H2O+O-Isoniazide-Parallel-Top-Al-AlN-vdw-opted

163

N 13.010987 13.038238 -0.085031

Al 12.115050 14.621977 -0.083753

Al 14.872386 16.187415 -0.048138

N 15.751129 11.415763 -0.074788

Al 14.847477 13.009312 -0.065575

Al 17.611298 14.572337 -0.042967

N 15.776746 14.584045 -0.053699

N 18.548131 16.151867 0.002733

Al 17.634562 17.744452 -0.019182

Al 20.393439 19.298036 -0.004761

N 18.480374 9.802958 -0.044708

Al 17.574699 11.404314 -0.065123

Al 20.342559 12.971580 0.015167

N 18.523126 12.984848 -0.039267

N 21.268574 14.529361 0.257491

Al 20.378922 16.127591 0.080430

Al 23.132893 17.700673 -0.031613

N 21.291818 17.709863 0.010935

N 24.058112 19.278696 -0.012507

Al 23.157442 20.869003 -0.000814

N 21.209860 8.193470 -0.028038

Al 20.306043 9.783235 -0.023463

Al 23.085881 11.366662 -0.006464

N 21.247433 11.360119 0.117589

N 23.991463 12.929912 -0.008763

Al 23.148522 14.569803 0.325502

Al 25.846132 16.097244 -0.036252

N 24.026717 16.116194 -0.099010

N 26.788973 17.662433 0.003313

Al 25.885238 19.260988 0.004839

N 23.936294 6.583461 -0.021522

Al 23.040421 8.184971 -0.027779

Al 25.802663 9.747264 0.000388

N 23.965597 9.762735 -0.020623

N 26.731301 11.324404 0.004754

Al 25.812133 12.921659 0.010789

Al 28.581009 14.475675 0.034244

N 26.747448 14.497577 0.026738

N 29.519260 16.056735 0.035137

Al 28.613913 17.649908 0.023774

N 26.711487 8.161530 0.007081

N 29.470996 9.720036 0.032971

Al 28.553061 11.305082 0.036008

Al 31.316809 12.864193 0.056232

N 29.483015 12.897414 0.057220

N 32.256081 14.452689 0.064351

Al 31.346790 16.037338 0.051397

N 32.225721 11.276363 0.070164

N 34.981097 12.841700 0.068965

Al 34.081844 14.425420 0.066610

C 25.362505 10.730009 4.454046

C 24.194160 11.414990 4.076279

C 24.329301 12.673308 3.433983

C 25.648360 13.167828 3.235164

C 26.745436 12.399985 3.659795

N 26.625305 11.184683 4.263325

C 23.229585 13.505787 2.881047

O 23.512500 14.599617 2.277339

N 21.897908 13.190226 2.915440

N 21.412502 11.898601 3.144057

H 25.311333 9.740546 4.950738

H 23.166807 10.969717 4.222441

H 25.806004 14.135385 2.741666

H 27.746116 12.733655 3.494746

H 21.406876 13.847650 2.267312

H 20.495827 11.982324 3.692687

H 21.216713 11.494536 2.196682

O 22.555628 17.132409 4.647907

H 21.920193 17.498456 4.017042

H 22.701337 16.220443 4.392121

O 23.440039 13.989459 5.810497

H 22.559350 14.274266 5.504956

H 23.964182 14.817889 5.821059

O 19.799570 13.374683 5.621795

H 20.205256 14.074086 6.145538

H 19.795981 12.630802 6.223538

O 26.026059 17.656153 3.870665

H 25.200592 18.073122 3.617275

H 26.603518 18.370199 4.065772

O 19.507064 15.990832 4.155412

H 18.919240 15.427093 4.626233

H 19.938112 16.523269 4.826007

O 25.461771 16.072013 6.053652

H 25.598761 16.673469 5.341544

H 25.298615 16.656575 6.791044

O 19.872644 10.142077 6.832416

H 20.779433 9.806140 6.768892

H 19.504587 9.994179 5.976366

O 22.540981 18.970150 6.847821

H 22.871650 18.439578 6.106333

H 23.095715 19.781385 6.850438

O 20.009998 18.946157 4.246446

H 19.364548 18.237124 4.049147

H 20.182024 19.385876 3.387225

O 24.448276 8.895210 7.510502

H 24.283395 9.113655 6.606384

H 24.261410 9.675667 8.026784

O 20.466404 15.828590 7.085925

H 20.045056 16.342413 7.804369

H 21.424498 15.768013 7.365358

O 23.759573 19.453207 4.198770

H 23.160937 20.008682 4.737653

H 23.364249 19.460653 3.342275

O 26.653481 14.895166 8.160240

H 27.362802 15.521609 8.338858

H 26.223753 15.230076 7.363018

O 26.660873 11.867150 8.346220

H 25.761016 11.686772 8.609753

H 26.757869 12.826982 8.473577

