70706228	-0.52277092
6	-6.51709164	-4.17887778	1.29494455
6	-5.25453978	2.19959118	-4.24835721
6	-6.72919079	0.48394843	-3.28560172
6	-7.99083125	-0.20411450	-3.20733176
6	-6.50023927	1.53019901	-4.17713087
6	3.47474638	-4.62011548	6.45438162
6	-8.19537089	-1.22519959	-2.32757864
1	-8.79387657	0.11355203	-3.87865185

6 1.18542489 -4.87048423 5.62818419
6 -1.11413822 -5.12376801 4.79611187
6 -3.41190596 -5.38351862 3.96081624
6 -5.69820213 -5.64208163 3.12734434
6 4.21497059 4.23054559 -1.87338011
6 1.91016966 3.98377042 -2.70286999
6 -0.40222792 3.74014863 -3.52551726
6 -2.71502609 3.50048988 -4.34196511
6 -5.01046256 3.26034045 -5.15275527
6 -3.77948392 3.91122510 -5.21738002
6 -1.45288654 4.14928339 -4.39243667
6 0.86178280 4.39036921 -3.57329229
6 5.49384525 4.88769061 -1.91456437
6 3.17275019 4.63630408 -2.74696578
6 -4.70193981 -6.02136061 3.97706527
6 -0.05936143 -5.49694682 5.66264647
6 -2.38093500 -5.75584488 4.82125539
6 2.26384579 -5.24441275 6.50450927
1 -7.30636611 1.84587800 -4.84703728
1 -5.81605829 3.57639576 -5.82321740
6 4.96793923 -2.90449025 5.45684774
6 5.21812554 -1.85716737 4.53888872
6 5.65094799 0.25297932 2.66651496
6 5.86887870 1.30518750 1.73948774
6 6.31571724 3.42718444 -0.11621312
6 6.50380099 4.47694535 -1.04710956
6 7.33572336 3.00547868 0.77018043
6 7.14177929 1.97289943 1.68525742
6 6.69980317 -0.15641432 3.56197599
6 6.46426220 -1.18937234 4.46680420
6 7.96269952 0.52903756 3.48221943
6 8.17238881 1.53934995 2.59143412

6	5.67573184	5.95532392	-2.86237945
6	3.38364363	5.70905913	-3.68199025
6	1.07939634	5.46322967	-4.50193003
6	-1.22675866	5.22455081	-5.32011034
6	-3.52217868	4.98964816	-6.13474450
6	-2.31064233	5.61282082	-6.18348378
6	2.34631839	6.09426002	-4.52861443
6	0.01856337	5.84974331	-5.35478859
6	4.67434322	6.34533364	-3.70101681
1	-2.13930942	6.42975907	-6.89042100
1	0.18454266	6.66728092	-6.06372393
1	2.51250626	6.91115223	-5.23817834
1	4.83739114	7.15980900	-4.41275117
1	-4.33007481	5.30273935	-6.80238914
1	-4.86874132	-6.82905412	4.69558663
1	-2.55161005	-6.56412537	5.53946218
1	-0.22920226	-6.30538579	6.38096083
1	2.08966038	-6.05219974	7.22117601
1	8.76219843	0.21778720	4.16078060
1	7.26609055	-1.49677156	5.14576597
1	5.76955293	-3.21123499	6.13642798
1	4.27929192	-4.92317501	7.13066907
1	-6.67013105	-6.14283793	3.15939760
1	-7.48955443	-4.68018509	1.33241883
1	-8.32079403	-3.20992508	-0.48337703
1	-9.16366016	-1.73239370	-2.28757723
1	9.14148033	2.04494944	2.54981181
1	8.30681222	3.50951295	0.73291369
1	7.47530195	4.98025063	-1.08347830
1	6.64844481	6.45451778	-2.89609482
42	-0.17950678	-1.88995194	-1.44809036
6	-0.06266299	-3.79241610	-1.23440038

6	1.54349620	-1.96005313	-2.29376931
6	-0.95010716	-2.22293514	-3.17261181
8	-1.43894558	-2.42083810	-4.21737965
8	2.60027978	-1.98228794	-2.79566073
8	-0.00741359	-4.95259226	-1.09084755

TS'(III)-Mo

6	1.07197617	-0.22983699	0.98229637
6	1.28402777	0.83157581	0.05763467
6	0.24609897	1.21829819	-0.83651376
6	-1.01750189	0.55735017	-0.80294333
6	-1.24881563	-0.48265058	0.15370509
6	-0.19017030	-0.89119598	1.03200188
6	-0.41486155	-1.95498794	1.95511160
6	2.10829614	-0.63140025	1.86389035
6	2.54134060	1.48636751	0.01285414
6	0.45914078	2.27554580	-1.75942105
6	-2.07509258	0.97252820	-1.66248102
6	-2.52296363	-1.13649965	0.20291436
6	1.88655018	-1.69164772	2.78945210
6	3.36807703	0.02880473	1.81865867
6	2.75925117	2.54061952	-0.91840956
6	3.58414115	1.08485116	0.89544980
6	-0.58932035	2.67802541	-2.63598164
6	1.71988805	2.93588049	-1.80019238
6	-1.69156161	-2.59077537	2.02169225
6	0.63076432	-2.35102604	2.83621365
6	-2.73474140	-2.19481099	1.13847506
6	-3.56900038	-0.71837090	-0.66989504
6	-3.34820498	0.34036466	-1.59100020
6	-1.85372094	2.03199711	-2.58429439
6	2.93228325	-2.09141544	3.67333897

