**Peroxide Splitting**

**OOH- Gas No Field**

O -1.7744643808 0.3825762858 -0.0102340706

O -0.2904619577 0.3917343337 -0.0006676011

H -0.1272136615 1.2876793805 0.3094516717

**OOH- Solvent No Field**

O -1.7756180793 0.3715121223 -0.0140600604

O -0.3088888786 0.3988256707 0.0017018783

H -0.1076330421 1.291652207 0.3109081821

**OH radical Gas No Field**

O -1.1530124938 -0.35393 -0.65976

H -0.1774475062 -0.35393 -0.65976

**OH radical Solvent No Field**

O -1.1543051134 -0.35393 -0.65976

H -0.1761548866 -0.35393 -0.65976

**OH anion Gas No Field**

O -1.1486097931 -0.35393 -0.65976

H -0.1818502069 -0.35393 -0.65976

**OH anion Solvent No Field**

O -1.1474688069 -0.35393 -0.65976

H -0.1829911931 -0.35393 -0.65976

**OO radical anion Gas No Field**

O -1.3285941438 -0.35393 -0.65976

O -0.0018658562 -0.35393 -0.65976

**OO radical anion Solvent No Field**

O -1.326835873 -0.35393 -0.65976

O -0.003624127 -0.35393 -0.65976

**OO neutral Gas No Field**

O -1.2635224927 -0.35393 -0.65976

O -0.0669375073 -0.35393 -0.65976

**OO neutral Solvent No Field**

O -1.2629283043 -0.35393 -0.65976

O -0.0675316957 -0.35393 -0.65976

**OOH- Gas Field + 2**

O -1.7739854368 0.3829656094 -0.0100975509

O -0.2908841114 0.3915645693 -0.0007280509

H -0.1272704518 1.2874598213 0.3093756018

**OOH- Solvent Field + 2**

O -1.7756180793 0.3715121223 -0.0140600604

O -0.3088888786 0.3988256707 0.0017018783

H -0.1076330421 1.291652207 0.3109081821

**OH radical Gas Field + 2**

O -1.1530263708 -0.35393 -0.65976

H -0.1774336292 -0.35393 -0.65976

**OH radical Solvent Field + 2**

O -1.1543367371 -0.35393 -0.65976

H -0.1761232629 -0.35393 -0.65976

**OH anion Gas Field + 2**

O -1.1486251219 -0.35393 -0.65976

H -0.1818348781 -0.35393 -0.65976

**OH anion Solvent Field + 2**

O -1.1475155583 -0.35393 -0.65976

H -0.1829444417 -0.35393 -0.65976

**OO radical anion Gas Field + 2**

O -1.3285943317 -0.35393 -0.65976

O -0.0018656683 -0.35393 -0.65976

**OO radical anion Solvent Field + 2**

O -1.3268362209 -0.35393 -0.65976

O -0.0036237791 -0.35393 -0.65976

**OO neutral Gas Field + 2**

O -1.2635225482 -0.35393 -0.65976

O -0.0669374518 -0.35393 -0.65976

**OO neutral Solvent Field + 2**

O -1.2629283922 -0.35393 -0.65976

O -0.0675316078 -0.35393 -0.65976

**OOH- Gas Field + 10**

O -1.2436850198 -0.5465809525 -0.475181372

H -0.2843952364 -0.6032580596 -0.4223505235

O -1.3975597437 0.6946790122 -1.2718681045

**OOH- Solvent Field + 10**

O -1.2371898933 -0.5321306943 -0.4843129091

H -0.2767745962 -0.6166055342 -0.4136805372

O -1.4116755105 0.6935762285 -1.2714065537

**OH radical Gas Field + 10**

O -1.1530833913 -0.35393 -0.65976

H -0.1773766087 -0.35393 -0.65976

**OH radical Solvent Field + 10**

O -1.1544649807 -0.35393 -0.65976

H -0.1759950193 -0.35393 -0.65976

**OH anion Gas Field + 10**

O -1.1486888858 -0.35393 -0.65976

H -0.1817711142 -0.35393 -0.65976

**OH anion Solvent Field + 10**

O -1.1477054535 -0.35393 -0.65976

H -0.1827545465 -0.35393 -0.65976

**OO radical anion Gas Field + 10**

O -1.3285988425 -0.35393 -0.65976

O -0.0018611575 -0.35393 -0.65976

**OO radical anion Solvent Field + 10**

O -1.3268446297 -0.35393 -0.65976

O -0.0036153703 -0.35393 -0.65976

**OO neutral Gas Field + 10**

O -1.2635238883 -0.35393 -0.65976

O -0.0669361117 -0.35393 -0.65976

**OO neutral Solvent Field + 10**

O -1.262930497 -0.35393 -0.65976

O -0.067529503 -0.35393 -0.65976

**Polymerization Mechanism**

**OH\_r**

O 0.000000 0.000000 0.108748

H 0.000000 0.000000 -0.869982

**H2O**

O -0.000000 -0.000000 0.117783

H 0.000000 0.765164 -0.471133

H -0.000000 -0.765164 -0.471133

**MA\_a**

C -1.753051 0.171198 -0.034078

C -2.054637 1.542788 -0.000954

C -0.402735 -0.233391 -0.022458

C -1.040016 2.490196 0.048021

C 0.297691 2.093229 0.064355

C 0.610812 0.733129 0.035555

C -0.058334 -1.704848 -0.149344

O 0.754118 -2.032559 -1.055358

O -0.634141 -2.509785 0.639509

C 2.069458 0.325981 0.149760

O 2.891981 0.896122 -0.620453

O 2.364360 -0.520724 1.037723

N -2.782182 -0.760758 -0.158898

H -2.565915 -1.664241 0.247544

H -3.687505 -0.409836 0.129533

H -3.096869 1.850870 -0.016583

H -1.294428 3.545580 0.080028

H 1.094332 2.828809 0.115259

**MA\_b**

C -1.810028 0.039587 0.034539

C -2.193175 1.418007 -0.010134

C -0.402155 -0.274618 0.008009

C -1.246699 2.417171 -0.072992

C 0.116275 2.087073 -0.083998

C 0.537417 0.747838 -0.050052

C 0.004270 -1.734996 0.109529

O -0.290542 -2.476577 -0.865654

O 0.549345 -2.097707 1.184405

C 2.029939 0.453247 -0.105902

O 2.794742 1.275261 0.469421

O 2.394234 -0.572471 -0.739385

N -2.782984 -0.872899 0.106703

H -2.377069 -1.812856 0.116745

H -3.254506 1.646239 0.010163

H -1.550413 3.458172 -0.110523

H 0.865581 2.870828 -0.127597

**MA\_e**

C -2.952147 1.152758 -2.112402

C -3.623653 0.959429 -0.817254

C -1.845952 0.484024 -2.451850

C -1.251738 -0.590592 -1.590720

C -1.881834 -0.671767 -0.217612

C -2.984972 0.011267 0.131522

C -1.197899 -1.645889 0.729572

C -3.602577 -0.156034 1.511922

N -4.704361 1.617765 -0.587249

O -3.923566 -1.319164 1.869846

O -1.069564 -2.825800 0.304847

N 0.212430 -0.570492 -1.570476

C 0.905423 0.325343 -0.745806

C 0.332409 1.538101 -0.328004

H -0.682796 1.787643 -0.612422

C 1.060709 2.435623 0.446725

H 0.592201 3.362585 0.763914

C 2.372075 2.152959 0.818401

H 2.939294 2.846776 1.431036

C 2.955161 0.951551 0.408498

C 4.354420 0.629648 0.903751

C 2.239146 0.038643 -0.374124

C 2.919808 -1.225169 -0.869923

H -3.389930 1.893005 -2.776046

H -1.353507 0.665112 -3.404206

H -1.500557 -1.541091 -2.085638

H 0.593795 -1.508380 -1.484799

O 4.514795 -0.464787 1.509832

O 4.041611 -1.094700 -1.427369

O 5.247666 1.503111 0.717964

O 2.304794 -2.320169 -0.713503

O -3.763161 0.897225 2.188272

O -0.789900 -1.199799 1.832738

H -5.046660 1.416723 0.355054

**MA\_eh\_PC**

C 1.991791 2.228238 -1.304327

C 3.237388 1.523796 -1.170031

C 0.810320 1.724952 -0.836585

C 0.766056 0.458312 -0.193668

C 1.981166 -0.279166 -0.046579

C 3.173484 0.230461 -0.520236

C 1.952604 -1.615895 0.678806

C 4.451940 -0.584124 -0.413145

N 4.335240 2.082585 -1.660804

O 4.472510 -1.701947 -0.986713

O 1.076291 -2.447730 0.318400

N -0.405218 -0.078236 0.264314

C -1.644135 0.583215 0.399999

C -1.719669 1.848126 0.990600

H -0.811644 2.340061 1.325820

C -2.958678 2.453921 1.169643

H -3.015550 3.438160 1.623302

C -4.121718 1.786536 0.794463

H -5.091407 2.247086 0.948723

C -4.059012 0.515990 0.214136

C -5.356010 -0.170908 -0.190398

C -2.811875 -0.086162 -0.003270

C -2.642640 -1.468237 -0.620938

H 2.011467 3.186124 -1.815821

H -0.108540 2.281314 -0.983991

H -0.390659 -1.084702 0.418679

O -5.290498 -1.079945 -1.060409

O -2.774721 -2.452433 0.155202

O -6.416402 0.229301 0.366590

O -2.307024 -1.518163 -1.833556

O 5.415720 -0.058549 0.215661

O 2.785742 -1.791971 1.609046

H 5.137524 1.475768 -1.479535

O 4.067786 0.443144 2.680669

H 3.538931 -0.332378 2.398297

H 4.678422 0.550134 1.930015

**MA\_eh\_RC**

C -3.003617 -0.430057 2.371027

C -3.667484 -0.709956 1.089107

C -1.879402 0.287861 2.449774

C -1.246187 0.943964 1.258209

C -1.857414 0.505246 -0.055480

C -2.985466 -0.220629 -0.136783

C -1.139540 0.982970 -1.307340

C -3.600206 -0.576098 -1.483629

N -4.776925 -1.359785 1.104027

O -3.923212 0.373797 -2.243117