O 29.609174 15.244944 6.541386

H 29.434442 15.207852 5.602141

H 30.232475 14.524306 6.681285

O 17.286746 11.593814 3.747889

H 17.708637 12.452738 3.737111

H 17.309238 11.334908 2.830485

O 17.075016 14.509165 5.409464

H 16.602488 14.892028 6.121563

H 17.396186 13.697298 5.793958

O 29.915443 15.111182 3.730235

H 29.695434 14.989095 2.807413

H 30.561567 14.435964 3.894484

O 23.873155 11.415628 9.304261

H 23.392165 11.930984 8.668805

H 24.384154 12.052999 9.755019

O 24.627416 18.656941 8.884899

H 23.775262 18.662855 8.468948

H 24.485342 18.122131 9.713407

O 20.507380 17.909001 9.072585

H 20.841387 18.298163 8.279641

H 21.057914 18.293148 9.776452

O 21.968697 15.381256 9.367747

H 21.371645 14.830275 9.865809

H 21.582060 16.268288 9.440656

O 24.787740 14.173124 10.021262

H 23.944934 14.462151 9.736924

H 25.399024 14.641705 9.436965

O 28.378528 16.414741 9.904828

H 29.199976 16.884766 9.782665

H 28.656743 15.554394 10.301158

O 19.373856 11.215662 10.161267

H 19.176075 10.990447 9.268332

H 19.558844 10.364728 10.573816

O 16.653070 15.043881 9.957672

H 16.699005 15.983836 10.252763

H 16.025477 15.048808 9.238217

O 15.360991 15.197036 7.692975

H 14.446062 15.306692 7.442388

H 15.515093 14.300703 7.507458

O 31.713490 13.507640 7.191609

H 32.292982 13.109730 6.505490

H 31.742659 12.895647 7.915958

O 19.951916 13.848829 10.400131

H 19.056765 14.111863 10.303228

H 19.892838 12.906514 10.315817

O 30.199216 11.030691 5.651571

H 29.325533 11.152701 5.285489

H 30.555541 11.915912 5.735049

O 13.121653 14.203349 6.809663

H 13.638173 13.816787 6.117491

H 13.135496 13.605300 7.531606

O 33.964638 14.517857 8.088161

H 33.051598 14.614709 7.876351

H 34.145871 13.565744 7.892764

H2O+O-Isoniazide-Top-B-vdw-opted

185

O 22.558000 17.133000 4.650000

H 21.923000 17.468000 4.016000

H 22.701000 16.223000 4.389000

O 23.359000 8.641000 10.634000

H 23.654000 8.161000 9.860000

H 23.855000 9.459000 10.613000

O 16.928000 12.089000 7.832000

H 17.278000 11.413000 8.413000

H 17.642000 12.274000 7.223000

O 26.021000 17.654000 3.869000

H 25.206000 18.086000 3.610000

H 26.614000 18.372000 4.089000

O 19.495000 15.993000 4.159000

H 18.899000 15.430000 4.653000

H 19.919000 16.535000 4.824000

O 25.459000 16.079000 6.057000

H 25.610000 16.667000 5.316000

H 25.286000 16.662000 6.795000

O 19.879000 10.144000 6.836000

H 20.770000 9.802000 6.751000

H 19.483000 9.994000 5.977000

O 22.540000 18.974000 6.848000

H 22.864000 18.449000 6.116000

H 23.076000 19.767000 6.829000

O 23.270000 8.287000 4.480000

H 22.410000 8.219000 4.065000

H 23.845000 7.759000 3.927000

O 24.446000 8.891000 7.515000

H 24.295000 9.139000 6.602000

H 24.237000 9.680000 8.015000

O 20.478000 15.834000 7.088000

H 20.066000 16.339000 7.790000

H 21.393000 15.756000 7.354000

O 27.795000 9.339000 4.181000

H 27.424000 10.104000 4.618000

H 27.155000 9.115000 3.505000

O 26.655000 14.898000 8.160000

H 27.353000 15.530000 8.336000

H 26.230000 15.224000 7.367000

O 26.659000 11.868000 8.347000

H 25.758000 11.680000 8.611000

H 26.747000 12.816000 8.454000

O 29.610000 15.242000 6.545000

H 29.410000 15.202000 5.610000

H 30.220000 14.520000 6.692000

O 27.754000 12.776000 4.222000

H 27.831000 13.695000 4.482000

H 28.658000 12.486000 4.098000

O 16.402000 14.722000 4.626000

H 16.609000 14.828000 5.555000

H 16.001000 13.856000 4.567000

O 29.438000 15.337000 3.435000

H 29.335000 16.256000 3.684000

H 30.374000 15.166000 3.533000

O 23.874000 11.413000 9.300000

H 23.381000 11.906000 8.645000