6	4.41212010	-0.37386084	2.70225868
6	4.84774157	1.74376459	0.84852284
6	4.02353957	3.19904402	-0.96300040
6	-4.00752638	-2.83501813	1.19751398
6	-4.83757644	-1.36285041	-0.60326194
6	-4.39827395	0.75413951	-2.45953315
6	-2.90778249	2.44820654	-3.45130442
6	2.70969224	-3.14839204	4.59901367
6	4.19142810	-1.43217437	3.62637721
6	5.06380730	2.79933997	-0.07970836
6	-4.22220384	-3.88473953	2.13236865
6	-5.05199378	-2.41769993	0.32788381
6	-5.66475349	0.10922476	-2.39596802
6	-4.17510792	1.80711496	-3.38863808
6	-5.88375345	-0.94502454	-1.47089397
6	-1.91038834	-3.64304481	2.95218238
6	0.40519459	-3.40429789	3.77069042
6	-3.17834045	-4.28861266	3.00399082
6	-0.86088316	-4.04878334	3.82418177
6	3.76933175	-3.54740681	5.48604653
6	1.45053715	-3.80172192	4.64878237
6	-5.50651197	-4.53006116	2.18541974
6	-6.33149071	-3.06575607	0.38919562
6	-7.16184850	-1.59987175	-1.40258897
6	-7.35527014	-2.63288480	-0.48645574
6	-6.51901265	-4.11283388	1.32388802
6	-5.23335394	2.22358633	-4.26451911
6	-6.71924951	0.53227831	-3.27696967
6	-7.98712630	-0.14212577	-3.18574885
6	-6.48436659	1.56746937	-4.18077891
6	3.51048518	-4.61978701	6.41023505
6	-8.19751323	-1.15383537	-2.29619208

1	-8.79066697	0.17717573	-3.85556978
6	1.22020134	-4.86771326	5.58627340
6	-1.08345869	-5.11070160	4.76264553
6	-3.39140554	-5.35242175	3.94746286
6	-5.68932348	-5.59174279	3.13947784
6	4.23851020	4.25366270	-1.89232667
6	1.93657760	3.99594791	-2.72930861
6	-0.37157260	3.74173535	-3.56050962
6	-2.68476791	3.50518799	-4.37586197
6	-4.98433290	3.27505496	-5.17861795
6	-3.74953429	3.91655919	-5.25139975
6	-1.42110124	4.14870184	-4.43086518
6	0.89149408	4.39473019	-3.60704049
6	5.51630078	4.91310426	-1.93274350
6	3.19816213	4.65141454	-2.77213154
6	-4.68532970	-5.98221576	3.97491910
6	-0.02510019	-5.49228385	5.62162446
6	-2.35365510	-5.73573327	4.79507663
6	2.30073006	-5.24634091	6.45803698
1	-7.29098294	1.88440303	-4.84951105
1	-5.79004874	3.59230371	-5.84837577
6	4.99752460	-2.89179381	5.42510762
6	5.24375944	-1.83626395	4.51493441
6	5.67103172	0.28570130	2.65478929
6	5.88817247	1.34102016	1.73058310
6	6.33619606	3.46173048	-0.12632666
6	6.52475436	4.50827469	-1.06040552
6	7.35474411	3.04276724	0.76268518
6	7.16045132	2.00997097	1.67790129
6	6.72061838	-0.12552108	3.54829403
6	6.48757966	-1.16424962	4.44757118
6	7.98202314	0.56292573	3.47205345

6	8.19065185	1.57633695	2.58436687
6	5.69912762	5.97593463	-2.88559657
6	3.41078397	5.71877656	-3.71250343
6	1.11073641	5.46292083	-4.54029092
6	-1.19272676	5.21969896	-5.36358364
6	-3.48878380	4.98758504	-6.17632927
6	-2.27518716	5.60592164	-6.22964767
6	2.37596392	6.09657132	-4.56571645
6	0.05235063	5.84411892	-5.39906578
6	4.69981133	6.35837719	-3.73023711
1	-2.10171975	6.41808443	-6.94139965
1	0.22008527	6.65814536	-6.11162133
1	2.54300962	6.90991282	-5.27918579
1	4.86331212	7.16917212	-4.44607835
1	-4.29624478	5.29963590	-6.84500314
1	-4.84869625	-6.79301513	4.69068349
1	-2.52240428	-6.54672329	5.51067830
1	-0.19414757	-6.30390552	6.33648263
1	2.12871946	-6.05891877	7.16979875
1	8.78162116	0.25101486	4.15021017
1	7.29028291	-1.47350255	5.12466979
1	5.80033647	-3.20051683	6.10235800
1	4.31642304	-4.92585091	7.08346995
1	-6.66393861	-6.08653495	3.18039152
1	-7.49403870	-4.60845756	1.36878078
1	-8.33049718	-3.12801456	-0.44059659
1	-9.17052491	-1.65110983	-2.24754611
1	9.15897619	2.08361441	2.54501067
1	8.32548777	3.54753935	0.72653893
1	7.49544503	5.01315215	-1.09656875
1	6.67068034	6.47745259	-2.91856556
42	-0.53508935	-2.33862372	-1.17861991

6	-0.49808685	-4.24665749	-0.97968795
6	1.20011764	-2.47055422	-1.98570385
6	-1.26403752	-2.61463492	-2.93073364
8	-1.71443464	-2.76370204	-4.00073724
8	2.26067932	-2.53146928	-2.47680838
8	-0.48702579	-5.40814106	-0.83560152

IM(IIIa-b)-Mo

6	1.07714245	-0.27176606	0.97363546
6	1.28890570	0.79811689	0.05644708
6	0.24908238	1.19323941	-0.83426387
6	-1.01601440	0.53639273	-0.79901784
6	-1.23684642	-0.52917822	0.13779169
6	-0.18204703	-0.93907577	1.02161205
6	-0.41566501	-1.98344863	1.96122239
6	2.11194761	-0.66651751	1.86207923
6	2.54320909	1.45636250	0.01532315
6	0.45825219	2.25913181	-1.74864331
6	-2.07353372	0.94958870	-1.65871167
6	-2.51025147	-1.18687127	0.18811335
6	1.88593559	-1.71873479	2.79468191
6	3.37049535	-0.00323111	1.81929028
6	2.75916660	2.51762206	-0.90985795
6	3.58673956	1.05351536	0.89715834
6	-0.59310906	2.66702963	-2.61827430
6	1.71869801	2.91904180	-1.78741679
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IIId-Mo