O -0.918782 2.230048 -1.398001

N 0.215981 0.890648 1.286941

C 0.902197 -0.236768 0.818692

C 0.325282 -1.516429 0.856890

H -0.688456 -1.645959 1.219179

C 1.050091 -2.629598 0.441645

H 0.581388 -3.608739 0.470932

C 2.361073 -2.496641 -0.007224

H 2.926717 -3.363052 -0.335198

C 2.947378 -1.228787 -0.050871

C 4.352666 -1.104853 -0.615409

C 2.230532 -0.098654 0.357269

C 2.894406 1.268062 0.358278

H -3.465335 -0.856177 3.257139

H -1.395161 0.465226 3.406839

H -1.478530 2.016496 1.350800

H 0.621478 1.749460 0.927255

O 4.542796 -0.247427 -1.520658

O 3.978119 1.384421 0.988688

O 5.224702 -1.899543 -0.164075

O 2.298260 2.202688 -0.251524

O -3.760797 -1.804456 -1.721006

O -0.809821 0.124979 -2.155936

H -5.112809 -1.512473 0.150475

O 0.134853 3.924775 0.346874

H -0.297477 3.287138 -0.299089

**MA\_eh\_TS**

C 2.885142 -0.449328 -2.369784

C 3.576604 -0.795650 -1.120271

C 1.768741 0.290036 -2.386933

C 1.200070 0.896928 -1.152920

C 1.831758 0.413577 0.123929

C 2.948004 -0.337035 0.143937

C 1.163275 0.882463 1.408341

C 3.591537 -0.746972 1.461618

N 4.667937 -1.472761 -1.196275

O 3.930343 0.173288 2.248850

O 1.002889 2.133962 1.534335

N -0.252710 0.974750 -1.139747

C -1.010358 -0.145903 -0.762443

C -0.503613 -1.450258 -0.872180

H 0.511742 -1.616320 -1.214349

C -1.300244 -2.545205 -0.549279

H -0.885755 -3.545287 -0.633611

C -2.612058 -2.367165 -0.119885

H -3.233496 -3.219217 0.137438

C -3.126414 -1.073231 -0.002718

C -4.534193 -0.907576 0.543603

C -2.340087 0.039099 -0.321948

C -2.933188 1.436242 -0.252581

H 3.311038 -0.848649 -3.285537

H 1.255502 0.515078 -3.317987

H 1.517656 2.007452 -1.226531

H -0.579861 1.810784 -0.660878

O -4.683923 -0.146653 1.538290

O -4.025739 1.629259 -0.847499

O -5.448488 -1.579334 -0.010752

O -2.275223 2.316273 0.374984

O 3.750694 -1.983916 1.647604

O 0.802275 0.010951 2.230664

H 5.028759 -1.672130 -0.260338

O 1.589755 3.456959 -0.718595

H 1.397304 3.127916 0.207972

**MA\_g**

C -4.226388 -2.191469 -1.574395

C -5.630132 -1.893266 -1.250907

C -3.210423 -1.716420 -0.848069

C -3.403549 -0.837540 0.354260

C -4.847231 -0.511777 0.631783

C -5.870298 -1.000113 -0.088491

C -5.078077 0.384182 1.838429

O -5.717575 1.452842 1.657258

O -8.011656 -0.131186 -0.623421

C -7.310163 -0.669118 0.276905

N -6.549873 -2.419875 -1.978294

O -7.700066 -0.975519 1.433750

O -4.589294 -0.018167 2.928744

N -2.646312 0.415442 0.248432

C -1.240698 0.372450 0.232731

C -0.522100 -0.666868 0.844661

H -1.038896 -1.501106 1.305957

C 0.864691 -0.642502 0.896219

H 1.392021 -1.449007 1.397263

C 1.595186 0.398770 0.315727

N 3.001774 0.426372 0.394272

C 0.888222 1.444772 -0.300128

C 1.659315 2.563294 -0.981301

C -0.512835 1.440425 -0.330346

C -1.245707 2.628256 -0.932967

H -4.055587 -2.814275 -2.448132

H -2.182699 -1.941939 -1.124839

H -3.048873 -1.370007 1.246489

H -2.997607 0.986093 -0.518356

O 1.428815 2.760374 -2.203982

O -0.920874 3.773543 -0.524263

O 2.502692 3.191263 -0.281116

O -2.147896 2.383588 -1.785617

C 3.844391 -0.618185 0.015228

C 5.234214 -0.486767 0.244834

C 6.101235 -1.525841 -0.108868

C 5.607930 -2.703935 -0.675771

C 4.241040 -2.826059 -0.913305

C 3.365519 -1.798624 -0.577257

C 5.764668 0.757210 0.933954

O 6.438516 0.591874 1.985940

O 8.135115 -0.328344 -0.404095

C 7.604820 -1.378560 0.051276

O 8.224499 -2.337248 0.591711

O 5.464531 1.874673 0.424211

H 3.421308 1.349952 0.338267

H 6.293119 -3.502221 -0.942985

H 3.847476 -3.726302 -1.376038

H 2.307035 -1.908574 -0.783839

H -7.472617 -2.111622 -1.662844

**MA\_h**

C -2.217696 2.286030 0.971768

C -3.467197 1.596117 0.809869

C -1.028695 1.752042 0.559533

C -0.981089 0.466507 -0.044529

C -2.202397 -0.257182 -0.221953

C -3.401903 0.289638 0.188002

C -2.180246 -1.620584 -0.898676

C -4.701691 -0.485355 0.040520

N -4.575189 2.179146 1.249231

O -4.825660 -1.536755 0.722433

O -1.271432 -2.425464 -0.539738

N 0.199681 -0.095152 -0.441476

C 1.451507 0.550796 -0.530144

C 1.574718 1.775742 -1.194255

H 0.691662 2.247557 -1.614911

C 2.826843 2.363456 -1.335912

H 2.919745 3.315551 -1.848533

C 3.960269 1.717654 -0.846023

H 4.941403 2.164131 -0.970193

C 3.847519 0.492265 -0.184297

C 5.101643 -0.163099 0.373087

C 2.584958 -0.090943 -0.007468

C 2.394662 -1.432015 0.688526

H -2.240136 3.257779 1.456471

H -0.106414 2.298566 0.722449

H 0.171986 -1.105818 -0.568063

O 4.980557 -0.842016 1.427842

O 2.709949 -2.459521 0.030542

O 6.182254 0.038660 -0.247873

O 1.884466 -1.415243 1.839937

O -5.577744 0.013152 -0.718066

O -3.049486 -1.846852 -1.776726

H -5.380177 1.580165 1.053408

**MB\_a**

C -0.010652 2.122703 0.000253

C -1.409843 2.303187 0.000673

C 0.482663 0.835733 -0.000044

C -0.371893 -0.293487 0.000042

C -1.779243 -0.109406 0.000125

C -2.267328 1.229225 0.000580

C 1.928696 0.605217 -0.000788

C 0.219440 -1.599537 0.000237

N 1.694480 -1.749675 0.001687

N 2.455140 -0.774723 0.001379

O -0.376573 -2.666903 -0.001094

O 2.778076 1.467316 -0.002540

N -2.649541 -1.132098 -0.000078

H -2.325885 -2.089165 -0.000570

H 0.665233 2.970195 0.000210

H -1.818155 3.308473 0.001031

H -3.343122 1.380417 0.000836

H -3.641692 -0.939550 0.000177

**MB\_b**

C 0.336588 -2.074669 0.016615

C 1.737758 -2.103984 0.031762

C -0.327504 -0.844298 0.008427

C 0.366574 0.364625 0.004647

C 1.813308 0.358912 0.011552

C 2.454026 -0.926765 0.029499

C -1.797347 -0.816329 -0.023523

C -0.420169 1.590092 -0.025652

N -1.888458 1.532182 0.168551

N -2.506203 0.462285 0.167857

O 0.009076 2.713983 -0.177006

O -2.505636 -1.780622 -0.177228

N 2.596185 1.427056 0.008394

H 2.029691 2.278604 0.002126

H -0.241985 -2.992024 0.013785

H 2.255448 -3.056486 0.043403

H 3.539248 -0.933148 0.040975

**MB\_bc\_RC**

C 3.194739 -0.121783 0.320119

C 3.488623 1.215152 0.622377

C 2.099468 -0.418318 -0.496804

C 1.275684 0.580278 -1.011799

C 1.551131 1.968663 -0.703821

C 2.696338 2.227814 0.126084

C 1.749188 -1.822954 -0.760995

H 3.800280 -0.931209 0.714002

H 4.340239 1.448848 1.251554

C 0.130008 0.153348 -1.802390

H 2.910803 3.267075 0.353767

N 0.047871 -1.244695 -2.283978

N 0.765375 -2.135526 -1.813766

O -0.805196 0.848586 -2.144179

O 2.224856 -2.775152 -0.193005

N 0.851940 3.012438 -1.117273

C -0.137588 1.016489 2.063814

C 0.617135 -0.056737 2.582784

C -1.176692 0.730357 1.203456

C -1.487305 -0.597533 0.820362

C -0.700196 -1.673179 1.311694

C 0.349902 -1.356671 2.222774

C -1.956765 1.816870 0.603856

N -3.158975 1.500460 -0.191390

N -3.430430 0.333983 -0.500206

C -2.574278 -0.805422 -0.096428

O -1.714941 2.997351 0.713275

O -2.911529 -1.871028 -0.589500

N -0.896705 -2.949692 0.943020

H -1.614654 -3.193431 0.274335

H -0.283884 -3.669280 1.302735

H 0.057763 2.705788 -1.685061

H 0.088918 2.043380 2.329519

H 1.434271 0.146938 3.267506

H 0.950873 -2.173188 2.613582

**MB\_bc\_TS**

C -4.070694 -1.326783 0.271313

C -3.398797 -2.549227 0.409685

C -3.361287 -0.215707 -0.167980

C -1.998937 -0.294765 -0.498101

C -1.319910 -1.544598 -0.408616

C -2.059078 -2.651790 0.085506

C -4.031319 1.082704 -0.300808

H -5.123515 -1.233452 0.515323

H -3.935868 -3.419870 0.770196

C -1.343699 0.935882 -0.916769

H -1.534545 -3.596925 0.189185

N -2.004535 2.234120 -0.651542

N -3.209100 2.305097 -0.382353

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C 3.797946 0.516628 -0.184238

