

Supporting Information for CP-ART-03-2014-001056

Cartesian coordinates of reaction intermediates, transition states, and products (in Å).

C₇H₇, p-tolyl

6	0	-0.004839	0.842257	0.000000
6	0	-0.007297	0.129292	1.204618
6	0	-0.007297	0.129292	-1.204618
6	0	-0.007297	-1.271651	1.219533
6	0	-0.007297	-1.271651	-1.219533
6	0	-0.006003	-1.904417	0.000000
6	0	0.027506	2.352855	0.000000
1	0	1.056779	2.728012	0.000000
1	0	-0.467084	2.765801	-0.882388
1	0	-0.467084	2.765801	0.882388
1	0	-0.012380	-1.817084	2.157994
1	0	-0.012380	-1.817084	-2.157994
1	0	-0.011347	0.669345	2.148265
1	0	-0.011347	0.669345	-2.148265

C₅H₈, isoprene

6	0	-1.583159	-0.912342	0.000003
6	0	-0.515323	-0.101212	-0.000008
6	0	-0.664444	1.399450	0.000000
6	0	0.834876	-0.675677	-0.000005
6	0	1.983193	0.008670	0.000002
1	0	-1.472073	-1.991394	0.000025
1	0	-2.595167	-0.523796	-0.000013
1	0	-0.187481	1.842680	-0.880078
1	0	-0.187868	1.842623	0.880320
1	0	-1.716157	1.689078	-0.000221
1	0	0.875392	-1.762702	-0.000004
1	0	2.938783	-0.502096	0.000007
1	0	2.013715	1.092277	0.000005

i0

6	0	3.549853	0.883812	0.397207
6	0	3.565226	-0.460088	0.006035
6	0	2.388795	-1.031208	-0.493514
6	0	1.207858	-0.285126	-0.601714
6	0	1.267572	1.025458	-0.194202
6	0	2.383572	1.654541	0.301179
6	0	4.822435	-1.287351	0.145092
1	0	4.457348	1.341300	0.780233
1	0	2.388565	-2.071156	-0.806718
1	0	0.299239	-0.730460	-0.991208
1	0	2.379676	2.696062	0.602905

1	0	4.875354	-2.063832	-0.621443
1	0	4.860012	-1.786329	1.119570
1	0	5.718329	-0.668243	0.060259
6	0	-2.642276	0.973919	-1.081019
6	0	-3.289808	0.294978	-0.121867
6	0	-4.569510	-0.354567	-0.427905
6	0	-5.321901	-1.056223	0.425761
6	0	-2.735048	0.184333	1.276254
1	0	-3.046694	1.054105	-2.084634
1	0	-1.696163	1.468052	-0.890735
1	0	-4.915109	-0.237080	-1.452715
1	0	-6.258008	-1.501880	0.110785
1	0	-5.036014	-1.210245	1.460005
1	0	-3.423068	0.621251	2.007371
1	0	-1.775695	0.696353	1.358313
1	0	-2.588387	-0.862766	1.560166

il

6	0	-2.713152	1.013290	-0.328955
6	0	-3.068124	-0.295806	0.001305
6	0	-2.048160	-1.164268	0.408112
6	0	-0.726153	-0.739979	0.476711
6	0	-0.372240	0.573404	0.146477
6	0	-1.387785	1.440121	-0.258884
6	0	1.073000	1.035170	0.241514
6	0	2.015736	0.225148	-0.599469
6	0	3.281557	-0.233069	-0.224081
6	0	4.059228	-0.954221	-1.113426
6	0	-4.497790	-0.770812	-0.101193
6	0	3.826569	0.058419	1.162106
1	0	-3.481850	1.711687	-0.645120
1	0	-2.294201	-2.187375	0.675993
1	0	0.044873	-1.436809	0.789853
1	0	-1.143045	2.465176	-0.519804
1	0	1.389864	1.021771	1.289370
1	0	1.117105	2.090034	-0.067513
1	0	1.677965	-0.002312	-1.607270
1	0	5.042536	-1.317746	-0.842233
1	0	3.702680	-1.177608	-2.112390
1	0	-4.672509	-1.296268	-1.046622
1	0	-5.199630	0.064871	-0.056308
1	0	-4.746400	-1.464655	0.705989
1	0	4.814493	-0.385607	1.292958
1	0	3.174353	-0.343784	1.943148
1	0	3.917645	1.134245	1.338640

i2

6	0	-0.712393	-0.734603	-0.546145
6	0	-2.008710	-1.189723	-0.341420
6	0	-3.019392	-0.326266	0.101747
6	0	-2.680368	1.007646	0.329628
6	0	-1.379547	1.466895	0.120717
6	0	-0.375632	0.606331	-0.321622
6	0	1.047071	1.093819	-0.546917
6	0	2.024023	0.490658	0.420192
6	0	3.213588	-0.178070	0.112621
6	0	3.667659	-0.398210	-1.174517
6	0	-4.425810	-0.831096	0.318810
6	0	4.057457	-0.667921	1.278473
1	0	0.053128	-1.426424	-0.882896
1	0	-2.242753	-2.233753	-0.527443
1	0	-3.441351	1.700925	0.674146
1	0	-1.146976	2.511601	0.302982
1	0	1.060054	2.186919	-0.440744
1	0	1.344026	0.886492	-1.578111
1	0	1.760984	0.593889	1.469965
1	0	4.595951	-0.926898	-1.352037
1	0	3.126244	-0.058313	-2.047677
1	0	-5.074498	-0.044657	0.709733
1	0	-4.444286	-1.663909	1.028549
1	0	-4.866596	-1.193257	-0.615566
1	0	4.796864	-1.402605	0.954580
1	0	3.436065	-1.129934	2.049706
1	0	4.595456	0.163167	1.745406

i3

6	0	-0.011750	1.075334	0.185136
6	0	-0.037676	-0.356940	0.646078
6	0	1.069806	-1.160912	-0.098887
6	0	2.399055	-0.439396	-0.135735
6	0	2.486709	0.876340	0.075188
6	0	1.305802	1.779537	0.341283
6	0	-1.124917	1.658722	-0.351349
6	0	-2.352144	0.969805	-0.463689
6	0	-2.472136	-0.379214	-0.015057
6	0	-1.384818	-1.006169	0.516832
6	0	3.605816	-1.288775	-0.436280
6	0	-3.805238	-1.078273	-0.140068
1	0	0.266076	-0.375458	1.709859
1	0	0.734211	-1.372462	-1.122452
1	0	1.192098	-2.137067	0.386876
1	0	3.463214	1.354831	0.053203

1	0	1.395880	2.185391	1.363579
1	0	1.346770	2.652822	-0.320441
1	0	-1.067626	2.686502	-0.700594
1	0	-3.212897	1.469497	-0.893749
1	0	-1.469466	-2.033355	0.861824
1	0	4.518195	-0.690788	-0.486377
1	0	3.488559	-1.811126	-1.393249
1	0	3.744412	-2.062821	0.327814
1	0	-3.758466	-2.099508	0.242878
1	0	-4.129159	-1.123113	-1.184974
1	0	-4.582853	-0.543705	0.415102

i4

6	0	-0.688287	-0.677433	-1.113441
6	0	-2.055674	-0.842874	-0.914113
6	0	-2.739022	-0.102724	0.055495
6	0	-2.000158	0.804304	0.820824
6	0	-0.632248	0.971295	0.621577
6	0	0.048527	0.231213	-0.349325
6	0	1.989429	1.823019	-0.509188
6	0	1.554254	0.386747	-0.576486
6	0	2.424707	-0.500970	0.316266
6	0	1.962006	-1.162445	1.376351
6	0	-4.228777	-0.255045	0.247391
6	0	3.872431	-0.583911	-0.102302
1	0	-0.183890	-1.268306	-1.871907
1	0	-2.600487	-1.557722	-1.523206
1	0	-2.501629	1.390974	1.584522
1	0	-0.087010	1.685500	1.228794
1	0	2.503518	2.214418	0.360080
1	0	1.668926	2.520087	-1.274118
1	0	1.732485	0.047875	-1.609467
1	0	2.623091	-1.773832	1.981583
1	0	0.921210	-1.123978	1.671795
1	0	-4.522487	-0.038540	1.277216
1	0	-4.560557	-1.267959	0.007148
1	0	-4.782368	0.432678	-0.401643
1	0	4.450992	-1.206752	0.582116
1	0	4.334802	0.407664	-0.142014
1	0	3.960278	-1.009166	-1.109198

i5

6	0	2.458378	-0.530182	-0.000595
6	0	2.561003	0.894374	-0.012283
6	0	1.402309	1.705430	-0.049930
6	0	0.168268	1.151194	-0.218012