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TS(IIId-e)-Mo

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1	2.03316949	6.66746473	-5.13716118
1	4.38623257	6.88533074	-4.39193866
1	-4.79718769	4.99307382	-6.66121630
1	-5.16589846	-7.13853203	4.82874784
1	-2.84606539	-6.86094114	5.65235357
1	-0.52556825	-6.58315206	6.48393059
1	1.78869430	-6.30694647	7.32044467
1	8.38717821	0.02564264	4.25021433
1	6.90904158	-1.69631389	5.24413395
1	5.43507428	-3.42492475	6.23643323
1	3.96620057	-5.15328093	7.23026278
1	-6.98696528	-6.45867709	3.31117248
1	-7.83259965	-4.99913455	1.49692081
1	-8.68561732	-3.53589781	-0.31489050
1	-9.54429478	-2.07286094	-2.11950190
1	8.75716609	1.83323616	2.61189063
1	7.93541523	3.23541245	0.74590069

1	7.13435928	4.63619365	-1.14219595
1	6.24775857	6.14608668	-2.95085542
42	5.81738943	2.79590332	-3.22768642
8	5.37940485	1.42289072	-4.55832971
8	7.29459336	1.70647857	-2.67068391
8	7.02186001	3.53608397	-4.50629098
8	7.76132783	4.00455555	-5.28578420
8	8.20288792	1.06801451	-2.30538905
8	5.11316568	0.60032776	-5.34016874

Ille-Mo

6	0.73518372	-0.58742580	1.16156102
6	0.95587832	0.46458799	0.22776612
6	-0.08831567	0.86696453	-0.64951383
6	-1.35432485	0.21773826	-0.59395161
6	-1.57337736	-0.83658000	0.33611972
6	-0.52861583	-1.23917185	1.21389026
6	-0.74851955	-2.29095962	2.14496295
6	1.77614355	-0.98567837	2.04348276
6	2.21962589	1.11597001	0.17559323
6	0.13033458	1.92102743	-1.57968653
6	-2.40082529	0.62379621	-1.46574640
6	-2.83692360	-1.48622048	0.39036664
6	1.55480037	-2.03750604	2.97624692
6	3.03891015	-0.32936406	1.99534711
6	2.44089057	2.16484994	-0.76002701
6	3.26015700	0.71905241	1.06385389
6	-0.92131389	2.33023096	-2.44908192
6	1.39667017	2.56723017	-1.63730896
6	-2.01315914	-2.94281653	2.19666798
6	0.29496739	-2.69027044	3.02573461
6	-3.05533332	-2.54124591	1.32107787

6	-3.88294770	-1.08045268	-0.48435103
6	-3.66578770	-0.02593514	-1.40981649
6	-2.18371475	1.68298910	-2.39233805
6	2.59930519	-2.43528884	3.86308951
6	4.08060948	-0.72541555	2.88551146
6	4.52364928	1.37869457	1.02164021
6	3.71248089	2.81382926	-0.80599373
6	-4.32297059	-3.19351620	1.37416905
6	-5.15100693	-1.73278663	-0.42945440
6	-4.71676988	0.38367048	-2.28352791
6	-3.23674725	2.09410459	-3.26210815
6	2.37647340	-3.48789860	4.79330419
6	3.85858084	-1.77780660	3.81591948
6	4.74412614	2.42906696	0.08794108
6	-4.53868462	-4.24750265	2.30458533
6	-5.36693753	-2.78792452	0.49847980
6	-5.97960660	-0.26827478	-2.22715499
6	-4.49973393	1.44275166	-3.20630987
6	-6.19573078	-1.32417164	-1.30329919
6	-2.23272079	-3.99889577	3.13032437
6	0.07375642	-3.74589767	3.96018000
6	-3.49688044	-4.64891078	3.17988146
6	-1.18863739	-4.39781658	4.00894018
6	3.43360891	-3.88357429	5.68401658
6	1.11747381	-4.14194458	4.84099732
6	-5.81950048	-4.90138537	2.35184021
6	-6.64266522	-3.44453749	0.55242342
6	-7.47088828	-1.98640151	-1.24338269
6	-7.66440528	-3.02012764	-0.32857338
6	-6.83069179	-4.49170732	1.48608170
6	-5.55838076	1.85582825	-4.08326503
6	-7.03419734	0.14967094	-3.11067992

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6	-8.50537452	-1.54712570	-2.14146146
1	-9.10024187	-0.21556895	-3.70084048
6	0.88812160	-5.20707194	5.77964448
6	-1.41018028	-5.46057090	4.94862421
6	-3.71081799	-5.71384228	4.12351129
6	-6.00261553	-5.96399286	3.30502009
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6	-3.02036856	3.15625907	-4.18295920
6	-5.31632478	2.91540876	-4.99076182
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6	-1.76101696	3.80531282	-4.23717254
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6	5.21829528	4.53632698	-1.77336232
6	2.87909622	4.27416282	-2.63178795
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6	-2.67662259	-6.09223058	4.97623733
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6	4.66202300	-3.22726865	5.62414905
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6	3.08215375	5.35953979	-3.56780213
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1	-2.45622863	6.08618263	-6.73609710
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1	2.19296717	6.55708048	-5.12208428
1	4.57722926	6.74877227	-4.36993545
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42	4.89329452	3.68629858	-4.13456464
8	4.48995349	1.78748680	-4.52810513
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8	4.83944636	4.02846584	-6.04109618
8	4.80479185	4.26236484	-7.18458443
8	7.90328664	3.06543042	-4.57838185
8	4.24860530	0.67306454	-4.75395663