C 2.540917 -0.084341 -0.064161

C 1.416912 0.576483 -0.577173

C 1.569099 1.807040 -1.215426

C 4.957447 -0.202717 0.361280

H 4.941837 2.190942 -0.896264

H 2.931715 3.344670 -1.827094

C 2.479947 -1.404717 0.571410

H 0.702768 2.296568 -1.649213

N 3.627368 -1.869012 1.380232

N 4.737946 -1.335954 1.285416

O 1.549622 -2.171306 0.516959

O 6.111180 0.075212 0.151035

N 0.143503 -0.043649 -0.501608

C -0.976409 0.496368 -0.075649

C -1.006551 1.807711 0.535787

C -2.212931 -0.273949 -0.193298

C -3.416718 0.283406 0.191016

C -3.463543 1.652290 0.752790

C -2.177835 2.339141 0.922082

C -2.205156 -1.622470 -0.721521

N -3.416064 -2.328680 -0.840324

N -4.524226 -1.815336 -0.495409

C -4.616210 -0.510174 0.029098

O -1.175290 -2.224933 -1.082107

O -5.759318 -0.116468 0.326922

N -4.518584 2.283254 1.120032

H -5.347174 1.702086 0.962021

H -0.075396 2.334736 0.704902

H -2.214876 3.314470 1.396717

H 0.067137 -1.032031 -0.802165

**MC\_a**

C 0.160351 2.114264 -0.011664

C -1.199015 2.417921 -0.022633

C 0.556309 0.776477 0.002054

C -0.404813 -0.257782 0.010791

C -1.791877 0.058506 0.015018

C -2.159374 1.414075 -0.008893

C 2.004051 0.439718 0.007031

C 0.071329 -1.638116 -0.007032

N 1.406092 -1.782830 -0.006711

N 2.392979 -0.821129 0.004304

O -0.671680 -2.659077 -0.028713

O 2.869796 1.386716 0.015093

N -2.764397 -0.906281 0.088148

H -2.483088 -1.854947 -0.122855

H 0.910586 2.895463 -0.017921

H -1.520643 3.455126 -0.040760

H -3.216557 1.664686 -0.012805

H -3.697111 -0.626578 -0.183257

H 1.757392 -2.733560 -0.021662

**MC\_b**

C -0.127130 -2.091936 0.000361

C -1.510331 -2.270612 0.000453

C 0.428126 -0.793463 0.000072

C -0.400503 0.329578 -0.000012

C -1.845907 0.166948 -0.000269

C -2.351419 -1.173375 0.000103

C 1.902934 -0.646159 -0.000170

C 0.228752 1.646923 0.000275

N 1.573363 1.625544 0.000046

N 2.437667 0.565161 -0.000309

O -0.383762 2.750233 0.000802

O 2.645569 -1.686639 -0.000394

N -2.730533 1.154867 -0.000954

H -2.225553 2.045268 -0.001147

H 0.543358 -2.943317 0.000478

H -1.925419 -3.273103 0.000783

H -3.430041 -1.295012 0.000056

H 2.032591 2.531003 0.000206

**MC\_e**

C -2.184735 2.373003 0.024610

C -0.889627 2.461162 0.515996

C -2.815611 1.126763 -0.009308

C -2.146974 -0.029538 0.445064

C -0.816687 0.066913 0.953213

C -0.213532 1.332915 0.974855

C -4.201160 1.032419 -0.538766

H -2.714563 3.248628 -0.330207

H -0.387756 3.423509 0.552802

C -2.866571 -1.303041 0.362073

H 0.786079 1.447852 1.375427

N -4.103840 -1.229334 -0.152191

N -4.809474 -0.136294 -0.601656

O -2.413787 -2.423115 0.730361

O -4.796680 2.097308 -0.933749

N -0.167480 -1.056943 1.445777

C 1.288973 -1.215090 1.331182

C 2.017300 -0.562795 2.468488

C 1.830179 -0.839007 -0.030526

C 2.861337 0.039573 -0.198698

C 3.552798 0.649091 0.973532

C 3.059707 0.254038 2.301566

C 1.204856 -1.505930 -1.186100

N 1.582662 -1.168128 -2.412800

N 2.569525 -0.242176 -2.524350

C 3.272447 0.377643 -1.559833

O 0.320017 -2.413016 -1.007364

O 4.190465 1.185133 -1.870750

N 4.530003 1.479302 0.909704

H 4.753013 1.668796 -0.069996

H 1.448882 -2.297236 1.432643

H 1.655054 -0.807183 3.463846

H 3.574757 0.695617 3.149720

H -0.655087 -1.901687 1.163040

H -4.612228 -2.104038 -0.219303

H 2.825754 -0.018434 -3.481435

**MC\_eh\_PC**

C -3.805160 1.865928 0.856390

C -2.596398 2.410343 1.263766

C -3.812635 0.662468 0.142781

C -2.603872 0.021471 -0.187956

C -1.367465 0.620467 0.177829

C -1.389209 1.794231 0.937380

C -5.111746 0.070589 -0.270179

H -4.746558 2.344560 1.098572

H -2.580322 3.320732 1.854602

C -2.681999 -1.268007 -0.882824

H -0.458608 2.217591 1.297751

N -3.925149 -1.671658 -1.186365

N -5.137427 -1.072445 -0.928769

O -1.693739 -1.989741 -1.177640

O -6.199047 0.685513 0.014107

N -0.165891 -0.006966 -0.149080

C 1.070314 0.562080 -0.259375

C 1.205071 1.935720 -0.611944

C 2.259065 -0.230116 -0.105981

C 3.518609 0.380822 -0.226013

C 3.658447 1.801500 -0.536829

C 2.425704 2.518767 -0.746316

C 2.185018 -1.679042 0.194919

N 3.284050 -2.381101 0.382746

N 4.472112 -1.730534 0.271794

C 4.707623 -0.437334 -0.018493

O 1.046696 -2.285001 0.273349

O 5.899703 -0.030934 -0.083699

N 4.783124 2.470975 -0.657957

H 5.565383 1.836013 -0.495481

H -0.635721 -0.790040 2.481921

H 0.310657 2.513456 -0.815779

H 2.505805 3.561390 -1.038460

H -0.183791 -1.027957 -0.219842

O -0.349658 -1.707954 2.577042

H 0.161192 -1.908071 1.761065

H 5.287377 -2.315855 0.423024

H -4.000976 -2.564122 -1.662145

**MC\_eh\_RC**

C -2.209534 -2.531935 -0.506611

C -0.900961 -2.506569 -0.995888

C -2.831718 -1.327015 -0.221338

C -2.166313 -0.094562 -0.412628

C -0.832250 -0.068777 -0.908123

C -0.227213 -1.313562 -1.193027

C -4.213631 -1.342990 0.306158

H -2.736344 -3.465988 -0.352089

H -0.397713 -3.438274 -1.234024

C -2.883282 1.119164 -0.072926

H 0.775162 -1.340200 -1.600816

N -4.181522 0.942370 0.432060

N -4.855442 -0.160321 0.629548

O -2.487250 2.279266 -0.177486

O -4.843877 -2.390964 0.482648

N -0.175311 1.115018 -1.131884

C 1.285881 1.234285 -1.029677

C 1.983130 0.823058 -2.290950

C 1.844345 0.587531 0.217929

C 2.890565 -0.288505 0.186927

C 3.573006 -0.628771 -1.094756

C 3.039346 0.007205 -2.308858

C 1.225419 0.988123 1.494306

N 1.622650 0.405452 2.618219

N 2.624063 -0.506676 2.522826

C 3.321695 -0.900332 1.442386

O 0.327186 1.899088 1.517738

O 4.248801 -1.746236 1.565449

N 4.574780 -1.422469 -1.214348

H 4.825408 -1.796646 -0.296475

H 1.447462 2.316075 -0.914202

H 1.593155 1.252982 -3.209880

H 3.540059 -0.249181 -3.237897

H -0.642187 1.920920 -0.728247

O 0.073217 4.352901 -0.322905

H 0.172222 3.616659 0.297793

H 2.893732 -0.925856 3.407808

H -4.671011 1.805353 0.671997

**MC\_eh\_TS**

C -2.557631 2.359966 0.600160

C -1.226926 2.410097 1.031028

C -3.098711 1.129617 0.266261

C -2.335796 -0.058088 0.361080

C -0.986610 -0.008733 0.815153

C -0.457503 1.265714 1.133748

C -4.496558 1.066972 -0.212457

H -3.158171 3.258181 0.520431

H -0.783546 3.366152 1.291077

C -2.962543 -1.300357 -0.037640

H 0.566899 1.344170 1.479522

N -4.288347 -1.196634 -0.492160

N -5.054104 -0.141433 -0.592286

O -2.473218 -2.430964 -0.025962

O -5.214516 2.069231 -0.299266

N -0.236529 -1.140224 0.960945

C 1.222096 -1.103015 0.921773

C 1.830591 -0.753975 2.216024

C 1.814078 -0.410487 -0.248955

C 2.946061 0.364529 -0.141140

C 3.616953 0.573379 1.171686

C 2.958232 -0.033467 2.328913

C 1.219813 -0.683193 -1.579051

N 1.703764 -0.069077 -2.649001

N 2.776207 0.747713 -2.468076

C 3.469618 1.002807 -1.344190

O 0.262201 -1.525383 -1.703980

O 4.475373 1.766157 -1.396787

N 4.707734 1.237262 1.359952

H 5.033787 1.612881 0.468866

H 1.508576 -2.285771 0.734351

H 1.345212 -1.156273 3.102812

H 3.416696 0.152378 3.295885

H -0.628764 -1.947530 0.491776

O 1.716101 -3.704510 0.486557

H 1.180351 -3.843442 -0.306200

H 3.116895 1.187312 -3.317086

H -4.717517 -2.078149 -0.775908

**MC\_g**

C -5.198384 -1.764469 -2.306464

C -6.241601 -1.392532 -1.338729

C -3.897210 -1.606587 -2.055609

C -3.371196 -1.022507 -0.778387

C -4.438438 -0.779653 0.258036

C -5.769900 -0.910423 -0.009099

C -3.962113 -0.383799 1.595518

N -4.849506 -0.092660 2.538524

N -6.162840 -0.196946 2.206477

C -6.725033 -0.587900 1.048816

N -7.470178 -1.514636 -1.688948

O -7.981001 -0.644128 0.945806

O -2.708292 -0.339409 1.845708

N -2.674177 0.244644 -1.054658

C -1.298636 0.323527 -0.885868

C -0.483104 -0.760547 -1.233748

H -0.926643 -1.656925 -1.655470

C 0.890851 -0.702135 -1.079066

H 1.488056 -1.557524 -1.378367

C 1.537635 0.434188 -0.580298

N 2.934543 0.437379 -0.448144

C 0.754520 1.579240 -0.307225

C 1.371413 2.883866 0.063165

C -0.659791 1.503087 -0.424697

C -1.446876 2.657435 0.020880

H -5.551212 -2.159361 -3.254823