H 24.381000 12.077000 9.768000

O 24.624000 18.653000 8.885000

H 23.766000 18.670000 8.465000

H 24.486000 18.158000 9.694000

O 20.505000 17.909000 9.073000

H 20.849000 18.297000 8.270000

H 21.049000 18.275000 9.771000

O 21.974000 15.383000 9.375000

H 21.371000 14.818000 9.860000

H 21.603000 16.261000 9.464000

O 24.790000 14.175000 10.020000

H 23.930000 14.477000 9.728000

H 25.409000 14.625000 9.447000

O 28.375000 16.414000 9.899000

H 29.199000 16.890000 9.792000

H 28.629000 15.586000 10.307000

O 19.374000 11.217000 10.159000

H 19.171000 10.986000 9.252000

H 19.575000 10.381000 10.579000

O 16.653000 15.043000 9.956000

H 16.704000 15.958000 10.234000

H 16.041000 15.049000 9.221000

O 17.657000 15.163000 7.950000

H 17.584000 16.012000 7.514000

H 17.919000 14.558000 7.256000

O 31.718000 13.509000 7.197000

H 32.263000 13.121000 6.512000

H 31.754000 12.881000 7.918000

O 19.955000 13.849000 10.397000

H 19.044000 14.135000 10.323000

H 19.914000 12.896000 10.334000

O 32.670000 13.697000 3.922000

H 31.761000 13.460000 3.736000

H 33.089000 12.873000 4.166000

O 13.635000 14.164000 6.787000

H 13.861000 13.753000 5.953000

H 13.874000 13.514000 7.448000

O 29.757000 11.393000 6.953000

H 29.376000 12.233000 6.697000

H 29.079000 10.749000 6.748000

B 23.659000 20.439000 0.273000

N 24.330000 19.187000 0.237000

B 25.752000 19.146000 0.205000

N 26.425000 17.897000 0.164000

B 27.845000 17.853000 0.163000

N 28.518000 16.602000 0.126000

B 29.939000 16.557000 0.136000

N 30.612000 15.305000 0.137000

B 32.032000 15.261000 0.212000

N 32.704000 14.010000 0.165000

B 34.125000 13.966000 0.192000

N 34.798000 12.716000 0.109000

B 21.492000 19.269000 0.334000

N 22.165000 18.018000 0.337000

B 23.585000 17.976000 0.283000

N 24.257000 16.726000 0.197000

B 25.676000 16.687000 0.139000

N 26.349000 15.437000 0.099000

B 27.770000 15.394000 0.092000

N 28.444000 14.144000 0.048000

B 29.864000 14.099000 0.051000

N 30.539000 12.848000 -0.018000

B 31.959000 12.803000 0.041000

N 32.630000 11.550000 0.068000

B 19.324000 18.105000 0.296000

N 19.996000 16.853000 0.291000

B 21.419000 16.808000 0.265000

N 22.090000 15.561000 0.147000

B 23.511000 15.519000 0.093000

N 24.182000 14.279000 -0.067000

B 25.597000 14.228000 0.040000

N 26.274000 12.978000 0.029000

B 27.693000 12.934000 0.013000

N 28.370000 11.684000 -0.034000

B 29.790000 11.639000 -0.018000

N 30.461000 10.386000 0.045000

B 17.155000 16.940000 0.252000

N 17.828000 15.687000 0.271000

B 19.249000 15.644000 0.228000

N 19.922000 14.396000 0.101000

B 21.344000 14.354000 0.038000

N 22.012000 13.114000 -0.158000

B 23.435000 13.068000 -0.117000

N 24.108000 11.813000 -0.144000

B 25.524000 11.771000 -0.039000

N 26.201000 10.520000 -0.065000

B 27.622000 10.475000 -0.060000

N 28.295000 9.222000 -0.065000

B 14.989000 15.779000 0.097000

N 15.661000 14.528000 0.099000

B 17.081000 14.481000 0.170000

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B 19.175000 13.192000 0.012000

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B 21.269000 11.903000 -0.149000

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N 24.034000 9.353000 -0.018000

B 25.453000 9.311000 -0.095000

N 26.127000 8.061000 -0.160000

B 12.819000 14.617000 0.045000

N 13.492000 13.367000 -0.012000

B 14.913000 13.322000 0.011000

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B 17.007000 12.028000 -0.024000

N 17.679000 10.777000 -0.076000

B 19.101000 10.734000 -0.063000

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B 21.194000 9.439000 0.022000