IIIa-W

6	1.03010600	-0.35871870	0.93701762
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6	-1.07466354	0.46150315	-0.83601455
6	-1.29938046	-0.60766404	0.10171401
6	-0.24905450	-1.01786345	0.98421644
6	-0.48152827	-2.05962506	1.93571276
6	2.06834967	-0.74713973	1.83963882
6	2.51369847	1.37891162	-0.02227786
6	0.40990241	2.19981214	-1.79255779
6	-2.13246027	0.89120469	-1.69686750
6	-2.57901533	-1.24118816	0.17054856
6	1.82677511	-1.78680587	2.77611036
6	3.31512858	-0.07712760	1.80084098
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6	1.66800839	2.85783430	-1.81297755
6	-1.75100033	-2.68405277	1.99218791
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6 4.35085551 -0.46538201 2.70126377
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6 5.00835683 2.71827530 -0.07413895
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6 -3.25468778 -4.35706790 2.99875046
6 -0.94070055 -4.12043479 3.82312271
6 3.68102464 -3.60741830 5.51423060
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6 -6.40117227 -3.13014063 0.37493138
6 -7.22416783 -1.66330846 -1.41965022
6 -7.42336041 -2.69308957 -0.50174440
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6 3.41267698 -4.66789084 6.44912705
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6 3.13991036 4.59793033 -2.74892978
6 -4.77532893 -6.02755809 3.98495708
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6 5.60634471 0.20257659 2.66395049
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6	7.09360655	1.93784951	1.70143019
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6	6.40759973	-1.23322793	4.47601214
6	7.90411658	0.49704510	3.50593472
6	8.11629208	1.51083325	2.61854201
6	5.63255712	5.93827474	-2.83491409
6	3.34719520	5.68229584	-3.67114292
6	1.04680104	5.43326609	-4.50515242
6	-1.25807918	5.19585163	-5.32826299
6	-3.55555903	4.96745332	-6.13977085
6	-2.34349431	5.59119539	-6.18553256
6	2.31103388	6.07042060	-4.51872911
6	-0.01318938	5.82527703	-5.35527265
6	4.63305057	6.32820118	-3.67622924
1	-2.17797730	6.41498595	-6.88586847
1	0.15053921	6.65150028	-6.05451999
1	2.47610710	6.89652887	-5.21785063
1	4.79411439	7.15082487	-4.37898727
1	-4.36281486	5.29061604	-6.80339717
1	-4.95007968	-6.82973132	4.70778224
1	-2.62071996	-6.58888633	5.53547034
1	-0.29475473	-6.34312969	6.37166983
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1	7.20431397	-1.53321319	5.16423742
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6	1.92738774	-0.97545096	-2.70410376
6	-0.47676145	-2.18321200	-2.64418299

8	-1.15474808	-2.71274189	-3.43380649
8	2.72492064	-0.76345531	-3.53028494
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1	-6.75242654	-6.12671599	3.19060459
1	-7.57468871	-4.65654094	1.36533647
1	-8.40223287	-3.18083136	-0.45282489
1	-9.23495598	-1.70368846	-2.26007126
1	9.08297228	2.02205308	2.59247508
1	8.25556925	3.48967353	0.76750831
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1	6.60126716	6.44581427	-2.85785612

IIIb-W

6	1.111662580	-0.249532050	0.891853540
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6	-0.992229700	0.594281250	-0.869357410
6	-1.205336400	-0.502010040	0.025561180
6	-0.149706430	-0.924670780	0.909988580
6	-0.372191360	-2.000944120	1.826277810
6	2.134365180	-0.655400560	1.780961270
6	2.563652190	1.503466150	-0.021183850
6	0.476085330	2.340971020	-1.768178760
6	-2.043024040	1.020318830	-1.715132240
6	-2.477471970	-1.155781260	0.065219160
6	1.911288390	-1.730978830	2.696367290
6	3.388369610	0.016411600	1.762646950
6	2.775736000	2.589620840	-0.918651520
6	3.603159500	1.090782790	0.860646140
6	-0.572310270	2.765957650	-2.633479910
6	1.735500340	3.006973380	-1.789102390
6	-1.651824230	-2.662308020	1.863315060

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6	-3.534643930	-0.714849150	-0.792649870
6	-3.313377370	0.365106140	-1.676047670
6	-1.830528240	2.110218490	-2.604742210
6	2.948248200	-2.130313210	3.590603250
6	4.426062380	-0.390832230	2.653573250
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6	-3.983850640	-2.879365010	1.044176590
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6	4.203515290	-1.461955810	3.563732560
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6	-5.630890370	0.155720860	-2.483054070
6	-4.148229690	1.888781090	-3.425333160
6	-5.849247750	-0.921044350	-1.581802360
6	-1.883668980	-3.721542720	2.802767160
6	0.427088080	-3.457408860	3.647661120
6	-3.152979380	-4.346736200	2.847275850
6	-0.842953280	-4.111876820	3.684104370
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6	1.460968980	-3.853563170	4.536536800
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6	-7.328813010	-2.620925020	-0.626954840
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6	-7.956341170	-0.075631210	-3.273873720
6	-6.456443700	1.661505640	-4.224383720
6	3.503984000	-4.672970000	6.317571500
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6	1.222361030	-4.925127150	5.468403950
6	-1.073646660	-5.172981910	4.620952500
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6	4.245766070	4.342021350	-1.835116220
6	1.947488100	4.096391840	-2.684593240
6	-0.358358160	3.857978130	-3.526888110
6	-2.667651940	3.628083260	-4.354885570
6	-4.963913590	3.406902640	-5.169592740
6	-3.733012910	4.058439400	-5.220352950
6	-1.407445430	4.283277270	-4.387087630
6	0.901089130	4.517684470	-3.551858110
6	5.519413420	5.011299060	-1.851538130
6	3.205458340	4.759447580	-2.705562050
6	-4.676233920	-6.030140350	3.807982050
6	-0.020411630	-5.552445960	5.490494710
6	-2.344191950	-5.797454940	4.641550860
6	2.296021910	-5.303393440	6.349813280
1	-7.264476580	1.995689610	-4.883053080
1	-5.770891890	3.739836110	-5.830199910
6	4.996016650	-2.933166640	5.359630000
6	5.247338330	-1.868125390	4.460231720
6	5.679063700	0.279134560	2.629470520
6	5.896578460	1.352636370	1.724622040
6	6.341059430	3.517610150	-0.080724770