H -3.150811 -1.864569 -2.803491

H -2.653963 -1.722532 -0.330729

H -3.144198 1.060586 -0.668715

N 0.620691 3.895371 0.455502

N -0.739326 3.704868 0.459643

O 2.642920 3.046063 -0.026341

O -2.709854 2.709823 0.042765

C 3.706247 -0.583769 0.063365

C 5.132453 -0.507088 -0.004262

C 5.922390 -1.569239 0.485789

C 5.327912 -2.690569 1.068595

C 3.943761 -2.737311 1.178581

C 3.144090 -1.709853 0.689547

C 5.829968 0.653802 -0.559103

N 7.169856 0.555234 -0.593283

N 7.990527 -0.462743 -0.163246

C 7.404474 -1.512124 0.378338

O 8.104559 -2.497209 0.811055

O 5.275092 1.704866 -0.980241

H 3.368328 1.357029 -0.491975

H 5.950022 -3.496268 1.438018

H 3.467018 -3.586128 1.660050

H 2.070279 -1.774561 0.814084

H -8.075215 -1.218056 -0.920018

H -6.802750 0.039319 2.958964

H -1.270822 4.504847 0.784497

H 7.666783 1.352676 -0.973565

**MC\_h**

C -3.826661 1.878008 0.776068

C -2.622108 2.470761 1.123734

C -3.828972 0.590305 0.229292

C -2.618036 -0.093688 0.007562

C -1.385697 0.540761 0.321176

C -1.414694 1.809553 0.907311

C -5.125589 -0.043194 -0.126301

H -4.769022 2.388545 0.934446

H -2.610711 3.455069 1.581061

C -2.693349 -1.454675 -0.536256

H -0.486725 2.273852 1.221584

N -3.934776 -1.883889 -0.814174

N -5.148224 -1.255437 -0.645915

O -1.706142 -2.207789 -0.734225

O -6.214100 0.603332 0.071355

N -0.174347 -0.121740 0.112974

C 1.041195 0.440100 -0.143513

C 1.147563 1.756609 -0.680439

C 2.245626 -0.316082 0.057876

C 3.493011 0.298607 -0.139037

C 3.604874 1.675500 -0.613174

C 2.356707 2.335241 -0.906966

C 2.193133 -1.738946 0.470886

N 3.307042 -2.397148 0.739730

N 4.481719 -1.726161 0.590665

C 4.695010 -0.469401 0.160896

O 1.069799 -2.359118 0.555502

O 5.880881 -0.046581 0.062420

N 4.716390 2.348593 -0.814116

H 5.510062 1.754145 -0.572919

H 0.241819 2.291968 -0.941568

H 2.415052 3.332259 -1.333020

H -0.150614 -1.145478 0.209592

H -4.007374 -2.822416 -1.191251

H 5.307300 -2.272966 0.812832

**MCAC\_e**

C -3.940815 1.610331 0.842563

C -2.870225 2.471746 1.048256

C -3.726524 0.410717 0.159091

C -2.441330 0.074697 -0.313669

C -1.346926 0.966177 -0.106311

C -1.595023 2.165418 0.580305

C -4.866380 -0.517751 -0.060022

H -4.934189 1.853002 1.199388

H -3.024599 3.410085 1.572856

C -2.276631 -1.214846 -0.982853

H -0.791260 2.879015 0.726530

N -3.394415 -1.948280 -1.095581

N -4.675999 -1.668314 -0.677159

O -1.185906 -1.663440 -1.437425

O -6.033903 -0.188763 0.356401

N -0.093302 0.678545 -0.600918

C 1.119154 1.172054 0.056969

C 1.763850 2.273826 -0.730876

C 2.040858 0.016101 0.350302

C 3.342069 0.011421 0.017651

C 3.950763 1.155871 -0.711018

C 3.056659 2.268069 -1.066361

C 1.392396 -1.139214 1.104798

O 1.652296 -2.308478 0.719826

O 4.475943 -1.340946 1.614618

C 4.265972 -1.139688 0.390519

O 0.624206 -0.821175 2.053150

O 4.786259 -1.773051 -0.567734

N 5.188487 1.233758 -1.047570

H 5.691543 0.388080 -0.768486

H 0.832528 1.579280 1.037496

H 1.115743 3.097742 -1.020987

H 3.500509 3.082682 -1.631426

H -0.025209 -0.253818 -1.002535

H -3.296825 -2.848782 -1.550996

**MCAC\_eh\_PC**

C -3.910846 -2.061641 0.553413

C -2.723197 -2.725592 0.826324

C -3.877192 -0.705676 0.214107

C -2.647881 -0.023560 0.122927

C -1.432772 -0.721973 0.364153

C -1.498367 -2.066313 0.742868

C -5.150959 0.009487 -0.057620

H -4.865162 -2.570743 0.613675

H -2.739734 -3.769883 1.122075

C -2.684517 1.401126 -0.211045

H -0.586236 -2.594563 0.997011

N -3.905016 1.904027 -0.432758

N -5.134876 1.290283 -0.378952

O -1.671207 2.151923 -0.286074

O -6.259231 -0.627616 0.020306

N -0.210788 -0.058579 0.287814

C 1.007338 -0.595994 -0.067928

C 1.120774 -1.807557 -0.798693

C 2.197414 0.114248 0.265735

C 3.437681 -0.383672 -0.076825

C 3.572258 -1.634723 -0.794232

C 2.348024 -2.299514 -1.148406

C 2.096665 1.415719 1.046755

O 2.675286 1.472496 2.157392

O 5.566561 -0.174925 0.958733

C 4.688248 0.408812 0.267148

O 1.412688 2.342607 0.521258

O 4.761734 1.580820 -0.187813

N 4.719253 -2.184959 -1.164264

H 5.495520 -1.607669 -0.833237

H 0.224549 -2.329758 -1.113417

H 2.423955 -3.213319 -1.730196

H -0.262219 0.959469 0.328826

H -3.947165 2.890725 -0.664443

O 0.528863 2.167036 -2.101254

H 1.000051 2.230564 -1.243725

H -0.397150 2.111972 -1.811905

**MCAC\_eh\_RC**

C -2.386140 -2.497360 -0.289790

C -1.025273 -2.491077 -0.617265

C -3.022137 -1.282250 -0.105267

C -2.326611 -0.056191 -0.236197

C -0.935613 -0.047175 -0.558729

C -0.318461 -1.312108 -0.750147

C -4.460697 -1.277554 0.241931

H -2.937251 -3.423753 -0.182673

H -0.505795 -3.431598 -0.771503

C -3.069374 1.164334 -0.026680

H 0.731177 -1.362639 -1.007688

N -4.429034 1.008935 0.300180

N -5.131550 -0.084539 0.440831

O -2.652074 2.319397 -0.102424

O -5.115389 -2.318682 0.369316

N -0.225603 1.100952 -0.684922

C 1.218723 1.159379 -0.882616

C 1.661740 0.725436 -2.249956

C 1.997981 0.507730 0.236565

C 3.106773 -0.224567 0.033955

C 3.596785 -0.497603 -1.341734

C 2.769841 0.006193 -2.450942

C 1.442528 0.781145 1.625170

O 1.023893 -0.208335 2.280885

O 4.175556 -0.051857 2.155096

C 3.855124 -0.824483 1.215275

O 1.409913 1.987332 1.983771

O 4.099602 -2.061615 1.158094

N 4.672481 -1.140293 -1.630171

H 5.130112 -1.461705 -0.774329

H 1.432415 2.236470 -0.810551

H 1.056816 1.069840 -3.085192

H 3.097949 -0.255318 -3.452965

H -0.648118 2.017672 -0.516203

H -4.937682 1.880925 0.449119

O -0.205897 4.009145 -0.539970

H -1.139648 4.128530 -0.329026

**MCAC\_eh\_TS**

C -2.749495 2.321994 0.471447

C -1.388184 2.427252 0.787825

C -3.268417 1.068373 0.198440

C -2.454070 -0.088223 0.236735

C -1.071000 0.018497 0.565801

C -0.567536 1.317286 0.836205

C -4.702144 0.939687 -0.141371

H -3.388612 3.196074 0.435465

H -0.962225 3.403099 0.998948

C -3.061508 -1.359263 -0.077200

H 0.481166 1.440903 1.081395

N -4.429428 -1.321119 -0.395723

N -5.243973 -0.298773 -0.438500

O -2.519771 -2.467231 -0.098996

O -5.466686 1.910412 -0.175905

N -0.263924 -1.069732 0.629851

C 1.176244 -1.010177 0.813499

C 1.615709 -0.627418 2.168561

C 1.913903 -0.327580 -0.276757

C 3.074670 0.340356 -0.073205

C 3.620151 0.502347 1.293182

C 2.774831 0.016822 2.388824

C 1.303136 -0.482661 -1.660222

O 0.865384 0.561075 -2.213487

O 4.011425 0.244727 -2.263557

C 3.812292 0.961707 -1.245741

O 1.242606 -1.653207 -2.122104

O 4.177914 2.165743 -1.121452

N 4.762957 1.033764 1.585425

H 5.221436 1.357988 0.732372

H 1.507231 -2.185466 0.719855

H 0.997170 -0.955201 3.001736

H 3.123612 0.218185 3.397870

H -0.660560 -1.954712 0.338607

H -4.848139 -2.225442 -0.615400

O 1.787345 -3.624046 0.618786

H 1.792266 -3.918203 1.539381

**MCAC\_g**

C 5.295829 -1.116680 2.552817

C 6.331226 -0.893234 1.532167

C 3.992533 -1.117108 2.264910

C 3.457293 -0.872331 0.884906

C 4.527272 -0.820495 -0.173527

C 5.857671 -0.780143 0.123123

C 4.053629 -0.811715 -1.568923

N 4.936667 -0.686253 -2.551682

N 6.245552 -0.593192 -2.197776

C 6.809286 -0.646707 -0.977566

N 7.556230 -0.824416 1.908536

O 8.062757 -0.569547 -0.858491

O 2.807461 -0.947493 -1.824251

N 2.702706 0.392331 0.862930

C 1.309674 0.366766 0.762404

C 0.562632 -0.696602 1.294207

H 1.064054 -1.521442 1.790001

C -0.823521 -0.695844 1.229372

H -1.379053 -1.523147 1.661344

C -1.514639 0.359023 0.628040

N -2.926582 0.375364 0.568884

C -0.782322 1.448363 0.132613

C -1.538389 2.593772 -0.521822

C 0.616597 1.461431 0.200720

C 1.375693 2.678743 -0.303401

H 5.654533 -1.257517 3.568393

H 3.249917 -1.251382 3.048319

H 2.783580 -1.692448 0.604804

H 3.098209 1.069674 0.215950

O -1.325502 2.799156 -1.746189

O 0.953573 3.810080 0.051070

O -2.354636 3.226671 0.203402

O 2.393476 2.474008 -1.027548

C -3.728921 -0.628102 0.084725

C -5.151453 -0.489773 0.119615

C -5.976113 -1.535224 -0.346057

C -5.419128 -2.705783 -0.864475