6	0	0.001523	-0.332814	-0.457780
6	0	1.238619	-1.124044	-0.152457
6	0	-1.184323	1.778805	0.022804
6	0	-2.028018	0.621804	0.582639
6	0	-1.291458	-0.683185	0.312125
6	0	-2.606734	-0.397442	-0.368057
6	0	3.711666	-1.348009	0.208451
6	0	-3.849868	-1.169900	0.017180
1	0	3.534740	1.356119	0.108707
1	0	1.499620	2.773164	0.127002
1	0	-0.213692	-0.485564	-1.536191
1	0	1.154293	-2.206946	-0.138035
1	0	-1.623943	2.178427	-0.902136
1	0	-1.121827	2.611769	0.727941
1	0	-2.539405	0.774900	1.526740
1	0	-1.246166	-1.463655	1.063950
1	0	-2.540497	-0.148280	-1.426507
1	0	4.436981	-1.164220	-0.591029
1	0	3.492318	-2.417338	0.223397
1	0	4.201088	-1.088687	1.152736
1	0	-3.904497	-2.124069	-0.516248
1	0	-4.757262	-0.602973	-0.213838
1	0	-3.859933	-1.388839	1.088998

i6

6	0	2.495340	1.035678	0.002494
6	0	2.865034	-0.301514	0.147802
6	0	1.884112	-1.276797	-0.075572
6	0	0.587585	-0.925715	-0.429581
6	0	0.218973	0.417253	-0.578121
6	0	1.193608	1.389252	-0.354583
6	0	-1.201665	0.792261	-0.979734
6	0	-2.263108	0.328465	-0.010076
6	0	-3.234222	-0.585911	-0.419325
6	0	-4.286607	-1.092669	0.317035
6	0	4.271739	-0.694639	0.530375
6	0	-2.228496	0.935327	1.361484
1	0	3.232182	1.815055	0.169889
1	0	2.141846	-2.326467	0.029862
1	0	-0.153238	-1.702595	-0.589071
1	0	0.936698	2.438638	-0.462231
1	0	-1.415533	0.383186	-1.972791
1	0	-1.251403	1.885268	-1.077671
1	0	-3.150995	-0.934642	-1.447693
1	0	-4.975456	-1.801631	-0.124135
1	0	-4.468366	-0.810000	1.346280

1	0	4.282578	-1.288115	1.449861
1	0	4.899935	0.183538	0.692441
1	0	4.740892	-1.301061	-0.250926
1	0	-2.871458	0.414281	2.070934
1	0	-2.551217	1.985227	1.329183
1	0	-1.210221	0.933369	1.762880

i7

6	0	-0.455354	-0.939624	0.022265
6	0	-1.778209	-1.199712	0.358208
6	0	-2.784751	-0.250838	0.136198
6	0	-2.413986	0.966268	-0.435816
6	0	-1.086429	1.228473	-0.775672
6	0	-0.086296	0.281441	-0.556237
6	0	1.362039	0.554339	-0.942555
6	0	2.324585	0.467415	0.217155
6	0	3.250851	-0.566314	0.359305
6	0	3.451295	-1.652207	-0.470307
6	0	-4.217426	-0.541377	0.514337
6	0	2.239093	1.566542	1.234814
1	0	0.303724	-1.691048	0.212592
1	0	-2.036214	-2.157022	0.801395
1	0	-3.170452	1.722721	-0.620171
1	0	-0.829339	2.183935	-1.222532
1	0	1.418801	1.560775	-1.375346
1	0	1.659613	-0.135607	-1.736385
1	0	3.892048	-0.505316	1.237420
1	0	4.216039	-2.383612	-0.242636
1	0	2.867888	-1.819026	-1.367217
1	0	-4.883411	0.263981	0.198074
1	0	-4.326336	-0.657528	1.597609
1	0	-4.570275	-1.468801	0.053171
1	0	2.936867	1.412986	2.060451
1	0	1.227965	1.644761	1.652108
1	0	2.460610	2.542358	0.781294

i8

6	0	0.163878	0.749389	0.218094
6	0	-0.204241	-0.672064	0.545875
6	0	0.653985	-1.637488	-0.327323
6	0	2.102306	-1.228663	-0.371749
6	0	2.556407	-0.014361	-0.051270
6	0	1.616066	1.096822	0.378631
6	0	-0.782314	1.636439	-0.212532
6	0	-2.143837	1.281523	-0.330441
6	0	-2.583336	-0.034577	0.001149

6	0	-1.672502	-0.956910	0.423141
6	0	4.017771	0.342677	-0.090930
6	0	-4.050561	-0.371348	-0.123010
1	0	0.113525	-0.873343	1.586264
1	0	0.236386	-1.666691	-1.342027
1	0	0.563048	-2.656257	0.067605
1	0	2.813169	-1.987707	-0.691473
1	0	1.832690	1.338546	1.433689
1	0	1.848834	2.011274	-0.180512
1	0	-0.481532	2.649011	-0.469106
1	0	-2.863910	2.015989	-0.673356
1	0	-2.000064	-1.961394	0.678124
1	0	4.363078	0.696541	0.887940
1	0	4.206445	1.155657	-0.802129
1	0	4.633604	-0.511430	-0.379730
1	0	-4.248905	-1.405342	0.165507
1	0	-4.399562	-0.233739	-1.151581
1	0	-4.658539	0.280257	0.512966

i9

6	0	-0.477920	1.133180	-0.526400
6	0	-1.868432	1.042540	-0.610591
6	0	-2.565937	-0.003129	-0.007639
6	0	-1.818697	-0.965711	0.682371
6	0	-0.435612	-0.875745	0.767650
6	0	0.267752	0.179435	0.167822
6	0	2.215267	-0.050340	1.705686
6	0	1.798475	0.222577	0.282694
6	0	2.466812	-0.809154	-0.624679
6	0	1.895611	-1.569459	-1.552366
6	0	-4.071283	-0.092746	-0.077324
6	0	2.380939	1.613942	-0.116433
1	0	0.014142	1.965428	-1.012990
1	0	-2.415897	1.804696	-1.156407
1	0	-2.328434	-1.797470	1.159514
1	0	0.116888	-1.638438	1.305334
1	0	3.197869	-0.456225	1.917653
1	0	1.629704	0.340052	2.528950
1	0	3.544300	-0.880818	-0.478220
1	0	2.488794	-2.251403	-2.151701
1	0	0.829645	-1.543928	-1.745861
1	0	-4.397833	-1.094557	-0.370739
1	0	-4.479532	0.618748	-0.798035
1	0	-4.525489	0.123338	0.895573
1	0	3.463732	1.613777	0.026614
1	0	1.955770	2.406599	0.503788

1	0	2.184487	1.837847	-1.168219
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i10

6	0	2.450117	-0.262526	0.116902
6	0	2.280255	1.147988	-0.030322
6	0	1.000106	1.704279	-0.261784
6	0	-0.077472	0.902031	-0.494918
6	0	0.072534	-0.598439	-0.602662
6	0	1.391781	-1.098666	-0.093484
6	0	-1.541594	1.260869	-0.442175
6	0	-2.212364	0.006355	0.163398
6	0	-1.212849	-1.135102	0.062550
6	0	-2.465571	-1.143827	-0.781354
6	0	3.803269	-0.793375	0.529715
6	0	-3.102044	0.196772	1.370577
1	0	3.127286	1.803849	0.138081
1	0	0.870029	2.780160	-0.181616
1	0	0.023130	-0.876968	-1.676246
1	0	1.513532	-2.171813	0.022831
1	0	-1.952047	1.485213	-1.436529
1	0	-1.716267	2.144530	0.178128
1	0	-1.112848	-1.855261	0.867331
1	0	-2.359135	-0.978092	-1.849912
1	0	-3.251873	-1.843059	-0.516013
1	0	4.564169	-0.549913	-0.219192
1	0	3.786244	-1.878259	0.650277
1	0	4.130529	-0.351682	1.476365
1	0	-3.437550	-0.765426	1.767484
1	0	-3.994578	0.780439	1.119473
1	0	-2.571807	0.722446	2.171669

p1

6	0	-2.612365	1.175695	-0.000004
6	0	-3.192788	-0.093424	-0.000001
6	0	-2.332783	-1.201531	0.000003
6	0	-0.955399	-1.048779	0.000005
6	0	-0.365413	0.228891	0.000001
6	0	-1.229764	1.333649	-0.000003
6	0	1.081515	0.457010	0.000002
6	0	2.054699	-0.473679	-0.000002
6	0	3.491011	-0.207068	-0.000001
6	0	4.360345	-1.231582	-0.000006
6	0	-4.690142	-0.278331	0.000000
6	0	3.974275	1.222993	0.000005
1	0	-3.249148	2.054597	-0.000008
1	0	-2.755169	-2.201893	0.000006