6	6.526426960	4.590135640	-0.986351280
6	7.356379250	3.086707450	0.805722590
6	7.163044330	2.033204400	1.697431350
6	6.722328420	-0.136626050	3.528354560
6	6.487460860	-1.187692690	4.412842250
6	7.979422720	0.562109330	3.474571480
6	8.188497340	1.591333230	2.605610980
6	5.698484400	6.102462010	-2.772956200
6	3.413754110	5.856222890	-3.613356360
6	1.116121490	5.614151860	-4.452526710
6	-1.184132270	5.382544180	-5.286878120
6	-3.477285490	5.159154620	-6.111662990
6	-2.267811670	5.787057090	-6.143379750
6	2.379047080	6.254311240	-4.456509850
6	0.057473860	6.015447850	-5.301373630
6	4.699415050	6.503339920	-3.608909970
1	-2.098293800	6.621714710	-6.829796070
1	0.221834470	6.851365680	-5.988922220
1	2.543366240	7.089676860	-5.144755730
1	4.859860280	7.335848290	-4.300091840
1	-4.285439540	5.486195480	-6.772304090
1	-4.848427040	-6.842172150	4.520283510
1	-2.519519640	-6.609057450	5.354758600
1	-0.194345830	-6.365099660	6.202974200
1	2.119560310	-6.119741050	7.056128280
1	8.774813800	0.245687750	4.155559940
1	7.285211030	-1.498675830	5.095009050
1	5.792645270	-3.242836190	6.043689430
1	4.303348670	-4.980269570	6.998117350
1	-6.653051710	-6.118495690	3.009435430
1	-7.476157510	-4.621125130	1.205066130
1	-8.306815770	-3.111062690	-0.587398030

1	-9.140692850	-1.603074640	-2.368609250
1	9.153038600	2.106851810	2.584176140
1	8.322813710	3.600733940	0.789193530
1	7.493221440	5.103500740	-1.003170820
1	6.666942820	6.610800270	-2.787974690
74	-0.806295840	-2.874237620	-0.413966420
6	0.093761340	-4.579901480	-0.096218890
6	0.488388880	-2.566505160	-1.848105660
6	-1.899900180	-3.815172010	-1.732868850
8	-2.586452480	-4.359765250	-2.503956340
8	1.264514940	-2.344825350	-2.690941820
8	0.626964200	-5.592291030	0.134631120

TS(III)-W

6	1.05392509	-0.27695144	0.98354528
6	1.26464345	0.79800678	0.06718292
6	0.22427440	1.19041765	-0.82908933
6	-1.05117519	0.54812991	-0.77871912
6	-1.26976563	-0.51061203	0.16785839
6	-0.21487358	-0.93097330	1.04830519
6	-0.44379234	-1.98119186	1.98317054
6	2.09069919	-0.67463957	1.87073982
6	2.51936823	1.44925446	0.02010143
6	0.43448397	2.25468191	-1.74746086
6	-2.10504999	0.95706792	-1.64562355
6	-2.52307618	-1.20426672	0.17992858
6	1.86144611	-1.71980727	2.80778441
6	3.34989014	-0.01332433	1.82294728
6	2.73678845	2.50745260	-0.91039689
6	3.56525515	1.04216596	0.89946048
6	-0.61869099	2.66679474	-2.61000412
6	1.69700368	2.91011258	-1.78789372

6	-1.71296516	-2.62563571	2.03326386
6	0.59864687	-2.37121858	2.86399449
6	-2.74169080	-2.24648036	1.13110295
6	-3.57371960	-0.77484159	-0.68637263
6	-3.36976624	0.30478092	-1.58570011
6	-1.88424421	2.02026611	-2.55962417
6	2.90495050	-2.11576087	3.69600609
6	4.39219721	-0.41231960	2.71046138
6	4.82837502	1.70026124	0.85125942
6	4.00127792	3.16312798	-0.95556446
6	-4.00921836	-2.89441961	1.17960045
6	-4.83776349	-1.42895489	-0.63021662
6	-4.41822810	0.71902054	-2.45450048
6	-2.93846006	2.43601710	-3.42612267
6	2.67719618	-3.16202436	4.63220664
6	4.16743612	-1.46264589	3.64234449
6	5.04356622	2.75813316	-0.07566811
6	-4.23058762	-3.93782745	2.12148142
6	-5.04908695	-2.48951097	0.29564102
6	-5.67706489	0.05873989	-2.40618026
6	-4.20123873	1.78516559	-3.37109636
6	-5.88648741	-1.00901150	-1.49547860
6	-1.93466069	-3.67370269	2.97033817
6	0.37195666	-3.41913361	3.80498287
6	-3.19675951	-4.32820829	3.01150014
6	-0.89273133	-4.06663121	3.85571521
6	3.73474628	-3.55712750	5.52262840
6	1.41516965	-3.81141771	4.68672091
6	-5.51053778	-4.59250583	2.16307746
6	-6.32442737	-3.14409285	0.34946754
6	-7.15944594	-1.67606065	-1.43857859
6	-7.34732527	-2.71660653	-0.53140112

6 -6.51511736 -4.18853732 1.28635699
6 -5.25937019 2.20108333 -4.24673240
6 -6.73259042 0.48240144 -3.28653032
6 -7.99354472 -0.20705788 -3.20885941
6 -6.50509698 1.53128924 -4.17540973
6 3.47154594 -4.61975616 6.45671642
6 -8.19630406 -1.23089229 -2.33186419
1 -8.79762925 0.11178287 -3.87838946
6 1.18185280 -4.87008627 5.63145965
6 -1.11790291 -5.12397881 4.79947249
6 -3.41452014 -5.38631523 3.96104134
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6 4.21549298 4.22272312 -1.88061309
6 1.91082258 3.97646165 -2.71010440
6 -0.40308159 3.73514043 -3.53018897
6 -2.71842081 3.49969137 -4.34254171
6 -5.01564788 3.26303770 -5.14969382
6 -3.78387686 3.91285082 -5.21538324
6 -1.45510010 4.14678275 -4.39437096
6 0.86165441 4.38428392 -3.57903222
6 5.49443869 4.87975309 -1.92159068
6 3.17335075 4.62905773 -2.75388236
6 -4.70426841 -6.02484901 3.97578270
6 -0.06360926 -5.49569020 5.66711066
6 -2.38490272 -5.75615375 4.82425142
6 2.26003691 -5.24286315 6.50852475
1 -7.31204837 1.84829089 -4.84368700
1 -5.82176914 3.58081530 -5.81870028
6 4.96655441 -2.90779132 5.45520900
6 5.21788305 -1.86260688 4.53529798
6 5.65188984 0.24529127 2.66046664
6 5.86968047 1.29699280 1.73296427