C -4.035000 -2.818517 -0.932482

C -3.199998 -1.806469 -0.471088

C -5.803455 0.722194 0.610274

N -7.145913 0.696540 0.602156

N -8.003374 -0.297746 0.187252

C -7.455127 -1.399420 -0.287188

O -8.190523 -2.367103 -0.698398

O -5.202694 1.756590 1.017740

H -3.390425 1.263211 0.742933

H -6.068418 -3.498953 -1.214103

H -3.585931 -3.711580 -1.357361

H -2.126482 -1.925324 -0.552848

H 8.154303 -0.664375 1.094722

H 6.883133 -0.491608 -2.981683

H -7.613350 1.530733 0.938581

**MCAC\_h**

C -3.857727 1.892149 -0.730254

C -2.657744 2.508511 -1.056150

C -3.843446 0.593328 -0.212552

C -2.623253 -0.076951 -0.000240

C -1.395879 0.580280 -0.291990

C -1.440721 1.863128 -0.848290

C -5.129612 -0.071188 0.123802

H -4.805650 2.393532 -0.883664

H -2.658063 3.503439 -1.490396

C -2.678535 -1.450933 0.505298

H -0.519047 2.350648 -1.144875

N -3.910805 -1.911513 0.765899

N -5.133686 -1.297864 0.610466

O -1.674953 -2.192225 0.687261

O -6.228415 0.562320 -0.057653

N -0.186299 -0.073997 -0.087291

C 1.042985 0.494699 0.162289

C 1.181612 1.795480 0.714056

C 2.218904 -0.271234 -0.091558

C 3.469738 0.254264 0.160382

C 3.629550 1.586423 0.706459

C 2.419429 2.312904 0.978648

C 2.085223 -1.665563 -0.687093

O 2.716087 -1.903684 -1.747950

O 4.815890 -1.668765 0.520589

C 4.711784 -0.580816 -0.104827

O 1.329319 -2.471025 -0.075724

O 5.558108 -0.105244 -0.910329

N 4.788617 2.161641 0.992279

H 5.553462 1.532915 0.737308

H 0.296180 2.368028 0.965957

H 2.515272 3.296400 1.429037

H -0.240270 -1.089438 0.003273

H -3.968798 -2.861304 1.116462

**MCBC\_e**

C -3.864546 1.397679 0.718040

C -3.027844 2.481137 0.957330

C -3.375087 0.287608 0.024142

C -2.043047 0.272541 -0.435824

C -1.217150 1.408903 -0.244989

C -1.721008 2.494215 0.470934

C -4.255780 -0.884302 -0.211874

H -4.889777 1.395905 1.068777

H -3.398534 3.340461 1.507497

C -1.532935 -0.977130 -1.006917

H -1.086530 3.362614 0.624640

N -2.432246 -1.963065 -1.108998

N -3.767323 -1.975668 -0.775226

O -0.331403 -1.178846 -1.346920

O -5.487101 -0.826295 0.132267

N 0.075514 1.484830 -0.794642

C 1.221186 1.627936 0.123358

C 2.265831 2.517617 -0.479236

C 1.761404 0.256569 0.432448

C 3.004794 -0.165870 0.127370

C 4.003462 0.762876 -0.474386

C 3.514463 2.123404 -0.744169

C 0.848508 -0.701953 1.090806

N 1.104406 -2.143347 0.961379

N 2.243051 -2.532200 0.679190

C 3.333895 -1.560173 0.465282

O -0.101799 -0.384636 1.761568

O 4.447466 -2.017844 0.564189

N 5.212951 0.465657 -0.771368

H 5.424380 -0.505324 -0.537165

H 0.857852 2.079361 1.054330

H 1.941514 3.527778 -0.713579

H 4.235230 2.801443 -1.191018

H 0.240896 0.700722 -1.421617

H -2.093663 -2.841777 -1.486933

**MCBC\_eh\_PC**

C -3.901744 1.733620 0.804298

C -2.755894 2.309436 1.326628

C -3.822808 0.534009 0.081793

C -2.579231 -0.078651 -0.126208

C -1.418108 0.548703 0.371269

C -1.507209 1.716124 1.116390

C -5.055924 -0.081887 -0.470808

H -4.872755 2.190737 0.956314

H -2.817902 3.221680 1.910008

C -2.539298 -1.359518 -0.842871

H -0.612106 2.149584 1.551761

N -3.732136 -1.786077 -1.277364

N -4.979362 -1.218819 -1.139979

O -1.495276 -2.032748 -1.030945

O -6.178494 0.503521 -0.296752

N -0.151898 -0.064335 0.179588

C 0.973556 0.518224 -0.146714

C 1.013617 1.889940 -0.614366

C 2.219238 -0.254876 -0.076230

C 3.424031 0.349028 -0.366996

C 3.473425 1.767661 -0.796379

C 2.187051 2.461350 -0.924971

C 2.220839 -1.641588 0.349935

N 3.432229 -2.337428 0.441879

N 4.546050 -1.782986 0.171480

C 4.632797 -0.442272 -0.234309

O 1.189146 -2.279556 0.651004

O 5.778226 -0.005814 -0.460635

N 4.532545 2.433939 -1.077557

H 5.359824 1.842064 -0.959801

H -0.273547 -0.339305 3.063018

H 0.081821 2.424305 -0.752544

H 2.226811 3.476292 -1.307273

H -0.103771 -1.085145 0.326727

H -3.738844 -2.673034 -1.770631

O 0.604055 -0.717423 3.210152

H 0.651186 -1.476894 2.610746

**MCBC\_eh\_RC**

C -2.044535 -2.525824 -0.504800

C -0.748659 -2.512315 -0.998823

C -2.705909 -1.313255 -0.286475

C -2.065460 -0.088698 -0.564702

C -0.738043 -0.082128 -1.081519

C -0.100784 -1.310915 -1.287221

C -4.087425 -1.326184 0.259287

H -2.551122 -3.457110 -0.282489

H -0.224172 -3.446846 -1.173050

C -2.801076 1.139304 -0.271880

H 0.904272 -1.333559 -1.695385

N -4.022164 0.970132 0.242465

N -4.709234 -0.188335 0.516509

O -2.368773 2.315710 -0.477271

O -4.666470 -2.445276 0.479109

N -0.089007 1.114277 -1.374505

C 1.345587 1.249598 -1.130648

C 2.195713 0.865193 -2.308931

C 1.802423 0.555551 0.130357

C 2.942851 -0.152736 0.236415

C 3.841359 -0.357748 -0.935955

C 3.331600 0.167860 -2.210091

C 0.970371 0.700155 1.343921

N 1.094496 -0.305818 2.413383

N 2.141975 -0.952363 2.513637

C 3.251051 -0.716358 1.564410

O 0.157213 1.569526 1.523019

O 4.341902 -1.046109 1.956850

N 4.968777 -0.964094 -0.910033

H 5.200149 -1.281145 0.032522

H 1.509101 2.324541 -0.960716

H 1.848561 1.226876 -3.272782

H 3.931722 -0.055138 -3.086951

H -0.619795 1.916663 -1.049959

H -4.541236 1.816270 0.452586

O -0.730848 4.036078 0.897046

H -1.349965 3.384431 0.475930

**MCBC\_eh\_TS**

C -2.341500 2.147692 1.106044

C -1.053025 2.095664 1.616983

C -2.900539 0.998946 0.536018

C -2.165384 -0.201093 0.482514

C -0.850013 -0.250259 1.020737

C -0.312663 0.913539 1.579877

C -4.271983 1.058822 -0.032763

H -2.920715 3.062558 1.137285

H -0.608576 2.980995 2.061160

C -2.786637 -1.355524 -0.170753

H 0.683869 0.894566 2.009955

N -4.019818 -1.142178 -0.649417

N -4.796276 -0.005908 -0.611257

O -2.245526 -2.489431 -0.306010

O -4.933387 2.153062 0.040697

N -0.112932 -1.436233 0.997055

C 1.317203 -1.372259 0.741704

C 2.175864 -1.338380 1.957873

C 1.718302 -0.350864 -0.279978

C 2.827418 0.409604 -0.193207

C 3.733603 0.314813 0.985265

C 3.284442 -0.591746 2.049972

C 0.903014 -0.237343 -1.507503

N 0.962927 1.009491 -2.283810

N 1.966503 1.724391 -2.197419

C 3.088659 1.330173 -1.316559

O 0.169855 -1.096884 -1.925434

O 4.148054 1.840896 -1.578937

N 4.828953 0.961934 1.135135

H 5.023925 1.555985 0.327523

H 1.556823 -2.387317 0.235681

H 1.865686 -1.982250 2.775544

H 3.898576 -0.609541 2.944992

H -0.584811 -2.148471 0.440734

H -4.465355 -1.929485 -1.108231

O 1.451992 -3.588120 -0.690659

H 0.816595 -3.204408 -1.331236

**MCBC\_g**

C 5.285538 -0.492292 2.691762

C 6.279289 -0.531191 1.606711

C 3.975720 -0.623756 2.475708

C 3.392720 -0.801842 1.104437

C 4.425443 -0.997822 0.020859

C 5.759918 -0.835895 0.243466

C 3.905379 -1.373841 -1.302498

N 4.752310 -1.503919 -2.315394

N 6.068139 -1.293356 -2.051504

C 6.672073 -0.990083 -0.887876

N 7.509149 -0.317269 1.900373

O 7.924316 -0.854211 -0.842415

O 2.653360 -1.584887 -1.461734

N 2.596892 0.382150 0.773012

C 1.279804 0.432049 0.526996

C 0.423809 -0.691540 0.801500

H 0.830750 -1.575795 1.275742

C -0.907023 -0.659054 0.540916

H -1.509946 -1.514432 0.820858

C -1.550587 0.499662 -0.015205

N -2.887903 0.514365 -0.253879

C -0.751841 1.641339 -0.221638

C -1.317722 2.861775 -0.711909

C 0.659020 1.607924 0.032669

C 1.425019 2.773339 -0.257636

H 5.680972 -0.335960 3.691126

H 3.261795 -0.568261 3.293357

H 2.742974 -1.678950 1.092500

H 3.120010 1.238238 0.595562

N -0.441255 3.955265 -1.094232

N 0.786223 3.917548 -0.884904

O -2.519292 3.096949 -0.868380

O 2.638787 2.923847 -0.055686

C -3.745147 -0.588331 -0.360351

C -5.104981 -0.461599 0.024437

C -5.956857 -1.577400 -0.062133

C -5.477952 -2.795816 -0.557489

C -4.164209 -2.890470 -0.989663

C -3.304112 -1.795158 -0.902992

C -5.680125 0.805954 0.487809

N -6.966995 0.739147 0.856076

N -7.836708 -0.327772 0.841679

C -7.370442 -1.474835 0.383659

O -8.122704 -2.508668 0.325383

O -5.061553 1.903039 0.530972

H -3.339286 1.429043 -0.286006

H -6.149273 -3.644510 -0.614256

H -3.794369 -3.819097 -1.412209