1	0	-0.330287	-1.934042	0.000009
1	0	-0.807785	2.333700	-0.000006
1	0	1.369137	1.504989	0.000005
1	0	1.785779	-1.526738	-0.000007
1	0	5.431981	-1.069773	-0.000005
1	0	4.019669	-2.261375	-0.000010
1	0	-5.021117	-0.838061	-0.880621
1	0	-5.209621	0.681862	-0.000023
1	0	-5.021121	-0.838021	0.880645
1	0	5.064188	1.265770	0.000005
1	0	3.612175	1.762962	0.880759
1	0	3.612175	1.762969	-0.880743

p2

6	0	1.276386	1.326541	0.294092
6	0	2.653172	1.123782	0.302083
6	0	3.199383	-0.126529	0.008121
6	0	2.312242	-1.167820	-0.301516
6	0	0.940407	-0.969905	-0.311867
6	0	0.385219	0.285810	-0.004866
6	0	-1.055732	0.551988	0.012934
6	0	-2.051326	-0.348271	-0.059015
6	0	-3.489519	-0.035606	-0.055920
6	0	-3.993461	1.074193	-0.612537
6	0	4.689915	-0.360181	0.019846
6	0	-4.379539	-1.066919	0.598833
1	0	0.880421	2.309751	0.527552
1	0	3.312560	1.952448	0.539689
1	0	2.708699	-2.148622	-0.546344
1	0	0.291630	-1.797206	-0.575460
1	0	-1.326142	1.599639	0.124203
1	0	-1.806269	-1.408379	-0.081075
1	0	-5.055151	1.290867	-0.574841
1	0	-3.364934	1.786762	-1.133699
1	0	5.034365	-0.779500	-0.930423
1	0	4.973712	-1.067457	0.806148
1	0	5.237004	0.568278	0.194519
1	0	-5.431357	-0.781550	0.545311
1	0	-4.111633	-1.205554	1.651603
1	0	-4.265792	-2.041975	0.111686

p3

6	0	-0.061409	0.998228	0.002472
6	0	-0.066268	-0.397806	0.004569
6	0	-1.291327	-1.078936	0.002426
6	0	-2.513602	-0.413598	-0.001413

6	0	-2.493210	0.987885	-0.003446
6	0	-1.288863	1.674138	-0.001691
6	0	1.228849	1.788707	0.004625
6	0	1.219370	-1.198492	0.009389
6	0	2.488552	-0.385378	-0.001091
6	0	2.471489	0.947683	-0.003083
6	0	-3.821965	-1.167485	-0.003515
6	0	3.769299	-1.176491	-0.007914
1	0	-1.282809	-2.166024	0.003786
1	0	-3.428084	1.540010	-0.006696
1	0	-1.292663	2.760401	-0.003619
1	0	1.242173	2.465367	-0.861718
1	0	1.245999	2.454441	0.879539
1	0	1.225868	-1.879296	-0.854379
1	0	1.230016	-1.862509	0.886256
1	0	3.415552	1.487728	-0.009995
1	0	-4.421306	-0.920868	-0.885616
1	0	-4.424933	-0.919407	0.875701
1	0	-3.659375	-2.247112	-0.002298
1	0	4.645218	-0.524911	-0.013332
1	0	3.824388	-1.829886	-0.886815
1	0	3.834466	-1.828664	0.871219

p4

6	0	0.539912	-0.737077	0.817491
6	0	1.914992	-0.933739	0.776795
6	0	2.744956	-0.105835	0.011146
6	0	2.145741	0.931737	-0.705316
6	0	0.768117	1.137036	-0.661837
6	0	-0.060055	0.307472	0.100106
6	0	-1.955554	1.759298	0.629006
6	0	-1.530799	0.564915	0.183370
6	0	-2.480504	-0.497226	-0.236388
6	0	-2.071800	-1.590312	-0.896659
6	0	4.234201	-0.345564	-0.050435
6	0	-3.946570	-0.300018	0.072013
1	0	-0.077762	-1.390344	1.423281
1	0	2.353586	-1.741995	1.354186
1	0	2.762756	1.590077	-1.308843
1	0	0.325609	1.946042	-1.232332
1	0	-3.005352	2.013778	0.697889
1	0	-1.249165	2.518497	0.942023
1	0	-2.781130	-2.349278	-1.207193
1	0	-1.033817	-1.754818	-1.153843
1	0	4.469826	-1.205099	-0.687349
1	0	4.645400	-0.555082	0.940816

1	0	4.760303	0.520261	-0.457896
1	0	-4.526424	-1.169486	-0.240266
1	0	-4.349064	0.574968	-0.448462
1	0	-4.110581	-0.141652	1.142236

p5

6	0	-2.426779	-0.488373	0.035110
6	0	-2.483691	0.873616	0.347212
6	0	-1.339975	1.675590	0.317069
6	0	-0.120964	1.112496	-0.034567
6	0	-0.045278	-0.257830	-0.328693
6	0	-1.186585	-1.050873	-0.297855
6	0	1.232430	1.782926	-0.194379
6	0	2.186741	0.627575	-0.504663
6	0	1.361316	-0.653276	-0.619049
6	0	2.351650	-0.461959	0.519441
6	0	-3.675883	-1.338477	0.040184
6	0	3.625569	-1.277192	0.546931
1	0	-3.438252	1.316572	0.612920
1	0	-1.414901	2.732207	0.554595
1	0	-1.120758	-2.110985	-0.525347
1	0	1.531373	2.338413	0.701739
1	0	1.213079	2.502148	-1.021368
1	0	3.013322	0.805128	-1.183199
1	0	1.573478	-1.411768	-1.364712
1	0	1.905582	-0.279089	1.494270
1	0	-4.034403	-1.520429	-0.978978
1	0	-4.484979	-0.854903	0.591693
1	0	-3.492724	-2.314553	0.497728
1	0	3.458695	-2.259617	0.999285
1	0	4.405561	-0.770360	1.124202
1	0	4.013622	-1.438103	-0.463267

p6

6	0	-0.180687	1.338153	-0.000215
6	0	1.204104	1.191811	-0.000461
6	0	1.794145	-0.072415	-0.000674
6	0	0.943977	-1.188241	-0.001039
6	0	-0.434677	-1.045933	-0.000742
6	0	-1.032188	0.226267	-0.000224
6	0	-3.447079	-0.493184	0.001130
6	0	-2.487689	0.436039	0.000004
6	0	3.292976	-0.245425	0.001311
1	0	-0.611591	2.334372	-0.000211
1	0	1.833772	2.075799	-0.000615
1	0	1.374854	-2.184949	-0.001736

1	0	-1.055717	-1.934242	-0.001254
1	0	-4.493026	-0.211383	0.001216
1	0	-3.235221	-1.556635	0.002039
1	0	-2.791368	1.480935	-0.000740
1	0	3.628864	-0.782536	0.894101
1	0	3.805030	0.718502	-0.020552
1	0	3.627094	-0.822295	-0.866776

p7

6	0	-2.507720	-1.169362	0.280095
6	0	-3.026910	0.100591	0.003885
6	0	-2.126547	1.100203	-0.375473
6	0	-0.759650	0.854566	-0.454308
6	0	-0.231102	-0.411278	-0.151671
6	0	-1.145308	-1.421893	0.195065
6	0	1.195334	-0.748142	-0.235812
6	0	2.288116	0.003996	0.036637
6	0	3.603598	-0.601074	-0.186696
6	0	4.794389	-0.012189	-0.021683
6	0	-4.504733	0.381237	0.121777
6	0	2.242006	1.408139	0.584323
1	0	-3.182155	-1.973084	0.558857
1	0	-2.502030	2.087123	-0.627519
1	0	-0.102313	1.644478	-0.794098
1	0	-0.772769	-2.418678	0.408341
1	0	1.386482	-1.775377	-0.541112
1	0	3.583843	-1.631194	-0.536311
1	0	5.713037	-0.549485	-0.224645
1	0	4.898352	1.013854	0.311172
1	0	-4.774036	0.644884	1.150781
1	0	-5.100543	-0.491655	-0.156185
1	0	-4.804977	1.214255	-0.517867
1	0	1.260877	1.654980	0.986604
1	0	2.493230	2.148951	-0.183217
1	0	2.974169	1.522189	1.388359

p8

6	0	0.992398	-1.346305	-0.414834
6	0	2.372160	-1.194656	-0.398045
6	0	2.964753	-0.013939	0.064326
6	0	2.118409	0.999529	0.522756
6	0	0.734956	0.854634	0.502127
6	0	0.134709	-0.318050	0.014708
6	0	-1.315694	-0.545925	-0.019399
6	0	-2.319805	0.334227	-0.226832
6	0	-3.722920	-0.113837	-0.159452

6	0	-4.226761	-1.007923	0.695897
6	0	4.463554	0.160292	0.057241
6	0	-2.130845	1.787321	-0.594535
1	0	0.561409	-2.275820	-0.772796
1	0	3.002109	-2.008529	-0.743624
1	0	2.548986	1.915162	0.916233
1	0	0.117479	1.646888	0.905416
1	0	-1.605571	-1.587376	0.096846
1	0	-4.401841	0.367894	-0.862255
1	0	-5.272449	-1.291224	0.661088
1	0	-3.615972	-1.473608	1.461829
1	0	4.976209	-0.781586	0.268004
1	0	4.783498	0.893924	0.800605
1	0	4.814401	0.509887	-0.920295
1	0	-1.134858	1.990588	-0.987828
1	0	-2.298175	2.444974	0.266523
1	0	-2.864697	2.076612	-1.353490