6	6.31587965	3.41890440	-0.12309558
6	6.50418367	4.46874817	-1.05411726
6	7.33614960	2.99726621	0.76330294
6	7.14248655	1.96487536	1.67855452
6	6.70046899	-0.16342291	3.55668363
6	6.46445488	-1.19529476	4.46253518
6	7.96341524	0.52196450	3.47642560
6	8.17310799	1.53168424	2.58497088
6	5.67635067	5.94768083	-2.86914761
6	3.38391285	5.70255508	-3.68824650
6	1.07873293	5.45830934	-4.50645906
6	-1.22933505	5.22286627	-5.32088833
6	-3.52668696	4.99216601	-6.13168955
6	-2.31430513	5.61371877	-6.18172661
6	2.34613756	6.08877216	-4.53375596
6	0.01687024	5.84673391	-5.35697673
6	4.67486421	6.33840978	-3.70732943
1	-2.14315727	6.43133307	-6.88792345
1	0.18229907	6.66505344	-6.06514263
1	2.51198509	6.90629030	-5.24266536
1	4.83800529	7.15320039	-4.41867773
1	-4.33523587	5.30730639	-6.79757165
1	-4.87224929	-6.83109908	4.69566060
1	-2.55645136	-6.56300178	5.54384938
1	-0.23385439	-6.30261438	6.38702259
1	2.08534256	-6.04882573	7.22711366
1	8.76292797	0.21119917	4.15518891
1	7.26595822	-1.50207461	5.14214722
1	5.76769271	-3.21385304	6.13566270
1	4.27586869	-4.92203512	7.13361465
1	-6.67063259	-6.14925532	3.15421363
1	-7.48765075	-4.68977049	1.32340894

1	-8.31872321	-3.21984674	-0.49185863
1	-9.16416564	-1.73890498	-2.29227269
1	9.14222249	2.03721508	2.54306055
1	8.30717960	3.50139104	0.72577953
1	7.47579122	4.97185255	-1.09036955
1	6.64918684	6.44662989	-2.90291236
74	-0.17357118	-1.82951287	-1.40225382
6	-0.04741234	-3.73710302	-1.17891407
6	1.57224148	-1.85708221	-2.21916642
6	-0.93930556	-2.14951490	-3.13896462
8	-1.44102659	-2.32625842	-4.18373538
8	2.64538953	-1.83516293	-2.68988321
8	0.00271723	-4.89629327	-1.01071159

TS'(III)-W

6	1.07865053	-0.23407353	0.97253545
6	1.28722773	0.83039232	0.05159239
6	0.25053039	1.21083433	-0.84829862
6	-1.01163613	0.54589888	-0.82087735
6	-1.24745580	-0.48867914	0.14461542
6	-0.18186346	-0.90224345	1.01626216
6	-0.40649307	-1.97264218	1.93461224
6	2.11349853	-0.63716407	1.85256784
6	2.54208548	1.48821546	0.00969416
6	0.46214591	2.26967231	-1.76930821
6	-2.07144554	0.96263098	-1.67727155
6	-2.52207777	-1.14662163	0.19057532
6	1.89344290	-1.70330697	2.77330233
6	3.37130856	0.02739577	1.81163166
6	2.75922841	2.54321389	-0.92108642
6	3.58509328	1.08725784	0.89268924
6	-0.58628614	2.67065722	-2.64709909

6 1.72085505 2.93490363 -1.80553481
6 -1.68893342 -2.59859574 2.01281714
6 0.64016609 -2.36703872 2.81643005
6 -2.73361802 -2.20256153 1.13044303
6 -3.56731374 -0.72601647 -0.68195713
6 -3.34584735 0.33305765 -1.60269828
6 -1.85057469 2.02348970 -2.59702217
6 2.93878039 -2.10150658 3.65805720
6 4.41527712 -0.37583127 2.69470708
6 4.84701940 1.74922747 0.84841857
6 4.02180218 3.20486994 -0.96251747
6 -4.00775584 -2.83799138 1.19350662
6 -4.83705286 -1.36705608 -0.61044439
6 -4.39685656 0.74870723 -2.46872677
6 -2.90579171 2.44140915 -3.46212564
6 2.71732462 -3.16047631 4.58195459
6 4.19617692 -1.43817349 3.61484516
6 5.06163694 2.80699425 -0.07764228
6 -4.22301508 -3.88491369 2.13156875
6 -5.05220030 -2.41916950 0.32436322
6 -5.66444491 0.10602902 -2.40242124
6 -4.17366381 1.80151028 -3.39808241
6 -5.88402427 -0.94719493 -1.47608273
6 -1.90778936 -3.64795163 2.94439573
6 0.41284618 -3.41752760 3.75359570
6 -3.17819081 -4.28967327 3.00109326
6 -0.85539487 -4.05748726 3.81213245
6 3.77697703 -3.55867497 5.46949188
6 1.45848578 -3.81437540 4.63171178
6 -5.50907091 -4.52624139 2.18844960
6 -6.33340901 -3.06335062 0.38991995
6 -7.16346755 -1.59857631 -1.40374206