H -2.291043 -1.877300 -1.281808

H 8.078110 -0.375212 1.052460

H 6.677179 -1.401432 -2.857157

H -7.386541 1.605279 1.176877

**MCBC\_h**

C 3.908502 1.759333 -0.774215

C 2.788516 2.388481 -1.290763

C 3.792670 0.502419 -0.163058

C 2.537980 -0.115961 -0.063043

C 1.402283 0.560346 -0.555652

C 1.529384 1.789108 -1.186913

C 4.998268 -0.168285 0.387074

H 4.887109 2.220171 -0.843680

H 2.879284 3.348803 -1.786708

C 2.460781 -1.450056 0.545857

H 0.655550 2.268542 -1.616386

N 3.632504 -1.922654 0.990140

N 4.886931 -1.357401 0.951927

O 1.405966 -2.125319 0.641718

O 6.131067 0.419060 0.312314

N 0.124503 -0.057098 -0.465778

C -0.995886 0.492453 -0.069585

C -1.031333 1.821554 0.509278

C -2.240504 -0.277783 -0.174299

C -3.442057 0.295857 0.183623

C -3.489259 1.681677 0.708868

C -2.201809 2.365455 0.875257

C -2.241330 -1.639771 -0.675373

N -3.454038 -2.332844 -0.796112

N -4.564670 -1.803379 -0.469592

C -4.648289 -0.494852 0.031442

O -1.211824 -2.258615 -1.011457

O -5.789848 -0.084534 0.320325

N -4.545957 2.325980 1.045228

H -5.373790 1.742462 0.894073

H -0.099409 2.346706 0.677503

H -2.237872 3.349176 1.332331

H 0.071012 -1.063326 -0.694200

H 3.612822 -2.845331 1.412183

**HO– Oxidation**

**1M-OH anion**

 H -2.16116901511835 0.10496764460614 0.24253157246660

 O -1.27521685332718 0.44157738330711 0.42089391644567

 H -0.62822002163050 3.31635922640150 0.52622472958561

 H -1.38784104369906 2.02188026686568 0.06663288613036

 O -1.41445656352094 3.02558562664214 -0.00219659942496

 H 1.02667631098851 -0.31621409073208 -1.18038750701117

 H -0.37108630846903 0.27344100086784 -0.88908291692235

 O 0.31079068648785 0.16090536000787 -1.63053592567337

 H -0.33917793946762 -1.57513077331942 2.55222903217478

 H -0.62616085462366 -0.89540980883515 1.14490825617825

 O -0.35351960983852 -1.75546282151407 1.59043947490989

 H 2.23518068272598 -0.08569840901840 0.80272217534839

 H 3.06037867383754 0.05505428611409 -0.53871027943859

 O 2.60658837033109 -0.60156797487873 0.04115233216662

 H -3.43867873413384 -1.49866779697035 -2.54196705735620

 H -2.34820251688597 -1.67483106578273 -1.46854512263305

 O -3.10046953644909 -1.09965596413486 -1.71527209387194

 H -1.32734028691382 -3.45659472657492 -2.16517030895382

 H -0.82310962804053 -3.56364466196948 -0.71621062221098

 O -0.91166279157679 -2.91721730851745 -1.44928417727152

 H -1.92990739625124 -2.59922549283874 1.44274857270894

 H -2.68065084365240 -3.80302146881025 2.02035071608456

 O -2.82965409966542 -3.00119221936934 1.49030340639138

 H 1.15184192986511 -2.68275801833695 1.36690477867661

 H 2.07788342304642 -3.57938638454973 2.24559124270396

 O 1.77519782529020 -3.44618529229462 1.32044478770706

 H -0.92723288307731 2.41020251946464 2.80803926356589

 H -1.01490165030324 1.10049808087646 1.90476604722837

 O -0.70383117503089 1.45250559219977 2.79192818587415

 H 2.55704273029016 1.54332750113956 2.11355829225633

 H 1.07155657559192 1.13409756640931 2.47483061461208

 O 1.96545000471190 0.76921339644433 2.28901435519824

 H 2.03591638452408 -2.25054792436396 -0.96344143850957

 H 0.76585002445169 -2.67280295831897 -1.75004988513060

 O 1.75744565576169 -2.69823337762484 -1.77905310836110

 H -4.09288607265398 0.98071731664302 1.77686087674510

 H -3.21138996671066 2.13008032295302 1.21923479333898

 O -4.12999320886679 1.90802892136167 1.42643382891974

 H 0.57268406299876 -0.17243391354643 -4.62998239373096

 H -0.10061024968418 -0.59574976157771 -3.31417678725236

 O -0.12313767554914 -0.78365404075293 -4.27526030984455

 H -1.73775756686824 -0.55717944609463 4.78433197905289

 H -1.76602087143633 0.69809444410059 3.91702235599327

 O -2.31259749333082 0.20220522849979 4.57797986923037

 H -3.55577765347889 -0.41360166848638 3.34540292575751

 H -3.78185302790051 -1.40704923876334 2.18505089707337

 O -4.12289619328048 -0.57724378328085 2.56343116361044

 H 2.00320461534169 -2.95781858271206 -4.88126612352998

 H 0.59466136338812 -2.38232099138841 -4.78397089373430

 O 1.08747437457404 -3.17378890376413 -5.09291216772140

 H -3.68359316692765 1.67546524255862 -2.52379298710307

 H -2.57331830777196 0.66747853996097 -2.57833429981966

 O -2.87055675277982 1.47425493973028 -3.03895963276700

 H -1.59893478836274 2.86245290441077 -3.00707145005544

 H -1.05859553696490 3.35402344640950 -1.67591673589314

 O -0.94321264391601 3.49573989569101 -2.64866875558751

 H 2.68684767299685 -1.72040975233652 -2.96845383004248

 H 4.19823120014225 -1.79188502924711 -3.16239062628796

 O 3.41050881785938 -1.29647470186588 -3.48286599953925

 H 2.77570763666864 -0.42011771667682 3.43800827039028

 H 4.02994068349830 -1.22379762587695 3.12622767471843

 O 3.36310516328654 -1.10076123153385 3.83316515402514

 H 5.02307160519391 -2.34943668316666 1.18584582817958

 H 4.02105995786103 -1.22486433970469 0.92648003976244

 O 4.84041386198618 -1.42924869910706 1.43699556441989

 H -1.46387082399596 6.11733624981143 1.17584579800446

 H -0.99205075210988 5.69839191153399 2.55437690305452

 O -0.71036380623081 6.23773607596170 1.78536039742024

 H -2.89422075357887 -3.77431512030476 -3.68064238315886

 H -3.02505253741911 -4.50326264951286 -2.33226204078378

 O -2.44369274324512 -4.43789021683850 -3.12270113749348

 H 2.22483942451131 5.06532382136013 -0.79725025736426

 H 2.23535908736790 3.58894031575783 -1.30589429785780

 O 2.59107792078340 4.16878579624020 -0.60274136102283

 H -4.54232821177513 -3.35251994707831 -1.08849174873841

 H -3.50791532122314 -3.76356397569148 -0.06550205519959

 O -4.02562602425164 -4.12054449990970 -0.81997078999474

 H 3.39998936987537 -3.71210741594164 0.39820469603960

 H 4.30064286442983 -4.82965933168799 -0.19696190208563

 O 4.31896233314780 -3.89506856240063 0.12128053373265

 H 3.40073116057630 -4.11133070624046 4.09599229644741

 H 2.83800535995284 -2.65910726140878 3.98363920076402

 O 2.58014699115404 -3.62957487502333 3.95216839066675

 H 1.41666012994987 4.02318298970961 0.65555414525450

 H 0.32728291887193 4.86018326046765 1.42258919788246

 O 0.73307012222548 3.96013619833162 1.36585588047092

 H 0.71577740737981 2.90922889849678 -2.78895482222657

 H 1.11312098706240 1.59037933106839 -2.15017338492051

 O 1.52751455977518 2.37971660308902 -2.58726692096912

 H 3.40101296007830 1.61800977095508 -2.15267035564769

 H 3.79136480564021 0.15812317092460 -2.50591982099298

 O 3.93677272981488 0.87346155206611 -1.83974792674485

 H 1.89350382279931 1.46975091675181 -4.24894204427377

 H 2.64368385838158 0.19037959693212 -4.66152833342696

 O 1.96926584776152 0.81489881390770 -4.97127628055139

 H 4.95653161716190 -3.05768953525153 -1.34701815971466

 H 6.01473886050173 -2.00725201210838 -1.71092371790306

 O 5.40976339724148 -2.63815517022822 -2.11480241404323

 H -4.00701459885016 3.17440709676202 4.58407362384530

 H -4.29583258309817 2.99627830627607 3.06541400366721

 O -4.13847875292139 3.67214044625054 3.75019789404083

 H -1.69805675693601 -0.38611830770517 -5.04551746282988

 H -2.88324794338405 0.51846843388593 -4.71084526283077

 O -2.62852054916042 -0.20767168777432 -5.31273539449411

 H 0.45324430776474 -4.75466306615884 -4.45969109648573

 H -0.79229032919448 -5.35337905586548 -3.78283994561729

 O 0.11906196927384 -5.57590991379639 -4.03511024758706

 H 5.65719130629194 0.21518086797223 0.80820300823819

 H 5.36889812052113 1.08473465657285 -0.41872805000931

 O 5.78101294830228 1.11611964857003 0.45925441337534

 H 0.89738088835692 6.75393754618706 0.07079817045924

 H 0.39408818626703 6.47127347572971 -1.34918409776826

 O 1.22180465528606 6.55859225866799 -0.81777051997101

 H -1.12995898521398 5.34769172096948 -2.58171375861328

 H -1.86881090178618 6.21605726617212 -1.57996443216969

 O -1.15600320711229 6.26208563107554 -2.23517892825291