p9

6	0	-0.117982	-0.691461	0.004440
6	0	0.242477	0.657290	0.003772
6	0	1.600540	1.003888	0.000374
6	0	2.613207	0.049536	-0.002127
6	0	2.236579	-1.300593	-0.001433
6	0	0.897084	-1.657549	0.001648
6	0	-1.566156	-1.133128	0.008326
6	0	-0.800571	1.754143	0.006561
6	0	-2.218894	1.264199	-0.002137
6	0	-2.581373	-0.018876	-0.001559
6	0	4.070480	0.445443	-0.005789
6	0	-4.023298	-0.450968	-0.009617
1	0	1.868833	2.057362	-0.000431
1	0	2.999894	-2.072703	-0.003568
1	0	0.624768	-2.709191	0.001882
1	0	-1.749190	-1.787853	-0.856237
1	0	-1.749593	-1.772126	0.884659
1	0	-0.637070	2.411578	-0.859142
1	0	-0.644187	2.400491	0.882076
1	0	-2.990243	2.030948	-0.008625
1	0	4.586470	0.053215	-0.887820
1	0	4.590970	0.052912	0.873456
1	0	4.188122	1.530891	-0.005930
1	0	-4.700664	0.405114	-0.014380
1	0	-4.255506	-1.065224	0.868594
1	0	-4.245161	-1.066956	-0.889282

p10

6	0	0.150582	-0.788207	0.778000
6	0	1.530388	-0.951055	0.726069
6	0	2.339008	-0.070175	-0.000930
6	0	1.714579	0.986783	-0.667386
6	0	0.333718	1.158080	-0.613345
6	0	-0.473845	0.275134	0.111620
6	0	-2.437518	1.664033	0.635168
6	0	-1.947631	0.489849	0.202490
6	0	-2.873907	-0.580583	-0.197248
6	0	-2.555997	-1.729934	-0.800289
6	0	3.832537	-0.274119	-0.082078
1	0	-0.449271	-1.480159	1.358001
1	0	1.988796	-1.774548	1.265018
1	0	2.315302	1.686871	-1.239585
1	0	-0.128570	1.981490	-1.146221
1	0	-3.506510	1.839740	0.690750
1	0	-1.786517	2.470799	0.949007
1	0	-3.921538	-0.373719	0.010388
1	0	-3.323750	-2.445027	-1.071512
1	0	-1.533281	-1.988109	-1.047554
1	0	4.088868	-1.004520	-0.857479
1	0	4.235662	-0.648437	0.862289
1	0	4.349329	0.656777	-0.325527

p11

6	0	-2.499173	-0.246409	-0.081290
6	0	-2.338754	1.133087	0.080545
6	0	-1.070239	1.715079	0.153229
6	0	0.055627	0.909207	0.059660
6	0	-0.090940	-0.479371	-0.081846
6	0	-1.354467	-1.053073	-0.154959
6	0	1.519742	1.304929	0.047751
6	0	2.283945	-0.027470	-0.007152
6	0	1.243273	-1.140026	-0.103545
6	0	2.074321	-0.956758	1.158672
6	0	-3.875325	-0.860942	-0.188397
6	0	3.586105	-0.068460	-0.772734
1	0	-3.219119	1.764494	0.145548
1	0	-0.975133	2.790337	0.268280
1	0	-1.460455	-2.128727	-0.262894
1	0	1.802082	1.904727	0.920198
1	0	1.749031	1.908894	-0.839046
1	0	1.406723	-2.024805	-0.708870
1	0	1.568257	-0.595281	2.047696
1	0	2.850549	-1.690802	1.347195

1	0	-4.103931	-1.141338	-1.222457
1	0	-4.649272	-0.165362	0.142794
1	0	-3.955875	-1.767593	0.417748
1	0	3.997161	-1.081105	-0.803471
1	0	4.337556	0.578706	-0.307201
1	0	3.447738	0.269097	-1.805125

p12

6	0	-0.002164	-1.139665	-0.225439
6	0	-1.394470	-1.175730	-0.230617
6	0	-2.150902	-0.024098	-0.009059
6	0	-1.458421	1.171311	0.220280
6	0	-0.071170	1.211867	0.222694
6	0	0.694274	0.057576	-0.013068
6	0	2.847611	1.197922	-0.421792
6	0	2.180997	0.105041	-0.030307
6	0	-3.659450	-0.062645	0.011725
6	0	2.927070	-1.136151	0.402857
1	0	0.543109	-2.057862	-0.407892
1	0	-1.899631	-2.119377	-0.411292
1	0	-2.016441	2.083046	0.411282
1	0	0.431612	2.148466	0.433464
1	0	3.931234	1.228216	-0.409685
1	0	2.340509	2.084742	-0.782443
1	0	-4.044284	0.060439	1.029797
1	0	-4.038669	-1.011831	-0.372260
1	0	-4.086686	0.741277	-0.594437
1	0	4.000118	-0.945604	0.453558
1	0	2.771723	-1.963012	-0.297962
1	0	2.587158	-1.481066	1.384232

CH₂C(CH₂)CHCH₂

6	0	1.998322	0.006097	0.024104
6	0	0.820354	-0.616138	-0.028707
6	0	-0.525693	0.004887	-0.006177
6	0	-1.622873	-0.844013	0.019684
6	0	-0.694623	1.390819	-0.013629
1	0	2.924708	-0.555380	0.002402
1	0	2.090383	1.084209	0.094030
1	0	0.815357	-1.701813	-0.089390
1	0	-2.632769	-0.452948	0.039447
1	0	-1.503182	-1.920347	0.021956
1	0	-1.688340	1.820129	0.011215
1	0	0.140922	2.076236	-0.051313

CH₂C(CH₃)CCH₂

6	0	1.106851	1.334653	0.000023
6	0	0.447997	0.099905	-0.000070
6	0	-0.899160	0.012624	-0.000012
6	0	-2.195572	-0.076762	0.000005
6	0	1.266175	-1.185909	0.000000
1	0	2.188854	1.381381	-0.000110
1	0	0.554361	2.264625	0.000216
1	0	-2.771365	-0.114783	0.924564
1	0	-2.771415	-0.114485	-0.924535
1	0	0.624191	-2.066618	-0.002987
1	0	1.906553	-1.229990	0.885206
1	0	1.911078	-1.227194	-0.882033

CH₂C(CH₃)CHCH

6	0	2.012584	0.096645	-0.000112
6	0	0.909082	-0.619297	-0.000029
6	0	-0.466406	-0.096597	-0.000098
6	0	-1.504981	-0.942851	-0.000021
6	0	-0.643164	1.399535	0.000047
1	0	3.078135	-0.074205	0.000089
1	0	0.998850	-1.711973	0.000678
1	0	-2.527968	-0.584687	-0.000372
1	0	-1.360427	-2.017815	0.000249
1	0	-1.699177	1.674028	-0.003533
1	0	-0.162843	1.845546	-0.876347
1	0	-0.169262	1.844489	0.880510

CH₂CHC(CH₃)CH

6	0	1.542288	-1.057072	0.000044
6	0	0.540823	-0.195027	-0.000023
6	0	-0.850525	-0.672843	-0.000050
6	0	-1.940319	0.100662	0.000040
6	0	0.803369	1.302715	-0.000022
1	0	2.622158	-1.021170	0.000088
1	0	-0.965821	-1.752802	-0.000133
1	0	-2.932191	-0.335406	0.000025
1	0	-1.887283	1.183339	0.000133
1	0	0.358057	1.769452	-0.883988
1	0	1.872552	1.516639	-0.000399
1	0	0.358704	1.769334	0.884335

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6	0	-2.896352	0.995658	0.201872
6	0	-3.099737	-0.377742	0.023265
6	0	-1.994658	-1.188865	-0.259066
6	0	-0.706277	-0.649670	-0.359183

6	0	-0.570272	0.705985	-0.168819
6	0	-1.616903	1.556897	0.107529
6	0	-4.481384	-0.975440	0.158344
1	0	-3.745290	1.639361	0.414862
1	0	-2.138405	-2.255497	-0.406908
1	0	0.145493	-1.283373	-0.582935
1	0	-1.473933	2.623819	0.245323
1	0	-4.701738	-1.229950	1.200931
1	0	-4.577922	-1.891434	-0.428888
1	0	-5.252662	-0.277655	-0.176428
6	0	1.864093	1.638348	-0.371175
6	0	2.631641	0.615641	-0.799483
6	0	3.303121	-0.365063	0.048246
6	0	4.020713	-1.354740	-0.512509
6	0	3.171581	-0.243030	1.546497
1	0	1.745452	1.869301	0.679764
1	0	1.440966	2.345085	-1.073143
1	0	2.753868	0.471619	-1.870377
1	0	4.533310	-2.097833	0.087419
1	0	4.114564	-1.442728	-1.589585
1	0	3.715394	-1.041272	2.053591
1	0	2.122305	-0.292861	1.853665
1	0	3.565201	0.715537	1.899606

TS i0-i4

6	0	-0.950860	1.365542	-0.034562
6	0	-2.321739	1.142554	0.132083
6	0	-2.857625	-0.148950	0.073626
6	0	-1.990110	-1.221986	-0.159164
6	0	-0.615388	-1.019344	-0.326356
6	0	-0.141906	0.272403	-0.258052
6	0	-4.335849	-0.381826	0.284277
1	0	-0.546004	2.370997	0.010637
1	0	-2.981643	1.987665	0.307585
1	0	-2.389419	-2.231040	-0.212036
1	0	0.050651	-1.858366	-0.499614
1	0	-4.679345	-1.271164	-0.249214
1	0	-4.926941	0.468894	-0.063056
1	0	-4.565696	-0.527880	1.345495
6	0	2.283564	1.954723	-0.328140
6	0	2.117510	0.653902	-0.707062
6	0	2.666577	-0.501862	0.031936
6	0	2.881438	-1.659816	-0.606370
6	0	2.990177	-0.330572	1.493624
1	0	2.647015	2.228084	0.654685
1	0	1.995814	2.764805	-0.986909