6 -7.35743109 -2.62943411 -0.48491728
6 -6.52193622 -4.10789768 1.32786738
6 -5.23283049 2.21952330 -4.27214043
6 -6.71971526 0.53072745 -3.28141663
6 -7.98876901 -0.14105633 -3.18712894
6 -6.48463963 1.56530295 -4.18619779
6 3.51879693 -4.63210251 6.39272432
6 -8.19979395 -1.15131592 -2.29592324
1 -8.79268635 0.17959102 -3.85597637
6 1.22777224 -4.87917880 5.57041167
6 -1.07864655 -5.11717479 4.75243454
6 -3.39101944 -5.35168532 3.94622056
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6 4.23577109 4.26047257 -1.89080961
6 1.93639570 3.99623428 -2.73334171
6 -0.36985085 3.73649829 -3.56922728
6 -2.68324321 3.49943743 -4.38549783
6 -4.98377243 3.27103120 -5.18635286
6 -3.74871617 3.91188363 -5.26004240
6 -1.41966138 4.14333315 -4.43950427
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6 5.51186073 4.92348744 -1.92807946
6 3.19613889 4.65562081 -2.77270971
6 -4.68695484 -5.97737738 3.97846747
6 -0.01868774 -5.50117933 5.60860552
6 -2.35130355 -5.73763541 4.79034419
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1 -7.29193153 1.88344285 -4.85350566
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6 5.24838394 -1.84180815 4.50348146
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6	5.88749437	1.34659466	1.73033739
6	6.33237340	3.47246712	-0.12143809
6	6.51969231	4.52064537	-1.05410864
6	7.35083212	3.05447353	0.76826914
6	7.15807093	2.01896033	1.68083760
6	6.72187278	-0.12366850	3.54431108
6	6.49047734	-1.16606709	4.43981343
6	7.98141144	0.56864034	3.47171098
6	8.18830749	1.58536601	2.58736358
6	5.69362989	5.98747376	-2.87988263
6	3.40779671	5.72418946	-3.71189829
6	1.11012916	5.46240126	-4.54439492
6	-1.19192718	5.21585222	-5.37053017
6	-3.48786424	4.98359339	-6.18413125
6	-2.27424429	5.60208332	-6.23650480
6	2.37368001	6.09956831	-4.56694335
6	0.05212156	5.84226191	-5.40420122
6	4.69502833	6.36754620	-3.72642032
1	-2.10046951	6.41508595	-6.94734359
1	0.21909937	6.65746471	-6.11558136
1	2.53972338	6.91397627	-5.27942140
1	4.85771534	7.17924252	-4.44141870
1	-4.29314092	5.29864955	-6.85398802
1	-4.85065713	-6.78663617	4.69589881
1	-2.52009580	-6.54724843	5.50746732
1	-0.18796721	-6.31181633	6.32450221
1	2.13733080	-6.07114175	7.15275401
1	8.78113938	0.25686717	4.14977588
1	7.29315114	-1.47532591	5.11694596
1	5.80657649	-3.20861489	6.08831229
1	4.32462735	-4.93875492	7.06569169
1	-6.66814486	-6.07753008	3.18988746

1	-7.49826531	-4.60065441	1.37562066
1	-8.33387335	-3.12191847	-0.43623681
1	-9.17388952	-1.64621945	-2.24482690
1	9.15534598	2.09528957	2.55069965
1	8.32034764	3.56173510	0.73436475
1	7.48910849	5.02811537	-1.08812123
1	6.66379611	6.49180975	-2.91052586
74	-0.53653845	-2.31246665	-1.11514880
6	-0.61216751	-4.22357517	-0.89399911
6	1.23217008	-2.51747576	-1.84895379
6	-1.22429816	-2.53625748	-2.89851276
8	-1.65915828	-2.63391805	-3.98304672
8	2.31749776	-2.60564555	-2.28311488
8	-0.68088048	-5.38045683	-0.71672594

IM(IIIa-b)-W

6	1.08560834	-0.28517731	0.95949130
6	1.29550311	0.78832871	0.04529825
6	0.25722670	1.18029590	-0.84946879
6	-1.00757783	0.52167610	-0.81862261
6	-1.23021294	-0.54271510	0.12357759
6	-0.17193268	-0.95665273	1.00616091
6	-0.40921796	-1.99791824	1.94898371
6	2.11821270	-0.67713100	1.85114674
6	2.54730198	1.44937565	0.00759259
6	0.46423774	2.24896319	-1.76055580
6	-2.06828631	0.93718656	-1.67403940
6	-2.50450512	-1.20592958	0.16987868
6	1.89085819	-1.72834653	2.78493273
6	3.37510347	-0.01027052	1.81154755
6	2.76278799	2.51219140	-0.91647173
6	3.59053035	1.04780879	0.89095292

6	-0.58834860	2.65771028	-2.62869983
6	1.72320044	2.91216445	-1.79551541
6	-1.68572466	-2.62939925	2.01761663
6	0.63085299	-2.38326090	2.83779224
6	-2.72241661	-2.24359519	1.12487011
6	-3.55470460	-0.77112649	-0.69282380
6	-3.34264366	0.30184639	-1.60076390
6	-1.85147856	2.00833879	-2.58278796
6	2.93226664	-2.11949524	3.67777532
6	4.41578415	-0.40693126	2.70185544
6	4.85097529	1.71247061	0.85014141
6	4.02424225	3.17506885	-0.95503339
6	-3.99817369	-2.87409039	1.19090086
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IIId-W

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TS(IIId-e)-W

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1	-7.87659491	-4.96486138	1.53254926
1	-8.72542500	-3.50284609	-0.28207417
1	-9.57810708	-2.04412158	-2.09307660
1	8.77278659	1.73888920	2.55002344
1	7.93366265	3.18294540	0.72661490
1	7.05518529	4.77008634	-0.96645275
1	6.20603362	6.19314949	-2.88484028
74	6.15976863	3.08438964	-3.19818774
6	5.88794431	1.27686437	-3.86702900
6	7.97964695	2.58099904	-2.84739921
6	6.77610090	3.61976989	-4.94149180
8	7.16188759	4.01258268	-5.97653232
8	9.08776568	2.29298779	-2.60089186
8	5.68634845	0.17656137	-4.20772335