 H -0.55949230619965 -4.79230437456670 3.99551518393790

 H 0.84539229042762 -4.36161255030534 4.49310795100598

 O -0.09482349949271 -4.36242916298940 4.73938095315336

 H 1.56853955561485 3.94554824529358 2.99523947512719

 H 2.87153132825321 3.51344897345303 3.65083566547697

 O 2.02219530287745 3.91927268366519 3.86479452075314

 H 0.55812932126559 -4.51432083809007 0.76749152660820

 H 0.29258731773816 -5.45916913052968 -0.40645300996329

 O -0.18028207906757 -5.00335072431774 0.32551351988881

 H -1.08921171561751 3.90068209763334 4.27870906197094

 H -2.47197563825249 4.01853095923487 3.54196904959707

 O -1.49089498769542 4.10360178343503 3.40947736823410

 H -2.49892487478721 4.45849897424671 0.05848125084562

 H -3.68738663781764 5.35190663350862 0.48056365015195

 O -2.82343235021130 5.38540301891568 0.05748942402721

 H 0.56347204294846 -1.40731089510968 4.78113035901172

 H -0.29026886709647 -2.69240782661217 4.60440750936853

 O -0.27943979610651 -1.71043453822074 4.42729257511570

 H -4.72934244459913 -2.28867781800138 -4.53134242613643

 H -3.39352282456501 -1.47821098403874 -4.70957325413549

 O -3.83126108604534 -2.23177217780003 -4.19194484441972

 H -2.04160579040369 -6.27556900954198 2.64594086738952

 H -1.11801791816378 -5.45895332091578 1.69762068159382

 O -1.61620460997784 -5.41788487930353 2.55279379666273

 H -4.78414105169265 1.56127403811157 -0.32369627465761

 H -4.60728794369278 0.30990920422185 -1.17231891266929

 O -4.95900161920773 1.21068720168086 -1.22035796811614

 H 1.74914808987444 -4.58021498726234 -1.77224385875703

 H 1.03930461429693 -5.65484701640527 -2.62928688119052

 O 1.54457435461435 -5.53822461425889 -1.77421079992667

 H 0.83048706603485 3.31954798460126 5.05359790564735

 H -0.09578977732398 2.11908347655267 5.20588550892856

 O 0.01609502106988 3.02176272120525 5.52523698409626

 H 3.11911371477161 -6.22580266110343 -1.36357846499575

 H 4.58518238562174 -6.42248864549042 -1.78346728507207

 O 4.02339874174112 -6.39149171147575 -1.00212947052197

 H 4.57231818033423 2.17646868906759 1.32687768539000

 H 3.54376101147616 3.26961941857346 0.95565992577525

 O 3.81074365334521 2.68691617478441 1.68627692593065

 H -2.92404379658073 1.51561003551152 5.72290231967209

 H -2.40040023834482 2.82963572554919 6.29401377268653

 O -3.22494084192691 2.36472050453473 6.10582400694171

**1M-OH-radical**

H -1.26431227777939 -1.29136662220366 0.10252332943964

 O -0.45376904717310 -0.81692262963408 -0.21752227976191

 H -0.63591071060776 2.13060207085371 -1.55652087161600

 H -0.56495024044500 0.89310653237997 -0.56607468621796

 O -0.44263647391958 1.87135052647535 -0.62377996033315

 H 0.11789856746458 -0.82233437094166 0.57840801086047

 H 0.88825685377580 -1.83584563047928 2.48335308457021

 O 0.73018795006100 -0.88882525102216 2.21563349934148

 H -2.07962728151042 0.73362396091971 2.10736806573745

 H -0.91561826583322 -0.23690117432500 2.58155068640556

 O -1.83877125454492 0.04098385782425 2.77833083190998

 H -0.14657746945832 -3.54401572383478 -2.19993698150550

 H 0.03283391604052 -2.39247068593026 -1.14900593006842

 O 0.17807245626718 -3.34254696780545 -1.29713317531801

 H -3.78177030623086 0.73887761889473 0.08269936165645

 H -3.47201184272729 -0.77702399298245 0.06065313325218

 O -3.98717361563949 -0.07618139393852 -0.40377005261595

 H -0.69450538648584 -0.97452139990196 -3.26621156815524

 H 0.29855004562102 -0.17781336183260 -4.18413549805031

 O 0.25552008073267 -0.86189794350320 -3.49055460020009

 H 1.47931402261977 0.96317160294927 -1.26443043594559

 H 1.22982513078006 -0.18480148478542 -2.26322664157105

 O 1.94367162257525 0.25071915914017 -1.72558163772769

 H 3.27122557063490 -1.93972013560365 0.41887984341283

 H 2.63023744023071 -1.15768230973989 -0.78688370095457

 O 3.06555705272041 -1.99582015324318 -0.53514500243702

 H 0.90382045614086 1.83316853927447 3.86614213981819

 H 1.06758204314655 2.83432177374560 2.68713947982317

 O 0.94327074325787 2.78538545497270 3.67143545519593

 H 0.86461964941384 2.66706910856206 0.42901006046812

 H 2.07528568107269 2.03413645432507 1.17309558321467

 O 1.58081654442421 2.88478812298136 1.05619749996906

 H -2.56435931692082 -2.56076621821572 1.45668672581556

 H -2.68827106527514 -2.92261875561498 -0.10534351505637

 O -2.60429344138860 -2.18430141967554 0.55555062739505

 H -2.40587816629825 2.67825840332242 1.93528298490390

 H -1.84216004846633 2.20934350247949 0.54848794356785

 O -2.57102818678305 2.05811756189812 1.18570461653100

 H 4.10833169747535 1.11944671468915 0.05816464190798

 H 4.87864789475326 2.38131472363520 0.43799241484282

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 H -2.94461389346771 -0.66225277536041 -2.28275619634196

 H -2.58534046036659 -2.14973659019775 -2.42836866057372

 O -2.46640302941265 -1.27387961304727 -2.86298215749928

 H 3.52586732756228 0.64343012191469 2.25316259178187

 H 2.18468910234769 -0.03300999919890 1.78950610748148

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 H 1.52774203410837 -2.35646478675161 -3.92228863130920

 H 2.32804258039547 -3.59631280652586 -3.44208838091627

 O 2.10520151875275 -3.07034377647928 -4.24272590917377

 H -0.16980044551901 -4.31643423603863 1.64052990173777

 H -0.36816888964595 -4.17603815531220 0.08025213169456

 O -0.50387026204261 -4.78576637885592 0.85103333548593

 H -0.24495991990163 2.33880099704008 -3.85919006902626

 H -1.75173392174654 2.42614194270873 -3.56130877633196

 O -0.89242579310054 2.66499654752112 -3.20005490976415

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 O 2.82047207182663 -4.48025906615526 -1.90976778892138

 H 1.04325214508833 -3.58648889371605 3.85452068282182

 H 1.83122872518611 -3.99869050669283 2.58235955137160

 O 1.01506172711183 -3.53435282243680 2.86843898616933

 H -3.70255492639002 -2.57861017051384 3.28800251438267

 H -2.62445909314986 -1.47434498888790 3.08911738609449

 O -2.74188894297809 -2.42516759976392 3.31764986822439

 H 5.32157839872294 -1.77171560683611 -2.70017993895958

 H 4.65703949307275 -1.96457654192813 -1.33106233366139

 O 5.54197013180187 -2.00439697007388 -1.76208288088581

 H -2.19501941887318 2.82788441181940 4.26694784113136

 H -0.92309196651570 3.33496743750587 3.61745005217835

 O -1.89481117225235 3.39992900988101 3.54404533388316

 H -7.01657460502298 -1.16603107169179 0.01093052242680

 H -5.48663502960648 -0.93848173331087 -0.11466466705751

 O -6.17308036696714 -1.62401307679856 0.08540548292228

 H 0.31432538825489 -0.71423160578131 4.64289607619846

 H 1.88454611198446 -0.66148209578561 4.32381748634349

 O 1.02488343507666 -0.13689625181248 4.25512402213230

 H -2.49287703949056 -4.48925639980416 -1.80073498614859

 H -3.92744431481813 -3.87843524065741 -1.56801394357748

 O -2.95610581093648 -3.66105998111905 -1.55042332207754

 H 1.87155886062986 1.45169598954775 -4.69778132702777

 H 0.92290912056981 1.61104650027651 -5.92793159655817

 O 0.91553731535802 1.46148174987821 -4.97756091506997

 H 4.21324162796105 3.77176429202216 2.25707669223579

 H 3.38426011746072 3.85900248201287 0.99216820275505

 O 4.30806518568493 3.83793382348189 1.29150101439694

 H -1.54797571975886 -2.06986011482156 4.84308078135717

 H -1.47392740675027 -0.81610347728505 5.72843857880032

 O -0.95163519582885 -1.59418732299083 5.45387076319100

 H -2.19269596205583 0.63433538271822 4.34336629766336

 H -3.30999100171259 0.79226488731370 5.40526247505831

 O -2.36278292838736 0.91279349070854 5.27893404656157

 H -1.32895925884337 -6.73799629722705 -2.06477358947296

 H -1.29611456024341 -5.57861291137058 -3.10470260219763

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 O -2.74933511018294 -3.24896394239383 -5.08965661096154

