**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

**i1**

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

**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

TS **i0**-**i1**

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

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 **i1-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

TS **i10-p11**

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