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6	0.73959363	-0.58499709	1.15723367
6	0.96048181	0.46712918	0.22335441
6	-0.08362354	0.86940433	-0.65376333
6	-1.34976113	0.22005168	-0.59811854
6	-1.56857959	-0.83483582	0.33129674
6	-0.52382176	-1.23736608	1.20905822
6	-0.74366885	-2.28977446	2.13970293
6	1.78009828	-0.98285505	2.04000962
6	2.22452870	1.11869445	0.17133242
6	0.13499073	1.92385475	-1.58406620
6	-2.39675028	0.62653628	-1.46920863
6	-2.83198802	-1.48518357	0.38513073
6	1.55871621	-2.03478924	2.97253760

6	3.04258401	-0.32570328	1.99296752
6	2.44660122	2.16650321	-0.76511501
6	3.26434263	0.72238674	1.06097048
6	-0.91754869	2.33383277	-2.45229892
6	1.40158435	2.56920292	-1.64299247
6	-2.00797837	-2.94263735	2.19057059
6	0.29931248	-2.68868825	3.02091044
6	-3.05005775	-2.54112660	1.31498011
6	-3.87815494	-1.07913603	-0.48900758
6	-3.66150851	-0.02342757	-1.41341386
6	-2.18022810	1.68674471	-2.39491679
6	2.60259139	-2.43177744	3.86045216
6	4.08324707	-0.72047746	2.88453533
6	4.52735185	1.38246241	1.02011008
6	3.71922551	2.81344249	-0.81064610
6	-4.31728205	-3.19420895	1.36725669
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6	-3.23388548	2.09896297	-3.26299779
6	2.37999186	-3.48490324	4.79031569
6	3.86109086	-1.77301246	3.81488714
6	4.74862725	2.43175841	0.08489065
6	-4.53254858	-4.24928032	2.29665725
6	-5.36139235	-2.78838601	0.49192622
6	-5.97575611	-0.26553310	-2.23025589
6	-4.49685119	1.44736742	-3.20727329
6	-6.19112175	-1.32292982	-1.30780784
6	-2.22719765	-3.99945797	3.12339651
6	0.07834479	-3.74492577	3.95486890
6	-3.49093042	-4.65058678	3.17187438
6	-1.18338341	-4.39803903	4.00239941
6	3.43630272	-3.87962942	5.68202640

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6	-5.55620895	1.86156554	-4.08272571
6	-7.03075177	0.15319081	-3.11252648
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6	-6.80098147	1.19593001	-4.00917681
6	3.17766288	-4.94946160	6.60812008
6	-8.50072603	-1.54585817	-2.14570906
1	-9.09664576	-0.21203668	-3.70285922
6	0.89257439	-5.20607621	5.77437989
6	-1.40462305	-5.46161874	4.94131054
6	-3.70445298	-5.71655611	4.11459839
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6	1.61169342	3.62561801	-2.58107361
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6	-3.01843545	3.16280018	-4.18235764
6	-5.31505437	2.92322599	-4.98854536
6	-4.08675105	3.57377503	-5.05493148
6	-1.75942734	3.81145762	-4.23696545
6	0.56067022	4.04566995	-3.43326082
6	5.22760072	4.53770834	-1.77899724
6	2.88507492	4.27491910	-2.64090796
6	-4.99484263	-6.35356336	4.13582563
6	-0.35028881	-5.83674948	5.80567238
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6	5.34157182	-0.05855074	2.84122554
6	5.56180027	0.99027525	1.91370074
6	6.02330549	3.10066845	0.04943835
6	6.23009258	4.13048931	-0.88380054
6	7.03525427	2.69005267	0.95345882
6	6.83465432	1.66392707	1.86885545
6	6.38694425	-0.46197825	3.74456308
6	6.15282699	-1.49548407	4.64645120
6	7.64759814	0.22940431	3.67503846
6	7.86009095	1.23867594	2.78527604
6	5.44459635	5.54416709	-2.79826207
6	3.08718121	5.36269604	-3.57681539
6	0.77057187	5.12497333	-4.36306767
6	-1.53887794	4.89067714	-5.16574000
6	-3.83549731	4.65419052	-5.97235319
6	-2.62655258	5.27962618	-6.02472534
6	2.02794915	5.75002506	-4.41357700
6	-0.29875327	5.51635317	-5.20760194
6	4.41212540	5.94204344	-3.66553695
1	-2.45805797	6.09775071	-6.73081901
1	-0.13499889	6.33399689	-5.91647821
1	2.19251667	6.56296977	-5.12730360
1	4.59089183	6.73218916	-4.39827229
1	-4.64707217	4.96597712	-6.63616190
1	-5.15763292	-7.16471707	4.85140919
1	-2.83865709	-6.90600247	5.68303635
1	-0.51881719	-6.64770986	6.52152089
1	1.79625548	-6.39097862	7.36478414
1	8.44241566	-0.07775679	4.36091309

1	6.95245906	-1.79899778	5.32978223
1	5.46498933	-3.52537385	6.30554751
1	3.98162061	-5.25080772	7.28586320
1	-6.96835280	-6.46711828	3.32993498
1	-7.79648189	-4.99597347	1.51719488
1	-8.63109480	-3.52235354	-0.29483576
1	-9.47031727	-2.05032112	-2.10189261
1	8.82673603	1.74917886	2.74962534
1	8.00461197	3.19717134	0.92122879
1	7.20184602	4.63226360	-0.91961202
1	6.42290288	6.02620189	-2.85938970
74	4.86066753	3.68270483	-4.09740310
6	4.39403354	1.78367900	-4.41659939
6	6.72795985	3.22074023	-4.38452774
6	4.78309974	3.97285923	-6.01889714
8	4.72205178	4.18457754	-7.16719549
8	7.86083500	2.97060081	-4.52992725
8	4.10333270	0.66903169	-4.58440424