 H 6.34488626625080 -1.21937941062602 -0.15968216447274

 H 5.82828994229676 0.07791442843625 0.46561841107805

 O 6.22652091845157 -0.78732316127837 0.70826145363243

 H 5.22794719040632 2.16453867132557 -1.83125623230043

 H 6.21188108861268 2.07775283806891 -3.00627934778423

 O 5.36942218483958 2.46996501522319 -2.75442069372420

 H -1.26243758830776 -3.78060046684836 -4.42033123490732

 H 0.30632433895747 -4.02548615112567 -4.34320470537877

 O -0.53234369009432 -4.17725922132471 -3.87456871823417

 H -5.25294522532308 -4.68688134341508 1.60082014747836

 H -4.37258198004394 -5.79128091460659 0.95444211367786

 O -5.28317875879005 -5.42434585225391 0.97018732420639

 H -6.27497873501308 -2.96202837606225 3.04386599966655

 H -5.74786144487086 -2.39456401408240 1.70724041727528

 O -5.47925644115480 -2.90127796942468 2.50562827346550

 H 5.94239911761848 -5.06190380067049 -2.61713208866762

 H 5.71158264139270 -3.75479549396960 -1.82459957106593

 O 5.55832688657829 -4.73153939678088 -1.79864259006254

 H 2.60392362601444 3.22739943031446 4.05326230059585

 H 3.70026591726348 4.03096211693487 4.81062410194464

 O 3.58147031926218 3.38401455045971 4.10856217524546

 H 3.57142364398959 -1.83263576095695 3.63323030314682

 H 3.88670169875563 -0.64918893596608 4.53342620311600

 O 3.30284819384963 -1.43516635785428 4.49205093905380

 H 4.98649233155077 -1.90353198302094 1.63594639583371

 H 4.22172336479949 -3.27037908675169 1.88100598192170

 O 4.16544213672568 -2.30453433756752 1.99141334158065

 H -4.93487920794590 -5.06945848198057 -3.33378536525216

 H -3.64003244394500 -5.85189635022414 -3.57793852492718

 O -4.32748636474555 -5.34093641031362 -4.03682775490203

 H 5.58911412194486 0.75590214910326 3.50693237252589

 H 4.44598976689096 1.73798098823042 3.99490746122793

 O 4.62527971130004 0.82516193385633 3.69957987497611

 H 2.13058047741806 -2.79291618847971 5.55748130517218

 H 0.63742001713933 -2.86015854052698 5.91424231450844

 O 1.37346610905018 -3.39883056752878 5.58785592713999

 H -2.75305326792103 -6.34949295104178 -0.43407837074556

 H -1.98658071154468 -5.80853406470017 0.76010689094682

 O -2.70242636332901 -6.43919586615014 0.52647707751403

 H -5.54474985475401 -4.70354921277569 -0.56681323105242

 H -5.93237633329977 -3.33322894486691 -1.15751883979644

 O -5.57116571635647 -4.19342927911091 -1.42189085737784

 H 7.85444615881612 1.00375122467355 2.84257422001258

 H 7.12277563913136 -0.17917261986634 2.18853912553184

 O 7.24281144089910 0.28775349902318 3.04081765831391

 H 3.79858168808284 -2.08746013757725 -4.37695821009802

 H 4.20543990587705 -0.60851441088090 -4.28479111596111

 O 4.58047998696655 -1.50919740313099 -4.27648527695872

 H -0.95977301504186 -7.81776077811988 -0.21561854806638

 H 0.43033497295549 -7.42672663733887 -0.72625850183174

 O -0.40695470689001 -7.84013852722565 -1.00959851996044

 H 0.95435848934455 -5.67280038503571 0.32074332443341

 H 2.07860018924806 -5.62181901379677 -0.76108973308489

 O 1.76749436866835 -6.14143637774868 0.02061583468337

 H 3.56240665836951 -5.66090886915632 2.55169869830872

 H 2.81141015807586 -5.47270538062304 1.20469337208522

 O 3.26182632359716 -4.97638318303199 1.94526524008049

**2M-OH-anion**

 H -1.14565804488928 0.49839152288201 0.50970467177340

 O -0.35663800994413 0.67446233210698 -0.03520395662682

 H -3.63706090560347 -1.55721044636939 4.33319411784338

 H -2.75650410033855 -4.47335934971782 4.24704729879518

 H -2.75987559778203 -3.28139523082261 5.21761131529521

 H -2.73824505827782 -1.01754951857070 5.46255180750384

 O -3.40923299502712 -1.70583996885535 5.26987880490672

 O -2.37809056210137 -4.19403237579636 5.08679820135477

 H -2.75454289978184 2.56035331597894 2.88476502906029

 H 1.41575365458801 -1.10820665017304 6.22454524979578

 H -0.06932507073870 -0.77037314353537 6.49911630011966

 H -1.91836455131479 3.61312549579434 3.66446704925925

 O 0.61275002892027 -1.45459581098850 6.65577194984541

 O -2.82121851512630 3.43295813662312 3.32104421126026

 H 1.42701699868847 1.22007997284551 0.60103289360880

 H 2.63144831627754 2.19756612188695 0.87231556698345

 O 2.35412267158850 1.38002527252779 0.36183432036305

 H -0.67026118667939 -2.34571002728428 -1.96938977633708

 H -0.55867188038334 -1.02070761204918 -2.80427549971879

 O -0.61104733060587 -2.05795831194162 -2.88822722128811

 H -0.65004201738658 0.62098723181542 -1.00071674152460

 H 0.17498930286579 0.83918756270925 -2.68405280617403

 O -0.72481361929261 0.48315238437128 -2.63264190064530

 H 2.06098491531133 1.71841916792117 -1.33848237813547

 H 2.76106863517118 2.14284707492956 -2.66564387813769

 O 1.86862648081573 1.97368246915556 -2.27144107032990

 H -0.82497328970910 0.92381201732702 2.71224465853720

 H 0.12242942599804 -0.26958036958673 2.96069907019973

 O -0.06727690792422 0.65204701533855 3.26405423771927

 H -3.66904703707497 1.73220166986036 -0.94911699329230

 H -3.56160055311970 0.22003724360137 -0.61102747026839

 O -3.97515391921983 1.08171317148747 -0.28123943683069

 H 0.82446039701810 -0.71100089916199 -0.41505631345438

 H 2.27283362441578 -1.22640795396505 -0.19303232328761

 O 1.49485617097857 -1.33439983970971 -0.76636758906149

 H 3.42569940617708 4.15019450026541 1.08050071389254

 H 4.18496512192710 2.96584154207288 1.86383202936658

 O 3.31315509370212 3.40495436072347 1.72553386821161

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 O 0.14549089749002 3.43148040267455 0.74531268718586

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 O -2.64458540978713 2.50943192596477 -2.29007479306112

 H -3.05721443336697 1.17864366562121 1.07919181561388

 H -2.92571784767059 0.15736743321291 2.22918081938593

 O -2.49585276550860 0.97923881448619 1.88843800085274

 H -3.10766082852593 -1.95307148977548 1.94291709462240

 H -4.53101530504883 -1.31866997090721 1.89308695091172

 O -3.73050752057021 -1.41203278537971 2.46853173148015

 H -2.54851773944349 -2.79668362595414 -5.39104620738374

 H -1.82394672747047 -1.99937740723165 -4.30220832057723

 O -2.42280169760852 -1.87351069013216 -5.06229446332330

 H -1.75701514780366 -3.39635346228770 0.45365545021532

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 O -1.74540398721873 -2.48208090441523 0.75765812117828

 H 2.68232175889827 -2.31123911784665 -3.42765160715215

 H 2.33196324766990 -1.17914133054378 -2.46856093751433

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 H 2.34040976394172 -0.77772032135344 4.10677917307965

 O 2.85382677197111 -0.97891078407718 4.89747060548606

 H 5.17563921766256 0.85346695952899 1.83234651073777

 H 5.10603156412712 1.59469519146523 3.17558555663128

 O 5.41834499581452 1.69887531461200 2.24115117783722

 H -3.16275859960461 1.60488305949633 -5.00852128614746

 H -4.36294386987612 1.01429674487667 -4.27949843419564

 O -3.99813981492681 1.87241605879754 -4.57846969432936

 H -0.96363277031349 0.42712007890485 4.87464549308251

 H -1.76415301714455 1.14307364585921 5.99364356642581

 O -1.41748873085562 0.25901459330274 5.72624433525075

 H -1.85639125693096 5.17317556073974 -0.88142245457454

 H -1.97377725262970 4.15474882161784 -2.02728091708241

 O -1.55429542062177 5.01326690046838 -1.79093799952241

 H 5.39255296285225 0.17630993812226 -2.16387860048832

 H 4.50394570990379 -1.05631092888508 -2.34916323570310

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 O -4.59554935918619 -0.75918878897959 -3.61547944826973

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 H 0.28128338080675 -2.67326807576017 5.48518632192812

 O 0.21252116454529 -3.33203910497206 4.74290473102144

 H -0.38069630638231 5.10531126966223 4.19780342027771

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 O -0.46769739493250 4.23231453250630 4.63869324960754

 H 3.42822716703309 1.95347517329981 4.60076629422315

 H 3.99890634813085 0.57090534844664 4.88780718589268

 O 4.27875587609888 1.49229815042627 4.73787132839103

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 H 3.10573872079663 -3.61733129561977 3.49057350879100

 O 3.05605519857389 -3.65725800052662 4.46818362210300

 H 1.20426160258701 -3.10886991540179 -0.61129701461091

 H 1.90620071642449 -4.27430444060426 0.01801782340658

 O 1.24489055646531 -4.08664400470846 -0.66493639723631

 H -2.96137351217553 2.91475854059354 5.40937672005158

 H -1.65563679260259 3.38738552145126 5.97343314007020

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 H 1.98692264480349 4.82112556953732 -3.66645064865009

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 H -5.67666173035785 -1.66479456445282 0.02388746546246

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 H -0.96299238289225 -5.74092765941964 -3.42361638834400

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 H -1.86800512775510 -4.96270662919395 -5.29665922719799

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 H -2.31542913322808 -0.98744256147402 -1.76294187615135

 O -2.96039940611535 -1.18120334890944 -1.07392672147641

**2M-OH-radical**

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 H -0.03926105709306 -2.03826193246738 2.55238903566055

 H 0.63568429054875 -3.73040813582522 5.63051477280647

 H -0.12050133862379 -2.59868231205508 4.86386570964230

 H 0.06673227060161 -0.59317169351348 3.11560297105613

 O -0.29777032415757 -1.48569830549037 3.31196116048472

 O -0.26144233176220 -3.41494277219874 5.37837609663966

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 H 1.27902050540790 1.54980148602108 2.92373744892204

 H -0.20798793527853 1.54834693939942 2.36636348535623

 H 3.70260344316111 2.66961024422209 0.67496613716820

 O 0.59215121473386 0.98411300821818 2.49151043604143

 O 3.68125719939600 3.53378550481608 1.15341571111395

 H 3.97048630543098 -3.55857910942237 2.35384297351460

 H 3.58211041834348 -2.04957052049661 2.10489485302467

 O 3.30237815586931 -2.86055395014477 2.58259215560335

 H -2.01393740367848 0.73879770724516 -1.74065739318507

 H -1.22185353439224 -0.10859057893618 -0.70076502002551

 O -1.89237999801563 0.62937662420362 -0.77420435055409

 H 2.06710936358037 -3.91552658519505 -0.60952696589176

 H 1.95987780464312 -5.01158290148471 0.51847156458182

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 H -3.35431831103846 -2.14079142843991 2.42042645153602

 H -2.13235804597125 -1.64270261690732 3.25075975865831

 O -3.10805473107851 -1.75394399486090 3.28586721401570

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 H -0.19221881119553 4.70533582481984 3.69516736371768

 O 0.76195252114981 4.75254793755607 3.54389163861808

 H -3.19290897605070 1.50949374077505 -3.24853882664278

 H -2.75334423747152 0.07782812366887 -3.67106188066419

 O -2.40365369730542 0.96786987035296 -3.49202807737875

 H -7.19448746356238 -2.69642445877743 -0.13965263008540

 H -5.66110384419826 -2.80884701820285 -0.18782062153820

 O -6.45928854142525 -2.71984130742310 -0.75982606276867

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 H 4.69734046831324 4.25049204338377 -0.40590045309683

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 H 3.80371069921260 1.18631944980812 4.13351633083705

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 H -4.68310889144648 3.65770205987806 1.75413553904127

 O -4.72702193437316 3.73887788336432 2.72612426590120

 H 1.99039631961755 3.31808680341593 3.80602960983790

 H 3.04978707847761 2.92887955473260 2.75853754812357

 O 2.56233617320279 2.57065006008311 3.53590483559638

 H -2.58388411798990 -4.08701832894806 5.41267870818131

 H -3.31349308440433 -3.37511281954462 4.29226160526077

 O -3.24405154292404 -4.24908744339440 4.72627542395399

 H 2.79430419098697 1.01557948719507 -0.37393576501235

 O 3.77624702621647 1.16114252712454 -0.18973203822774

3M-ANION

 H 0.61762582168851 -0.59812131141169 1.38947660094007

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3M-RADICAL

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