1	0	1.864612	0.457715	-1.744748
1	0	3.303164	-2.519443	-0.097829
1	0	2.653149	-1.776213	-1.660497
1	0	3.337604	-1.268287	1.929492
1	0	2.109287	0.005152	2.049420
1	0	3.773030	0.420467	1.641559

TS **i0**-CH₂C(CH₂)CHCH₂

6	0	-2.719330	1.037427	0.413391
6	0	-3.108491	-0.214626	-0.072840
6	0	-2.120317	-1.083298	-0.552738
6	0	-0.772148	-0.717191	-0.545957
6	0	-0.435160	0.528872	-0.052153
6	0	-1.373800	1.420566	0.427308
6	0	-4.560099	-0.634102	-0.062427
1	0	-3.473969	1.725111	0.783957
1	0	-2.406572	-2.057701	-0.938440
1	0	-0.015435	-1.397926	-0.921600
1	0	-1.088668	2.397911	0.803860
1	0	-5.223070	0.228399	0.033160
1	0	-4.770694	-1.306163	0.776547
1	0	-4.828366	-1.165538	-0.979218
6	0	2.778500	-0.825180	1.886778
6	0	3.326121	-0.831632	0.668089
6	0	3.073788	0.141768	-0.404677
6	0	3.624144	-0.056866	-1.619688
6	0	2.190700	1.302217	-0.140481
1	0	3.021803	-1.593055	2.611559
1	0	2.065946	-0.071537	2.200860
1	0	4.022047	-1.627632	0.412987
1	0	3.459339	0.633704	-2.438531
1	0	4.255075	-0.915985	-1.819301
1	0	1.010675	0.925523	-0.082816
1	0	2.198503	2.041897	-0.940341
1	0	2.349947	1.775260	0.829694

TS **i0**-CH₂C(CH₃)CCH₂

6	0	2.490393	0.135300	-1.194508
6	0	3.199190	-0.072270	-0.005434
6	0	2.485220	-0.128429	1.196522
6	0	1.095522	0.014302	1.217086
6	0	0.430641	0.214578	0.019849
6	0	1.101324	0.279336	-1.189721
6	0	4.698606	-0.256426	-0.023974
1	0	3.030180	0.188042	-2.135613
1	0	3.020718	-0.282388	2.128816

1	0	0.554791	-0.027320	2.157033
1	0	0.564552	0.443269	-2.118491
1	0	4.964989	-1.302987	-0.208672
1	0	5.147258	0.031673	0.929352
1	0	5.164160	0.341672	-0.811043
6	0	-2.556380	-1.774819	-0.143074
6	0	-3.077706	-0.543238	-0.045314
6	0	-2.214667	0.629131	0.053379
6	0	-2.522591	1.917149	0.159358
6	0	-4.573245	-0.312654	-0.032625
1	0	-3.190808	-2.650824	-0.216237
1	0	-1.485164	-1.935996	-0.152225
1	0	-1.750081	2.676353	0.224122
1	0	-3.551603	2.270332	0.186590
1	0	-4.877572	0.328800	-0.865623
1	0	-4.884952	0.186563	0.890198
1	0	-5.113333	-1.257533	-0.111494
1	0	-0.930982	0.378587	0.034024

TS **i0**-CH₂C(CH₃)CHCH

6	0	-2.506775	0.018934	1.202478
6	0	-3.192975	-0.183492	-0.000281
6	0	-2.506749	0.021753	-1.202498
6	0	-1.165897	0.412616	-1.209723
6	0	-0.518619	0.592883	0.000687
6	0	-1.165960	0.409757	1.210679
6	0	-4.634243	-0.636167	-0.000721
1	0	-3.026570	-0.126644	2.144929
1	0	-3.026504	-0.121601	-2.145306
1	0	-0.648274	0.574215	-2.149736
1	0	0.761108	1.000670	0.001102
1	0	-0.648365	0.569127	2.151088
1	0	-5.164391	-0.278592	-0.886448
1	0	-5.166673	-0.273107	0.881432
1	0	-4.703219	-1.729565	0.002643
6	0	1.951624	1.601484	0.001460
6	0	3.136308	0.996447	0.000801
6	0	3.441239	-0.440563	-0.000416
6	0	4.723375	-0.834636	-0.000933
6	0	2.310450	-1.435810	-0.001071
1	0	1.809041	2.677049	0.002340
1	0	4.019201	1.641127	0.001192
1	0	4.995615	-1.883836	-0.001838
1	0	5.536428	-0.116683	-0.000466
1	0	2.692756	-2.457792	-0.001942
1	0	1.669479	-1.306097	-0.877451

1	0	1.669702	-1.307508	0.875680
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TS i0-CH₂CHC(CH₃)CH

6	0	-2.587435	0.041986	1.201260
6	0	-3.279495	0.132565	-0.012336
6	0	-2.585868	-0.134150	-1.197587
6	0	-1.232213	-0.478641	-1.178570
6	0	-0.580652	-0.554127	0.040578
6	0	-1.234659	-0.300944	1.235366
6	0	-4.735607	0.534193	-0.040138
1	0	-3.112409	0.239751	2.131339
1	0	-3.109088	-0.074582	-2.147401
1	0	-0.706958	-0.685382	-2.105330
1	0	-0.711023	-0.369921	2.183290
1	0	-4.844201	1.623572	0.000285
1	0	-5.279795	0.121468	0.812985
1	0	-5.226715	0.189726	-0.952796
6	0	1.986586	-1.292908	0.073092
6	0	2.968955	-0.391606	0.019606
6	0	2.668684	1.045162	-0.045664
6	0	3.571266	2.029633	-0.101095
6	0	4.420705	-0.827526	0.024449
1	0	2.099991	-2.371041	0.122567
1	0	1.612724	1.299650	-0.047519
1	0	3.261668	3.067021	-0.147219
1	0	4.639114	1.843159	-0.102609
1	0	4.932353	-0.482851	-0.879776
1	0	4.505154	-1.913617	0.072877
1	0	4.951166	-0.402746	0.882596
1	0	0.706413	-0.906025	0.062942

TS i1-i2

6	0	1.192788	-1.309887	0.206796
6	0	2.549965	-1.182752	-0.088721
6	0	3.160761	0.070597	-0.148364
6	0	2.364592	1.196637	0.095496
6	0	1.011890	1.070650	0.388455
6	0	0.401522	-0.187477	0.451030
6	0	-1.078292	-0.313138	0.746247
6	0	-1.957049	0.036431	-0.420952
6	0	-3.420583	0.204544	-0.267371
6	0	-3.981849	1.411064	-0.156678
6	0	4.633355	0.215721	-0.449848
6	0	-4.245800	-1.066547	-0.245551
1	0	0.745835	-2.298455	0.248558
1	0	3.141235	-2.074095	-0.273733

1	0	2.812317	2.185188	0.056501
1	0	0.417872	1.960506	0.571891
1	0	-1.346766	0.327454	1.597404
1	0	-1.288305	-1.340846	1.087013
1	0	-1.540221	-0.045044	-1.421138
1	0	-5.055314	1.529597	-0.045884
1	0	-3.385551	2.316419	-0.178660
1	0	4.806655	0.940282	-1.250924
1	0	5.071970	-0.735676	-0.757575
1	0	5.185018	0.566781	0.428606
1	0	-5.310371	-0.850749	-0.130439
1	0	-3.936966	-1.721398	0.576492
1	0	-4.105200	-1.635018	-1.171340

TS i1-i4

6	0	-0.544502	0.764481	0.886782
6	0	-1.815485	1.089781	0.498804
6	0	-2.641307	0.198879	-0.229360
6	0	-2.128574	-1.097604	-0.489139
6	0	-0.869743	-1.469941	-0.112358
6	0	0.060062	-0.528425	0.535150
6	0	1.192304	-1.085230	1.392688
6	0	1.564023	-0.663254	0.004695
6	0	2.543104	0.412142	-0.329352
6	0	2.454831	1.707426	-0.015734
6	0	-4.007639	0.607847	-0.704211
6	0	3.739939	-0.110379	-1.095402
1	0	0.014483	1.448355	1.511762
1	0	-2.217597	2.057812	0.784262
1	0	-2.764829	-1.821508	-0.990325
1	0	-0.517445	-2.477926	-0.308004
1	0	1.169727	-2.143043	1.633716
1	0	1.526443	-0.444028	2.201235
1	0	1.624830	-1.493400	-0.693250
1	0	3.246845	2.392869	-0.296375
1	0	1.607970	2.135964	0.498376
1	0	-4.693316	-0.243703	-0.735089
1	0	-3.973552	1.029102	-1.717801
1	0	-4.445510	1.371033	-0.055038
1	0	4.457120	0.684608	-1.306729
1	0	3.428591	-0.552327	-2.048672
1	0	4.254160	-0.898142	-0.533447