N 21.866000 8.184000 0.053000

B 23.287000 8.143000 -0.019000

N 23.957000 6.896000 -0.149000

C 20.237000 13.144000 5.929000

C 21.602000 13.265000 5.627000

C 22.053000 12.795000 4.382000

C 21.104000 12.219000 3.516000

C 19.770000 12.139000 3.925000

N 19.323000 12.592000 5.112000

C 23.445000 12.934000 3.835000

O 23.638000 12.980000 2.611000

N 24.539000 13.036000 4.666000

N 24.527000 12.758000 6.040000

H 19.860000 13.516000 6.890000

H 22.290000 13.714000 6.345000

H 21.427000 11.852000 2.537000

H 19.019000 11.692000 3.260000

H 25.427000 13.057000 4.153000

H 24.957000 11.845000 6.223000

H 25.059000 13.479000 6.535000

H2O-O-Isoniazide-parallel-Top-Si-vdw-opted

163

Si 34.014184 14.515262 0.108433

C 34.886438 13.001768 0.110412

Si 12.306316 14.551104 -0.013314

Si 15.003102 16.150595 -0.009485

C 15.886373 14.595570 -0.062048

Si 14.983624 13.029289 0.080629

C 13.206152 13.032683 0.034764

Si 17.697964 17.662747 -0.019298

C 18.638445 16.113187 0.010984

Si 17.737773 14.585525 0.053962

C 18.634373 13.014906 0.076698

Si 20.454573 13.008735 0.153630

C 21.335040 14.569502 0.189880

Si 20.391873 16.083835 0.117167

C 21.318428 17.680722 0.196305

Si 20.416914 19.250829 0.100794

Si 23.140496 20.801523 0.074742

C 24.083214 19.249830 0.161839

Si 23.125279 17.706302 0.161183

C 24.022669 16.146079 0.199784

Si 23.163727 14.556876 0.363581

C 24.065586 12.979867 0.008339

Si 23.154760 11.426531 -0.010826

C 21.281217 11.470878 0.174538

Si 20.412954 9.890530 0.092145

C 18.636867 9.786200 0.119654

Si 17.711013 11.418121 0.043681

C 15.917443 11.477829 -0.049119

Si 25.867205 19.295732 0.049482

C 26.745601 17.690837 0.019175

Si 25.876381 16.161624 0.075886

C 26.804745 14.556300 -0.008398

Si 25.851549 13.023242 -0.088971

C 26.759725 11.417134 -0.185500

Si 25.850944 9.877953 -0.078009

C 24.052118 9.809779 0.034250

Si 23.124931 8.299950 0.061597

C 21.344069 8.293302 0.129090

C 24.035669 6.717390 0.095728

C 26.759623 8.298866 -0.009895

Si 28.522180 11.382437 -0.099360

C 29.440069 12.946345 -0.063272

Si 28.593082 14.559018 -0.040524

C 29.491651 16.127216 0.046051

Si 28.587463 17.628859 0.013087

Si 31.249600 16.085833 0.038650

C 32.173476 14.535563 0.078488

Si 31.266918 12.973246 -0.030354

C 32.186823 11.381245 0.065038

C 29.456229 9.867184 -0.041723

C 27.676524 12.815817 3.384418

C 26.328160 12.464029 3.279823

C 25.356406 13.468230 3.263553

C 25.768279 14.822288 3.383594

C 27.163764 15.063401 3.527412

N 28.097191 14.081422 3.440345

C 23.963282 13.287295 2.925409

O 23.357551 14.323664 2.486291

N 23.290756 12.143118 3.093948

N 23.803553 10.891789 3.564778

H 28.426460 11.949368 3.323791

H 26.109897 11.359166 3.285311

H 25.040845 15.601642 3.279892

H 27.587668 15.975362 3.625797

H 22.358975 12.203392 2.867081

H 23.109480 10.484672 4.328433

H 23.699206 10.250056 2.762901

O 22.585892 17.139934 4.658029

H 21.875815 17.278439 4.017186

H 22.727521 16.196214 4.503142

O 23.626730 13.322847 6.392736

H 24.026062 12.759863 5.708940

H 24.332669 13.991448 6.459422

O 19.830504 13.407270 5.588394

H 20.085549 14.205411 6.078875

H 19.943059 12.687313 6.215669

O 25.977186 17.656945 3.860704

H 25.237726 18.176909 3.558994

H 26.593735 18.279314 4.219164

O 19.382466 16.012437 4.195480

H 18.756083 15.532015 4.712527

H 19.740900 16.557843 4.903440

O 25.426025 16.142758 6.090947

H 25.688653 16.603984 5.323501

H 25.133572 16.803502 6.717263

O 19.927330 10.169503 6.861405

H 20.750122 9.737759 6.627796

H 19.324682 9.964607 6.147267

O 22.529223 19.001960 6.860569

H 22.666282 18.358834 6.125666

H 22.963056 19.835758 6.622006

O 23.289320 8.325044 4.505147

H 22.574340 8.275964 3.854336

H 23.931076 7.698938 4.145094

O 24.417027 8.869773 7.546581

H 24.438025 9.207117 6.652830

H 24.157901 9.635690 8.046159

O 20.563537 15.877081 7.067854

H 20.186221 16.311202 7.867036

H 21.423845 15.558844 7.551696

O 27.739390 9.279036 4.137013

H 27.283886 10.046041 4.484034

H 27.146693 8.915662 3.477917

O 26.668198 14.918416 8.167977

H 27.356634 15.558637 8.404222

H 26.386866 15.173994 7.259047

O 26.648965 11.866786 8.348541

H 25.742538 11.637218 8.581259

H 26.618014 12.832801 8.259329

O 29.602772 15.221064 6.585777

H 29.386325 15.091421 5.661599

H 30.212917 14.501134 6.776005

O 17.109122 11.474089 3.084464

H 17.916467 11.979383 2.991743

H 16.599510 11.670901 2.315747

O 17.072609 14.468903 5.431284

H 16.582727 14.978350 6.032848

H 17.529513 13.721212 5.801658

O 30.392851 15.111819 3.830119