TS i1-i5

6	0	-2.559114	-0.464511	-0.032111
6	0	-2.484995	0.890418	-0.393675

6	0	-1.312668	1.630103	-0.186762
6	0	-0.201821	1.057562	0.403564
6	0	-0.247765	-0.325068	0.772665
6	0	-1.452488	-1.048193	0.573244
6	0	1.179154	1.661754	0.370764
6	0	2.035852	0.667042	-0.449536
6	0	1.450686	-0.696856	-0.516341
6	0	2.710494	-0.516810	0.239285
6	0	-3.822234	-1.254180	-0.283209
6	0	4.020757	-1.080428	-0.279535
1	0	-3.344222	1.369114	-0.852621
1	0	-1.267263	2.661929	-0.522149
1	0	0.421044	-0.687082	1.547412
1	0	-1.510070	-2.077272	0.913638
1	0	1.593932	1.788398	1.377990
1	0	1.169788	2.647765	-0.098886
1	0	2.531623	1.076547	-1.326379
1	0	1.256642	-1.327948	-1.373773
1	0	2.635599	-0.514848	1.328499
1	0	-3.954538	-1.457787	-1.351293
1	0	-4.707948	-0.708203	0.054109
1	0	-3.800956	-2.214671	0.235911
1	0	4.135925	-2.131776	0.001970
1	0	4.875108	-0.528238	0.125711
1	0	4.070180	-1.020925	-1.370263

TS il-p1

6	0	2.622688	1.160911	-0.169683
6	0	3.201094	-0.103380	-0.041545
6	0	2.343390	-1.194452	0.155620
6	0	0.967451	-1.031160	0.213045
6	0	0.382450	0.238284	0.071072
6	0	1.242969	1.329350	-0.110788
6	0	-1.069084	0.467608	0.105517
6	0	-2.033714	-0.475378	-0.056213
6	0	-3.466069	-0.227404	-0.095505
6	0	-4.315886	-1.258667	-0.258464
6	0	4.695154	-0.298498	-0.119946
6	0	-3.973463	1.185490	0.056729
1	0	3.259536	2.027787	-0.313947
1	0	2.765097	-2.187815	0.274880
1	0	0.341844	-1.898484	0.389278
1	0	0.822341	2.325033	-0.208787
1	0	-1.363752	1.512391	0.108695
1	0	-1.740441	-1.516838	-0.154091
1	0	-5.389107	-1.112273	-0.292389

1	0	-3.955174	-2.276310	-0.361447
1	0	5.225334	0.653584	-0.052473
1	0	4.982479	-0.771360	-1.065404
1	0	5.055581	-0.943619	0.686252
1	0	-5.062871	1.215964	0.013286
1	0	-3.584009	1.834943	-0.733876
1	0	-3.655772	1.613115	1.013108
1	0	-1.282967	0.767677	2.197880

TS i2-i3

6	0	-0.046138	1.063366	0.277589
6	0	-0.183678	-0.250242	0.831824
6	0	2.477104	0.842436	0.131549
6	0	1.292767	1.753589	0.366760
6	0	-1.099898	1.582834	-0.454209
6	0	-2.307219	0.887325	-0.594239
6	0	-2.495309	-0.363303	0.021294
6	0	-1.450572	-0.895792	0.761474
6	0	-3.814769	-1.086228	-0.110224
6	0	1.158371	-1.138618	-0.546332
6	0	2.422224	-0.449839	-0.241072
6	0	3.676150	-1.297826	-0.285063
1	0	0.487994	-0.541773	1.632132
1	0	3.448991	1.280290	0.345169
1	0	1.415424	2.209190	1.360809
1	0	1.317699	2.593878	-0.339144
1	0	-0.986484	2.550498	-0.934177
1	0	-3.114641	1.327738	-1.170263
1	0	-1.583807	-1.842742	1.275005
1	0	-4.649874	-0.448053	0.194142
1	0	-3.838223	-1.987929	0.505150
1	0	-3.998636	-1.385670	-1.147260
1	0	0.599137	-0.844353	-1.427034
1	0	1.137146	-2.211836	-0.363667
1	0	3.586192	-2.153406	0.394586
1	0	4.559726	-0.724857	0.005108
1	0	3.845167	-1.707192	-1.286668

TS i2-p2

6	0	-1.290729	1.315580	-0.339814
6	0	-2.663875	1.094832	-0.388109
6	0	-3.207398	-0.144540	-0.045770
6	0	-2.322143	-1.156319	0.352623
6	0	-0.953466	-0.940557	0.402439
6	0	-0.403082	0.302253	0.045403
6	0	1.040699	0.577797	0.053655

6	0	2.033761	-0.344425	0.034861
6	0	3.471978	-0.064734	-0.014113
6	0	4.015540	1.063924	0.466681
6	0	-4.695142	-0.392644	-0.085468
6	0	4.325965	-1.152685	-0.625586
1	0	-0.896584	2.289797	-0.610826
1	0	-3.322651	1.900626	-0.695581
1	0	-2.717179	-2.126791	0.637435
1	0	-0.305274	-1.741073	0.739981
1	0	1.310896	1.619986	-0.092056
1	0	1.763344	-1.398036	0.029641
1	0	5.081667	1.247275	0.396849
1	0	3.418797	1.820762	0.961749
1	0	-5.086137	-0.618506	0.911909
1	0	-4.938620	-1.244567	-0.727842
1	0	-5.233807	0.477749	-0.464956
1	0	5.383859	-0.886151	-0.611737
1	0	4.033291	-1.347366	-1.662697
1	0	4.204988	-2.094229	-0.078407
1	0	1.190760	1.149637	2.125735

TS i3-p3

6	0	-0.062836	1.015290	-0.025319
6	0	-0.060804	-0.395893	0.073602
6	0	1.216996	-1.185220	-0.163572
6	0	2.487183	-0.384072	-0.031502
6	0	2.470329	0.947480	0.033420
6	0	1.231155	1.794141	-0.011105
6	0	-1.287445	1.682213	-0.051008
6	0	-2.492149	0.990880	-0.032943
6	0	-2.514019	-0.414294	-0.006099
6	0	-1.300498	-1.081917	0.018734
6	0	3.763600	-1.180208	0.000521
6	0	-3.825659	-1.161653	-0.006437
1	0	0.155259	-0.394366	1.892500
1	0	1.175093	-1.615438	-1.175803
1	0	1.250839	-2.044531	0.515869
1	0	3.412031	1.484499	0.119015
1	0	1.228259	2.476343	0.851250
1	0	1.269508	2.453547	-0.890223
1	0	-1.296357	2.767625	-0.090168
1	0	-3.427577	1.540959	-0.056543
1	0	-1.287991	-2.168085	0.027939
1	0	4.641260	-0.532755	0.050407
1	0	3.856922	-1.812656	-0.890554
1	0	3.784186	-1.852508	0.866295

1	0	-3.671643	-2.236137	-0.123309
1	0	-4.476798	-0.823528	-0.817918
1	0	-4.368112	-1.003461	0.931493

TS i4-p4

6	0	0.583474	-0.769506	0.828815
6	0	1.956074	-0.962379	0.737951
6	0	2.761969	-0.106480	-0.022824
6	0	2.138180	0.946849	-0.693220
6	0	0.761907	1.145881	-0.601739
6	0	-0.040316	0.295894	0.165934
6	0	-1.962943	1.799819	0.508936
6	0	-1.519829	0.535040	0.253481
6	0	-2.452700	-0.512278	-0.265888
6	0	-2.010288	-1.555109	-0.979035
6	0	4.255854	-0.309749	-0.095608
6	0	-3.926319	-0.334464	0.007284
1	0	-0.016881	-1.441863	1.430686
1	0	2.411814	-1.790985	1.271273
1	0	2.732951	1.620813	-1.301614
1	0	0.300758	1.961815	-1.146685
1	0	-3.013199	2.056893	0.486621
1	0	-1.272336	2.574547	0.816675
1	0	-2.703166	-2.294067	-1.365588
1	0	-0.962490	-1.697968	-1.206753
1	0	4.509289	-1.365562	-0.223674
1	0	4.744284	0.031619	0.823552
1	0	4.693530	0.246389	-0.927185
1	0	-4.487900	-1.207390	-0.327727
1	0	-4.328494	0.539988	-0.514557
1	0	-4.112805	-0.190685	1.075982
1	0	-1.765727	-0.084658	2.044472

TS i4-p6

6	0	0.726515	0.007442	1.344211
6	0	2.058677	-0.356661	1.171584
6	0	2.710129	-0.154326	-0.047478
6	0	1.972248	0.417399	-1.091346
6	0	0.643098	0.783572	-0.921340
6	0	-0.006389	0.596374	0.307201
6	0	-2.033521	2.023757	-0.120464
6	0	-1.412107	0.996987	0.539506
6	0	4.162770	-0.520398	-0.231376
1	0	0.245134	-0.167705	2.300951
1	0	2.598758	-0.808084	1.997953
1	0	2.446073	0.571413	-2.056038

1	0	0.098632	1.203477	-1.759299
1	0	-3.004584	2.381823	0.198044
1	0	-1.612801	2.476781	-1.009775
1	0	-1.798130	0.729411	1.519027
1	0	4.352736	-0.909510	-1.234977
1	0	4.477550	-1.277575	0.490156
1	0	4.809719	0.353217	-0.093745
6	0	-2.513738	-0.891466	-0.160057
6	0	-1.775420	-1.871971	-0.625252
6	0	-3.967811	-0.697720	0.019198
1	0	-2.234618	-2.799157	-0.979731
1	0	-0.693179	-1.816369	-0.680637
1	0	-4.327177	0.154539	-0.565541
1	0	-4.220423	-0.500785	1.066824
1	0	-4.524399	-1.589403	-0.299542