H 29.925954 14.872980 3.025372

H 31.260389 14.736403 3.769820

O 23.890156 11.397624 9.263885

H 23.410567 11.803049 8.543846

H 24.121010 12.238489 9.648806

O 24.595042 18.628490 8.862690

H 23.738054 18.662877 8.430144

H 24.444495 18.279688 9.751993

O 20.485699 17.910238 9.062634

H 20.979267 18.269382 8.327654

H 20.996640 18.247586 9.807112

O 22.038920 15.382490 9.444727

H 21.276145 14.796643 9.713344

H 21.689850 16.252587 9.671755

O 24.784631 14.182782 10.011531

H 24.019652 14.663852 9.755394

H 25.491985 14.472685 9.393225

O 28.337220 16.421748 9.838114

H 29.188975 16.874587 9.855990

H 28.475322 15.683310 10.450500

O 19.369693 11.228497 10.128692

H 19.256546 10.920813 9.233490

H 19.749464 10.483512 10.591523

O 16.664179 15.016102 9.950031

H 16.760440 15.961041 10.159429

H 16.217778 15.175284 9.104428

O 15.384628 15.281920 7.707046

H 14.432455 15.292148 7.623648

H 15.526399 14.365222 7.537191

O 31.759945 13.526182 7.258539

H 32.069826 13.084657 6.446916

H 31.751144 12.752112 7.835325

O 19.982971 13.859003 10.373315

H 19.101549 14.181605 10.439274

H 19.908821 12.919782 10.455325

O 33.065150 13.209722 3.157523

H 32.707811 13.790989 2.484810

H 33.390056 13.828641 3.813746

O 13.041674 14.168380 6.836037

H 13.716875 13.909366 6.218382

H 13.090708 13.461890 7.458808

O 29.776507 11.371002 6.871021

H 29.438895 12.220848 6.621092

H 28.961478 10.855405 6.822680

O-Isoniazide-Parallel-Top-B-Cluster-MP2-AIM

115

C 5.442000001 -4.551000001 23.339900003

C 5.328900001 -3.142900000 23.347900003

C 6.514000001 -2.367900000 23.349000003

C 7.748000001 -3.064900000 23.349000003

C 7.742000001 -4.474000001 23.353900003

N 6.613900001 -5.232000001 23.344900003

C 6.604000001 -0.874000000 23.243900003

O 7.639900001 -0.324000000 22.833900003

N 5.508000001 -0.068000000 23.545000003

N 4.423000001 -0.492000000 24.344000003

N 1.233000000 -3.674900000 19.914900002

N 1.231000000 -7.936000001 20.039900002

B 1.234000000 -6.517000001 19.940000002

N 2.468000000 -5.807900001 19.926900002

B 2.462000000 -8.647900001 20.065900002

N 3.693900000 -7.937000001 20.079900002

N 1.231000000 0.590000000 19.900900002

B 1.229000000 2.012000000 19.920900002

N 2.462000000 2.719900000 19.902900002

B 2.460900000 4.142000000 19.937000002

N 3.692000000 4.851000001 19.902000002

B 1.231000000 -2.253000000 19.934000002

N 2.460900000 -1.543000000 20.001000002

B 2.460900000 -0.122000000 19.943900002

N 3.692000000 0.588000000 19.989900002

B 3.693000000 2.008900000 19.937000002

N 4.924000001 2.718000000 19.966900002

B 4.923000001 4.139900000 19.936000002

N 6.153900001 4.851000001 19.974000002

B 2.464000000 -4.386000001 19.943900002

N 3.692000000 -3.674900000 20.039900002

B 3.693000000 -2.254000000 20.053000002

N 4.924900001 -1.544900000 20.057900002

B 4.924000001 -0.122000000 20.062000002

N 6.152000001 0.587000000 20.105000002

B 6.153900001 2.008000000 20.067000002

N 7.383000001 2.721000000 20.109900002

B 7.384000001 4.141000000 20.056900002

N 8.615000001 4.852900001 20.039900002

B 3.694900000 -6.514900001 20.067000002

N 4.921900001 -5.804000001 20.172900002

B 4.924000001 -4.384900001 20.073000002

N 6.152900001 -3.676000000 19.995000002

B 6.155000001 -2.254000000 19.952900002

N 7.381900001 -1.540000000 19.899000002

B 7.384900001 -0.124000000 20.056900002

N 8.614000001 0.589000000 20.036000002

B 8.614000001 2.007000000 20.079000002

N 9.845000001 2.719900000 20.085000002

B 9.846000001 4.141000000 20.065900002

N 11.076900001 4.852000001 20.079900002

B 4.924900001 -8.647000001 20.074900002

N 6.155000001 -7.939000001 20.170900002

B 6.155000001 -6.514900001 20.204000002

N 7.387900001 -5.804000001 20.175000002

B 7.384000001 -4.386000001 20.051900002

N 8.611000001 -3.674900000 19.928900002

B 8.612000001 -2.251900000 19.940900002

N 9.842000001 -1.544900000 20.051900002

B 9.843000001 -0.122000000 20.071000002

N 11.076900001 0.588000000 20.105000002

B 11.076000001 2.008900000 20.064000002

N 12.304900001 2.722000000 19.992900002

B 7.384000001 -8.646000001 20.065000002

N 8.618000001 -7.937900001 20.056000002

B 8.614000001 -6.514900001 20.068900002

N 9.843000001 -5.806000001 19.955900002

B 9.843000001 -4.383000001 19.940000002

N 11.076000001 -3.673000000 19.960000002

B 11.074900001 -2.253000000 20.053000002

N 12.310000001 -1.544900000 20.071000002

B 12.307000001 -0.122000000 20.059000002

N 13.535000002 0.588000000 19.954000002

B 12.307900001 4.142000000 20.074900002

B 13.535000002 2.011000000 19.945000002

B 9.843900001 -8.647000001 19.937000002

N 11.076000001 -7.937900001 19.902000002

B 11.073900001 -6.516000001 19.928000002

N 12.305900001 -5.806000001 19.914000002

B 12.305900001 -4.384000001 19.932900002

N 13.538900002 -3.674900000 19.923900002

B 13.535900002 -2.253000000 19.946900002

B 12.307000001 -8.647900001 19.936000002

N 13.538000002 -7.937000001 19.974000002

B 13.538000002 -6.516000001 19.931000002

H 4.522000001 -5.174900001 23.320000003

H 4.336000001 -2.661900000 23.347900003

H 8.692900001 -2.484900000 23.321900003

H 8.702000001 -5.033900001 23.347900003

H 5.743000001 0.935000000 23.495900003

H 4.536900001 -0.136000000 25.309000003

H 3.557900000 -0.090000000 23.952900003

H 2.460900000 -9.788000001 20.076000002

H 4.926900001 -9.784000001 19.993900002

H 7.381000001 -9.782900001 19.986900002

H 9.839900001 -9.785000001 19.870000002

H 12.307000001 -9.788000001 19.932900002

H 0.249000000 -5.948000001 19.870000002

H 0.242000000 2.581900000 19.951000002

H 1.475000000 4.711900001 19.992000002

H 0.244000000 -1.683000000 19.896000002

H 13.294900002 4.708900001 20.137000002

H 14.521000002 2.581000000 19.899000002

H 14.518000002 -1.680000000 19.865900002

H 14.525000002 -5.945900001 19.910000002

H 0.382000000 -4.142000000 19.954900002

H 0.389000000 -8.374000001 20.033000002

H 14.458000002 -8.442000001 20.054900002

H 14.519000002 -4.242000001 19.981000002

H 14.406000002 0.060000000 19.995000002

H 11.064900001 5.865000001 19.990900002

H 8.646000001 5.908900001 19.998900002

H 6.128000001 6.044900001 19.896900002

H 0.475000000 0.125000000 19.878000002

H 3.724000000 5.953900001 19.960900002

O-Isoniazide-Parallel-Top-B-vdw-opted

89

B -0.000774 -0.120828 -0.073563

N 1.230632 0.589829 -0.098564

B 1.228976 2.012250 -0.078607

N 2.461622 2.720261 -0.096697

B 2.460600 4.142153 -0.062554

N 3.692270 4.851063 -0.097884

B 3.690640 6.273061 -0.072230

N 4.922592 6.982821 -0.086126

B 4.922354 8.404609 -0.067168

N 6.154999 9.113960 -0.076364

B 6.152856 10.535715 -0.053152

N 7.384065 11.246168 -0.091523

B 1.231427 -2.253485 -0.066009

N 2.461329 -1.542510 0.001198

B 2.461397 -0.121573 -0.056139

N 3.692243 0.588006 -0.010380

B 3.692748 2.009223 -0.062625

N 4.924434 2.718483 -0.032698

B 4.923448 4.140470 -0.064080

N 6.153950 4.851502 -0.025588

B 6.153976 6.272524 -0.068696

N 7.386455 6.982089 -0.086680

B 7.385176 8.403524 -0.080506

N 8.616578 9.113875 -0.085442

B 2.464094 -4.385757 -0.056069

N 3.691570 -3.675084 0.039525

B 3.693388 -2.253568 0.052525

N 4.925077 -1.544686 0.057915

B 4.923733 -0.122486 0.061734

N 6.152242 0.587355 0.104997

B 6.154014 2.007788 0.066976

N 7.382714 2.721152 0.109832

B 7.383916 4.141380 0.056970

N 8.614813 4.853043 0.040322

B 8.617770 6.271309 -0.059653

N 9.851546 6.980915 -0.072555

B 3.694838 -6.515361 0.067405

N 4.921905 -5.804407 0.173385

B 4.924438 -4.385240 0.073163

N 6.153100 -3.676394 -0.005342

B 6.155133 -2.254198 -0.046909

N 7.382078 -1.540050 -0.100593

B 7.385090 -0.124446 0.056790

N 8.614353 0.588719 0.035732

B 8.613734 2.006982 0.079222

N 9.844813 2.719826 0.085266

B 9.845878 4.140776 0.066421

N 11.077323 4.851933 0.080220

B 4.924865 -8.647121 0.075449

N 6.154945 -7.938652 0.171138

B 6.155454 -6.514990 0.203658

N 7.387885 -5.803775 0.175186

B 7.383785 -4.385993 0.052201

N 8.610592 -3.675404 -0.071002

B 8.611936 -2.251679 -0.059186

N 9.842479 -1.545468 0.051935

B 9.842832 -0.122102 0.071251

N 11.076634 0.587883 0.105034

B 11.075617 2.009406 0.063632

N 12.305433 2.721507 -0.007233

B 6.151648 -10.777765 -0.055287

N 7.381920 -10.064135 -0.061091

B 7.383854 -8.646180 0.065305

N 8.617745 -7.938068 0.056008

B 8.613989 -6.514816 0.068879

N 9.842795 -5.805821 -0.043708

B 9.842748 -4.383347 -0.059962

N 11.075576 -3.673480 -0.039567

B 11.074641 -2.253179 0.053156

N 12.310162 -1.545032 0.071031

B 12.306498 -0.122061 0.059282

N 13.535330 0.588482 -0.045597

C 5.441722 -4.551252 3.340471

C 5.329179 -3.142878 3.348209

C 6.514364 -2.368136 3.349241

C 7.747753 -3.065075 3.349171

C 7.741917 -4.473801 3.354255

N 6.614363 -5.231535 3.345385

C 6.603498 -0.873665 3.244128

O 7.640438 -0.323841 2.833640

N 5.507563 -0.068377 3.544732

N 4.423027 -0.491544 4.344284

H 4.521950 -5.175345 3.319967

H 4.336113 -2.661680 3.347543

H 8.692606 -2.485492 3.322164

H 8.702339 -5.033981 3.348156

H 5.743463 0.935290 3.495786

H 4.536810 -0.136298 5.308916

H 3.557648 -0.090268 3.953186

O-Isoniazide-parallel-Top-Si-Cluster-MP2-AIM

99

Si 23.140000003 5.160000001 0.090000000