TS i5-p5

6	0	-2.464236	-0.495686	-0.007144
6	0	-2.532397	0.885165	0.243326
6	0	-1.386239	1.685968	0.242221
6	0	-0.146547	1.105553	0.038692
6	0	-0.040273	-0.308188	-0.065764
6	0	-1.216460	-1.081105	-0.198434
6	0	1.196246	1.772370	-0.181991
6	0	2.137491	0.625179	-0.567517
6	0	1.350795	-0.685365	-0.489358
6	0	2.491096	-0.405345	0.467294
6	0	-3.725232	-1.326228	-0.053095
6	0	3.781142	-1.184681	0.340674
1	0	-3.503421	1.347783	0.388625
1	0	-1.481768	2.761672	0.352614
1	0	-1.138943	-2.146478	-0.390640
1	0	1.546265	2.307072	0.709368
1	0	1.130274	2.511965	-0.986980
1	0	2.842409	0.789773	-1.375148
1	0	1.474236	-1.472050	-1.225667
1	0	2.184754	-0.189210	1.488136
1	0	-3.553570	-2.281277	-0.554149
1	0	-4.528083	-0.805986	-0.582189
1	0	-4.088606	-1.544769	0.956929
1	0	3.715732	-2.144324	0.862320
1	0	4.620993	-0.627164	0.767210
1	0	4.018769	-1.390910	-0.707316
1	0	0.088639	-0.641920	1.683450

TS i0-i6

6	0	2.887098	1.019809	-0.140511
6	0	3.112376	-0.346061	0.068977
6	0	2.010621	-1.206486	0.129972
6	0	0.703657	-0.722311	-0.009104
6	0	0.547401	0.629390	-0.209177
6	0	1.589642	1.526436	-0.282048
6	0	4.517181	-0.873536	0.249794
1	0	3.732921	1.699496	-0.196776
1	0	2.170750	-2.269724	0.285192
1	0	-0.145281	-1.396472	0.034870
1	0	1.429404	2.586917	-0.447564
1	0	4.575227	-1.939372	0.018410
1	0	4.858567	-0.742722	1.282482
1	0	5.226376	-0.349690	-0.396029
6	0	-1.948829	1.426706	-0.600247
6	0	-2.733712	0.504157	-0.000014
6	0	-3.187556	-0.659401	-0.757182
6	0	-3.943910	-1.662162	-0.289695
6	0	-3.124484	0.633209	1.449386
1	0	-1.701825	1.354884	-1.652611
1	0	-1.636585	2.325565	-0.083619
1	0	-2.867903	-0.690797	-1.796530
1	0	-4.235655	-2.487240	-0.928426
1	0	-4.296907	-1.693775	0.734726
1	0	-4.213184	0.644669	1.565470
1	0	-2.724816	1.550807	1.882846
1	0	-2.748000	-0.211042	2.036651

TS i0-i9

6	0	-0.841756	-1.321812	-0.177332
6	0	-2.229056	-1.145964	-0.129626
6	0	-2.792701	0.126113	0.013493
6	0	-1.935118	1.228034	0.113164
6	0	-0.545999	1.071471	0.066255
6	0	-0.041780	-0.204202	-0.072947
6	0	-4.292204	0.312522	0.030093
1	0	-0.417528	-2.313893	-0.290828
1	0	-2.878994	-2.013310	-0.204613
1	0	-2.354742	2.223893	0.226747
1	0	0.109108	1.934074	0.133627
1	0	-4.802862	-0.592991	0.365512
1	0	-4.671705	0.551520	-0.969516
1	0	-4.585455	1.130192	0.693156
6	0	2.334179	-1.739134	-0.610184
6	0	2.248203	-0.517075	0.012059
6	0	2.568645	0.686132	-0.781577

6	0	2.968346	1.865133	-0.298713
6	0	2.376052	-0.439321	1.521422
1	0	2.405489	-1.816163	-1.688904
1	0	2.266806	-2.663473	-0.048792
1	0	2.483403	0.561240	-1.858367
1	0	3.209267	2.686287	-0.963528
1	0	3.080171	2.051437	0.763283
1	0	1.828820	0.406747	1.938500
1	0	3.430199	-0.327448	1.798756
1	0	1.997164	-1.349493	1.988333

TS i6-i7

6	0	-1.121907	-1.293201	-0.546656
6	0	-2.456559	-1.047561	-0.221579
6	0	-2.897832	0.238661	0.089248
6	0	-1.955454	1.275304	0.063447
6	0	-0.626731	1.031103	-0.259752
6	0	-0.184973	-0.260762	-0.572385
6	0	1.268077	-0.511977	-0.930613
6	0	2.249250	-0.296938	0.198726
6	0	3.641730	0.047967	-0.153948
6	0	4.181935	1.263503	-0.084713
6	0	-4.339443	0.513265	0.445186
6	0	1.992574	-0.925015	1.535100
1	0	-0.808828	-2.304548	-0.787162
1	0	-3.163200	-1.871536	-0.212144
1	0	-2.270272	2.288008	0.297258
1	0	0.082664	1.852567	-0.271401
1	0	1.553391	0.132810	-1.768838
1	0	1.360210	-1.545405	-1.308962
1	0	4.277020	-0.776607	-0.499442
1	0	5.216082	1.440154	-0.360591
1	0	3.607584	2.120960	0.251587
1	0	-4.432245	0.879955	1.472569
1	0	-4.948796	-0.388468	0.357717
1	0	-4.772856	1.275193	-0.209916
1	0	2.554003	-0.419446	2.325355
1	0	2.310348	-1.982549	1.549460
1	0	0.930891	-0.907184	1.792149

TS i6-i9

6	0	-0.360953	0.905462	0.801547
6	0	-1.676785	1.115910	0.490956
6	0	-2.480148	0.123615	-0.120347
6	0	-1.875163	-1.132420	-0.378441
6	0	-0.566517	-1.390959	-0.080341

6	0	0.313024	-0.368632	0.507887
6	0	1.465359	-0.812567	1.435751
6	0	1.853593	-0.334350	0.079677
6	0	2.542483	0.990129	-0.041074
6	0	2.245804	1.934045	-0.930791
6	0	-3.930111	0.365703	-0.437461
6	0	2.344371	-1.350025	-0.942713
1	0	0.215952	1.694412	1.267095
1	0	-2.122664	2.078518	0.725145
1	0	-2.477669	-1.922273	-0.818752
1	0	-0.163591	-2.377191	-0.274673
1	0	1.532314	-1.874156	1.652060
1	0	1.656458	-0.167139	2.287406
1	0	3.378174	1.148238	0.641230
1	0	2.819069	2.852442	-0.991909
1	0	1.414222	1.826781	-1.619542
1	0	-4.590580	-0.106715	0.301649
1	0	-4.202134	-0.046062	-1.414558
1	0	-4.164156	1.432902	-0.446489
1	0	3.435574	-1.425373	-0.890194
1	0	2.081499	-1.042545	-1.958136
1	0	1.937794	-2.347297	-0.768222

TS i6-i10

6	0	2.523344	-0.140736	0.149485
6	0	2.132795	1.208055	0.165326
6	0	0.854273	1.594592	-0.258339
6	0	-0.054025	0.664133	-0.728852
6	0	0.315532	-0.718047	-0.744247
6	0	1.622771	-1.083766	-0.331743
6	0	-1.527047	0.931532	-0.892414
6	0	-2.232335	0.012329	0.147678
6	0	-1.375950	-1.133744	0.542560
6	0	-2.570113	-1.411237	-0.290015
6	0	3.899900	-0.542342	0.624803
6	0	-3.123335	0.712787	1.154941
1	0	2.827282	1.961724	0.522809
1	0	0.563016	2.638421	-0.190083
1	0	-0.195399	-1.394905	-1.421721
1	0	1.925557	-2.123535	-0.404958
1	0	-1.876420	0.703362	-1.906044
1	0	-1.763046	1.980881	-0.700062
1	0	-1.133682	-1.509966	1.527863
1	0	-2.441729	-1.664888	-1.341670
1	0	-3.422757	-1.907927	0.169816
1	0	4.009314	-0.376883	1.701766

1	0	4.679913	0.041710	0.127316
1	0	4.095284	-1.598843	0.430291
1	0	-3.540965	0.004572	1.875673
1	0	-3.960142	1.217392	0.658919
1	0	-2.561086	1.467551	1.714981