Si 20.426900002 6.730000001 0.084000000

C 21.332000003 5.166000001 0.099000000

Si 17.716000002 8.295900001 0.050000000

C 18.620000002 6.730900001 0.059000000

Si 25.852000003 6.729000001 0.021000000

Si 28.565000003 8.295900001 -0.035000000

C 29.466900004 6.730000001 0.001000000

Si 28.562900003 5.163900001 0.016000000

C 26.754900003 5.163900001 0.034000000

Si 31.277000004 9.861000001 0.025000000

C 32.179900004 8.297000001 0.075000000

Si 31.277000004 6.732900001 0.047000000

Si 17.719900002 17.689000002 0.014000000

C 18.623000002 16.125000002 0.065000000

Si 17.719900002 14.560900002 0.037000000

C 18.621900002 12.993000002 0.068000000

Si 20.431900002 13.009000002 0.125000000

C 21.335000003 14.560000002 0.190000000

Si 20.435900002 16.117000002 0.149000000

C 21.332900003 17.689000002 0.183000000

Si 20.431000002 19.250000002 0.110000000

Si 23.140000003 20.815900002 0.094000000

C 24.042900003 19.251900002 0.111000000

Si 23.144900003 17.675900002 0.171000000

C 24.047000003 16.117900002 0.200000000

Si 23.152900003 14.535900002 0.387000000

C 24.044000003 12.996000002 -0.070000000

Si 23.147900003 11.442000001 -0.010000000

C 21.341000003 11.432900001 0.172900000

Si 20.429900002 9.867000001 0.112000000

C 18.623000002 9.862000001 0.090000000

Si 17.718000002 11.429000001 0.050000000

Si 25.850000003 19.251000002 0.070900000

C 26.754000003 17.684900002 0.055000000

Si 25.841900003 16.117900002 0.059000000

C 26.754900003 14.557000002 -0.062000000

Si 25.844000003 12.994900002 -0.114000000

C 26.754900003 11.426000001 -0.166000000

Si 25.856000003 9.864000001 -0.067000000

C 24.045000003 9.865000001 0.057000000

Si 23.138900003 8.294000001 0.063000000

C 21.332900003 8.298900001 0.104000000

C 24.044000003 6.730900001 0.066000000

C 26.754000003 8.295900001 -0.032000000

Si 28.562900003 11.428000001 -0.106000000

C 29.468000004 12.990900002 -0.066000000

Si 28.559000003 14.556000002 -0.024000000

C 29.466000004 16.121900002 0.019000000

Si 28.560900003 17.685900002 0.027000000

Si 31.272900004 16.123000002 0.064000000

C 32.176900004 14.557900002 0.073000000

Si 31.272900004 12.990900002 0.022000000

C 32.179000004 11.428000001 0.059000000

C 29.466900004 9.862000001 -0.048000000

C 27.684000003 12.836000002 3.354000000

C 26.335000003 12.462900001 3.262000000

C 25.359900003 13.480000002 3.266000000

C 25.797000003 14.813000002 3.415000000

C 27.167000003 15.064900002 3.530000000

N 28.109900003 14.103900002 3.477900000

C 23.920900003 13.291900002 2.940900000

O 23.263900003 14.265000002 2.443900000

N 23.253000003 12.130000001 3.093900000

N 23.815000003 10.916900001 3.516900000

C 21.332000003 20.821900002 0.103000000

C 18.621900002 19.256000002 0.049000000

Si 28.562900003 20.820000002 0.020000000

C 26.754000003 20.818900002 0.039000000

C 32.179000004 17.690000002 0.104000000

Si 31.274900004 19.256000002 0.065000000

C 29.466900004 19.253000002 0.033000000

H 28.464900003 12.066000001 3.306000000

H 26.056900003 11.413900001 3.158900000

H 25.067000003 15.628000002 3.402000000

H 27.530900003 16.094000002 3.637900000

H 22.307900003 12.131900001 2.680000000

H 23.221000003 10.522000001 4.251900001

H 23.823000003 10.272000001 2.710000000

H 23.853900003 3.921000000 0.101900000

H 20.791000002 4.230900001 0.113000000

H 16.286900002 8.297000001 0.011000000

H 18.079900002 5.796000001 0.049000000

H 29.277900003 3.926000000 0.014000000

H 26.214900003 4.229000001 0.053000000

H 33.259000004 8.297000001 0.122000000

H 31.992900004 5.495000001 0.061000000

H 16.292000002 17.687900002 -0.054000000

H 16.291000002 14.561900002 -0.010000000

H 23.856900003 22.053000003 0.073000000

H 16.289000002 11.429000001 0.004000000

H 33.256000004 14.557900002 0.109000000

H 33.258000004 11.429900001 0.101000000

H 20.792000002 21.757000003 0.104000000

H 18.082900002 20.192000002 0.034000000

H 29.277900003 22.057900003 -0.005000000

H 26.213000003 21.754000003 0.031000000

H 33.258000004 17.690000002 0.151000000

H 31.989000004 20.495000002 0.059000000

O-Isoniazide-parallel-Top-Si-vdw-opted

67

Si 33.98395128 14.55724061 0.09823861

C 34.88875608 12.99366329 0.11404234

Si 12.29511246 14.55708678 0.01005814

Si 15.00769433 16.12395087 -0.04579002

C 15.90997308 14.55824327 -0.00990594

Si 15.00615978 12.99236953 0.00544758

C 13.19763259 12.99178812 0.02392123

Si 17.72001766 17.68865804 0.01444097

C 18.62324376 16.12467118 0.06472728

Si 17.71993424 14.56074715 0.03652568

C 18.6224556 12.99297504 0.0680951