TS i6-p7

6	0	2.519763	1.174045	0.192977
6	0	3.044234	-0.107932	0.006874
6	0	2.148139	-1.136244	-0.307071
6	0	0.783044	-0.900895	-0.412793
6	0	0.248477	0.382955	-0.203994
6	0	1.155802	1.416814	0.079229
6	0	-1.179233	0.705297	-0.321840
6	0	-2.269892	-0.032822	-0.003350
6	0	-3.587525	0.540895	-0.287847
6	0	-4.774576	-0.047222	-0.095687
6	0	4.524566	-0.378552	0.119524
6	0	-2.218008	-1.389970	0.651421
1	0	3.189407	1.995809	0.426127
1	0	2.527348	-2.138472	-0.482782
1	0	0.128974	-1.715498	-0.695976
1	0	0.779328	2.424208	0.224560
1	0	-1.374068	1.704473	-0.707075
1	0	-3.572758	1.542648	-0.712214
1	0	-5.695572	0.463314	-0.350457
1	0	-4.872898	-1.046862	0.311052
1	0	4.936598	-0.734520	-0.830217
1	0	4.731420	-1.148163	0.869632
1	0	5.073020	0.521500	0.404100
1	0	-1.239218	-1.595312	1.081483
1	0	-2.455002	-2.190396	-0.058602
1	0	-2.957633	-1.447734	1.454632
1	0	-1.567683	2.006794	2.561081

TS i7-i8

6	0	-0.137329	-0.758273	0.257117
6	0	0.280326	0.523900	0.745839
6	0	-2.550217	0.014698	-0.056610
6	0	-1.601938	-1.116056	0.305872
6	0	0.795333	-1.554673	-0.383174
6	0	2.138464	-1.170294	-0.489297
6	0	2.588631	0.038605	0.071278
6	0	1.667878	0.846631	0.720486
6	0	-4.009050	-0.276265	0.167632
6	0	4.045287	0.426620	-0.022457

6	0	-0.736514	1.594432	-0.752441
6	0	-2.123800	1.216270	-0.493914
1	0	-0.336084	1.012523	1.492783
1	0	-1.873065	-1.455207	1.317447
1	0	-1.790751	-1.979405	-0.345860
1	0	0.478605	-2.499456	-0.815372
1	0	2.844039	-1.823698	-0.992022
1	0	1.998613	1.766835	1.191667
1	0	-4.633359	0.587013	-0.071367
1	0	-4.203524	-0.564222	1.208065
1	0	-4.344414	-1.115655	-0.454371
1	0	4.322329	0.670351	-1.053586
1	0	4.696613	-0.390002	0.302565
1	0	4.264901	1.299881	0.595149
1	0	-0.202352	1.124461	-1.570546
1	0	-0.492537	2.648532	-0.635897
1	0	-2.871437	2.004494	-0.590630

TS i7-p8

6	0	0.992824	-1.337663	-0.418966
6	0	2.374126	-1.192384	-0.431913
6	0	2.982508	-0.021921	0.033897
6	0	2.151765	0.988774	0.527424
6	0	0.768107	0.850200	0.536915
6	0	0.152849	-0.312178	0.045421
6	0	-1.302685	-0.530521	0.027697
6	0	-2.297017	0.356027	-0.244653
6	0	-3.703633	-0.075099	-0.239645
6	0	-4.250758	-1.007361	0.547212
6	0	4.481295	0.147758	-0.005159
1	0	0.549373	-2.259895	-0.780461
1	0	2.991708	-2.003983	-0.803817
1	0	2.595594	1.895944	0.925689
1	0	0.162881	1.637253	0.968268
1	0	-1.597950	-1.572961	0.108690
1	0	-4.352124	0.456038	-0.934952
1	0	-5.299641	-1.266185	0.460600
1	0	-3.677385	-1.522692	1.309619
1	0	4.994510	-0.811088	0.099276
1	0	4.829431	0.807416	0.793092
1	0	4.802264	0.587895	-0.956039
1	0	-1.581670	-0.519624	2.273245
6	0	-2.071007	1.803335	-0.605941
1	0	-2.242574	2.459819	0.255587
1	0	-2.782719	2.110587	-1.378165
1	0	-1.061947	1.987664	-0.974361

TS i8-p9

6	0	-0.121755	-0.711120	-0.028181
6	0	0.236128	0.653057	0.082120
6	0	-0.800304	1.741489	-0.147362
6	0	-2.218754	1.258433	-0.073137
6	0	-2.581588	-0.023176	-0.014410
6	0	-1.569724	-1.141769	-0.016249
6	0	0.892912	-1.667736	-0.061770
6	0	2.234088	-1.306564	-0.039460
6	0	2.613345	0.046409	-0.002481
6	0	1.609833	1.000547	0.028469
6	0	-4.022684	-0.452445	0.052193
6	0	4.072119	0.435127	0.000246
1	0	0.033112	0.685280	1.900208
1	0	-0.619569	2.183255	-1.138730
1	0	-0.645259	2.557378	0.567087
1	0	-2.988764	2.026069	-0.082198
1	0	-1.746343	-1.779027	0.863183
1	0	-1.762897	-1.795854	-0.878831
1	0	0.625485	-2.719382	-0.110169
1	0	2.998257	-2.076841	-0.068886
1	0	1.874130	2.054056	0.044507
1	0	-4.220141	-1.026444	0.965352
1	0	-4.279237	-1.105748	-0.790399
1	0	-4.699107	0.404227	0.036404
1	0	4.196573	1.514794	-0.103319
1	0	4.614761	-0.047476	-0.817972
1	0	4.557312	0.132194	0.933897

TS i9-p10

6	0	0.359234	-0.897337	0.492241
6	0	1.739732	-1.056967	0.510453
6	0	2.594192	-0.065975	0.014845
6	0	2.007759	1.085462	-0.512782
6	0	0.624599	1.246770	-0.534889
6	0	-0.232485	0.266043	-0.020295
6	0	-2.230047	1.750571	0.017883
6	0	-1.723274	0.465094	-0.072527
6	0	-2.548729	-0.531554	-0.805283
6	0	-2.113848	-1.554818	-1.541435
6	0	4.093307	-0.232032	0.067415
6	0	-2.336805	-0.263432	1.975951
1	0	-0.265560	-1.687748	0.887669
1	0	2.161646	-1.969666	0.920082
1	0	2.638832	1.866977	-0.924411
1	0	0.201686	2.139424	-0.979992

1	0	-3.271921	1.950517	-0.202203
1	0	-1.642194	2.563504	0.424087
1	0	-3.619778	-0.351342	-0.744023
1	0	-2.815132	-2.197161	-2.061285
1	0	-1.060519	-1.778080	-1.659395
1	0	4.590680	0.403194	-0.668776
1	0	4.387699	-1.267073	-0.124097
1	0	4.484856	0.039922	1.053941
1	0	-3.344990	0.126175	2.050664
1	0	-1.590867	0.231002	2.586143
1	0	-2.256249	-1.340592	1.892136

TS i9-p12

6	0	0.502481	-1.136282	-0.668084
6	0	1.877794	-0.944442	-0.785808
6	0	2.548281	0.000463	-0.009359
6	0	1.783903	0.759024	0.886171
6	0	0.413946	0.570562	1.006281
6	0	-0.262040	-0.393302	0.239533
6	0	-2.325088	-0.450332	1.620453
6	0	-1.729239	-0.629343	0.397362
6	0	4.041355	0.193236	-0.113879
1	0	0.029468	-1.884546	-1.291152
1	0	2.435907	-1.544556	-1.497707
1	0	2.269673	1.516844	1.493480
1	0	-0.144500	1.198475	1.690063
1	0	-3.362619	-0.723342	1.773908
1	0	-1.813375	0.017475	2.450888
1	0	4.436185	-0.241776	-1.034386
1	0	4.559951	-0.283680	0.725135
1	0	4.309304	1.253220	-0.098799
6	0	-2.501597	1.282367	-0.637753
6	0	-1.710953	2.228490	-1.084034
1	0	-3.581916	1.210622	-0.599631
1	0	-2.107997	3.142471	-1.532050
1	0	-0.627737	2.148893	-1.036075
6	0	-2.410949	-1.550649	-0.601180
1	0	-3.492969	-1.526600	-0.461434
1	0	-2.082913	-2.584694	-0.445955
1	0	-2.193815	-1.277554	-1.634504

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6	0	-2.491260	-0.248676	-0.139705
6	0	-2.336433	1.135700	0.042282
6	0	-1.072643	1.718171	0.180981
6	0	0.053272	0.913769	0.192301

6	0	-0.091639	-0.499706	0.161831
6	0	-1.359492	-1.058405	-0.117234
6	0	1.512699	1.311083	0.143305
6	0	2.279404	-0.007548	-0.072219
6	0	1.251861	-1.140076	-0.033795
6	0	2.272210	-0.979165	1.075218
6	0	-3.865298	-0.843469	-0.339895
6	0	3.437748	0.001107	-1.043220
1	0	-3.215269	1.772265	0.021138
1	0	-0.981020	2.798740	0.230476
1	0	-1.454680	-2.131029	-0.252924
1	0	1.839196	1.826177	1.054656
1	0	1.693518	2.000537	-0.689238
1	0	1.328867	-1.998327	-0.692097
1	0	1.905744	-0.660874	2.045342
1	0	3.077833	-1.705094	1.109685
1	0	-3.806091	-1.840644	-0.781490
1	0	-4.480390	-0.219669	-0.993807
1	0	-4.395233	-0.937146	0.614230
1	0	3.856548	-1.001093	-1.168036
1	0	4.243360	0.653467	-0.688717
1	0	3.125697	0.360379	-2.029396
1	0	-0.280658	-0.734403	1.921081