Si 20.43217693 13.00930433 0.12507207

C 21.3354401 14.55971956 0.18990559

Si 20.43553538 16.11666251 0.14918147

C 21.3333215 17.68949253 0.18307726

Si 20.43099064 19.25036086 0.11032534

Si 23.13954623 20.81588188 0.09380459

C 24.04293611 19.25194787 0.1107026

Si 23.14493724 17.67634203 0.17067118

C 24.04717522 16.11825877 0.2004582

Si 23.15338655 14.53606604 0.38724807

C 24.04367189 12.9959613 -0.06961456

Si 23.14845839 11.44180649 -0.00996269

C 21.34091476 11.4326 0.17274933

Si 20.43036837 9.86726766 0.11203733

C 18.62254945 9.86219467 0.08961349

Si 17.71801756 11.42890152 0.05025302

C 15.90967237 11.42587291 0.01789878

Si 25.84991455 19.25065501 0.07126087

C 26.75400131 17.68518196 0.05493068

Si 25.84214833 16.11791242 0.05927242

C 26.75451108 14.55704265 -0.06248801

Si 25.84399384 12.99512926 -0.11360084

C 26.7546554 11.42599359 -0.16628317

Si 25.85601399 9.86414284 -0.06732219

C 24.04499425 9.86478928 0.05717699

Si 23.13932926 8.29419603 0.06258022

C 21.33257909 8.29859411 0.10391683

C 24.04361581 6.73058346 0.06626374

C 26.75443625 8.29613031 -0.03201213

Si 28.56287066 11.4278839 -0.10642475

C 29.46752349 12.99133819 -0.06592326

Si 28.55875292 14.55620166 -0.02362844

C 29.46625826 16.12165016 0.01932305

Si 28.56101125 17.68617161 0.02733804

Si 31.2725204 16.12308082 0.06412395

C 32.17732605 14.55820958 0.07328265

Si 31.27300359 12.99147071 0.02241253

C 32.17880994 11.42779779 0.05943339

C 29.46721992 9.86243813 -0.04770031

C 27.68411215 12.83570777 3.35402374

C 26.33510999 12.4629567 3.26162685

C 25.35991634 13.48036701 3.26588178

C 25.7966204 14.81306905 3.41481618

C 27.16728634 15.06478177 3.53045527

N 28.11034605 14.1044671 3.477513

C 23.92083388 13.29181163 2.94120787

O 23.26389112 14.26548287 2.4440614

N 23.2529525 12.12978228 3.09391315

N 23.81541407 10.91704937 3.51681203

H 28.46523979 12.06621278 3.30614268

H 26.05731315 11.41427202 3.15883526

H 25.06673837 15.6284689 3.40244149

H 27.53096062 16.09422695 3.63798003

H 22.30840323 12.13215471 2.68024607

H 23.22098154 10.52224003 4.25193211

H 23.82311259 10.27173114 2.70978235

O-Isoniazide-Top-Al-AlN-Cluster-MP2-AIM

99

Al 31.464900004 11.099000001 -0.079000000

Al 34.213000004 12.683900002 -0.037000000

Al 20.481000002 20.612900002 -0.037000000

N 21.405900003 15.859000002 -0.039000000

Al 20.481900002 17.443000002 -0.020000000

Al 23.234000003 19.025900002 0.141900000

N 21.402900003 19.027900002 0.045000000

N 24.161000003 20.609900002 0.189000000

Al 23.234900003 22.193000003 0.064000000

Al 25.977000003 23.780900003 0.116000000

N 24.144900003 14.274000002 -0.013000000

Al 23.237900003 15.862900002 0.037000000

Al 25.998000003 17.449900002 0.268000000

N 24.161000003 17.445000002 0.188000000

N 26.908900003 19.025900002 0.601000000

Al 25.995000003 20.597900002 0.284900000

Al 28.728000003 22.187900003 0.094000000

N 26.893000003 22.196000003 0.256000000

N 29.632000004 23.783900003 0.013000000

Al 28.719900003 25.370000003 -0.002000000

N 26.887000003 12.686900002 -0.064000000

Al 25.978000003 14.278900002 -0.008000000

Al 28.727000003 15.865900002 -0.099000000

N 26.893900003 15.864000002 0.070900000

N 29.617900004 17.446900002 -0.177000000

Al 28.804900003 18.989000002 0.450000000

Al 31.446000004 20.611900002 -0.066000000

N 29.623000004 20.609000002 0.042000000

N 32.381000004 22.195000003 -0.074000000

Al 31.463900004 23.780900003 -0.044000000

N 29.632900004 11.099000001 -0.070900000

Al 28.719000003 12.686900002 -0.103000000

Al 31.463000004 14.272900002 -0.164000000

N 29.631000004 14.268000002 -0.181000000

N 32.381900004 15.856900002 -0.189000000

Al 31.443900004 17.440000002 -0.151000000

Al 34.203000004 19.024900002 -0.082000000

N 32.371900004 19.027000002 -0.078000000

N 35.127000004 20.611900002 -0.066000000

Al 34.213000004 22.199900003 -0.072000000

N 32.381000004 12.685000002 -0.101000000

N 35.137000004 14.266900002 -0.046000000

Al 34.210000004 15.852900002 -0.105000000

Al 36.957900004 17.439000002 -0.021000000

N 35.128000004 17.439000002 -0.072000000

N 37.872900005 19.024900002 -0.042900000

Al 36.959000004 20.614000002 -0.049000000

C 30.593000004 20.548900002 6.626900001

C 29.573000004 20.126000002 5.764900001

C 29.882900004 19.960000002 4.403000001

C 31.199900004 20.228000002 3.984900000

C 32.128900004 20.673000002 4.929900001

N 31.847900004 20.832000002 6.235000001

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O-Isoniazide-Top-Al-AlN-vdw-opted

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