

H2O+O-Isoniazide-Parallel-Top-Al-AIN-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-optimized

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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
N	17.755000	13.233000	0.075000
B	19.175000	13.192000	0.012000
N	19.846000	11.943000	-0.119000
B	21.269000	11.903000	-0.149000
N	21.938000	10.648000	-0.072000
B	23.362000	10.607000	-0.070000
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
N	15.587000	12.073000	-0.035000
B	17.007000	12.028000	-0.024000
N	17.679000	10.777000	-0.076000
B	19.101000	10.734000	-0.063000
N	19.772000	9.484000	0.027000
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

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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

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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

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
C	28.943900003	19.478900002	3.354000000
O	29.437000004	18.876900002	2.347900000
N	27.611900003	19.667900002	3.386000000
N	26.986000003	20.524900002	4.312000001
N	21.405900003	22.196900003	-0.046000000
Al	23.225900003	25.367900003	-0.021000000
N	24.141900003	26.954000003	-0.042900000
N	24.144900003	23.782000003	0.069000000
N	26.887000003	25.368900003	0.046000000
Al	25.974000003	26.957000003	-0.024000000
N	32.381900004	25.370000003	-0.061000000
Al	31.464900004	26.955900003	-0.079000000
N	35.137000004	23.786900003	-0.039000000
Al	34.213900004	25.370900003	-0.020000000
N	37.877000005	22.202000003	-0.013000000
Al	36.969900004	23.791000003	0.037000000
N	26.887000003	28.544000003	-0.064000000
N	29.632900004	26.955900003	-0.070900000
Al	28.719000003	28.544000003	-0.103000000
H	30.385000004	20.670900002	7.697000001
H	28.568000003	19.932900002	6.141000001
H	31.481900004	20.083900002	2.937000000
H	33.155900004	20.905900002	4.623900001
H	27.126900003	19.373000002	2.492000000
H	26.745900003	21.403900003	3.834000000
H	26.111900003	20.082000002	4.612000001
H	18.981900002	20.612900002	-0.096000000
H	32.215000004	9.800000001	-0.068000000
H	34.957900004	11.384000001	0.023000000
H	37.707000005	16.140900002	0.039000000
H	21.727000003	25.364900003	-0.076000000
H	32.215000004	28.254900003	-0.100000000
H	34.960000004	26.670900003	0.029000000
H	37.719000005	25.085900003	0.139000000
H	29.469000004	29.841900004	-0.161000000
H	23.518900003	27.850000003	-0.038000000
H	26.205900003	29.504900004	-0.057000000
H	39.201900005	22.219900003	-0.058000000
H	39.045900005	19.013900002	-0.018000000
H	36.402900004	14.256000002	-0.059000000
H	29.155000003	10.102900001	-0.011000000
H	26.385000003	11.708900001	-0.033000000
H	23.628000003	13.263900002	0.046000000
H	20.719900002	14.864000002	-0.076000000
H	20.782000002	23.012000003	-0.079000000
H	18.981900002	17.442000002	-0.057000000

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

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N	18.6505	17.44212	-0.06127
Al	17.7332	19.02854	-0.07923
Al	20.4814	20.61312	-0.03676
N	21.4058	15.85932	-0.03927
Al	20.4825	17.44274	-0.01998
Al	23.2342	19.02555	0.142207
N	21.4034	19.02822	0.045077
N	24.1608	20.60956	0.188687
Al	23.2351	22.19285	0.063924
Al	25.9766	23.7813	0.116071
N	24.145	14.27399	-0.01321
Al	23.238	15.86311	0.037097
Al	25.9982	17.45019	0.26755
N	24.1608	17.44455	0.188135
N	26.9093	19.0259	0.60086
Al	25.9947	20.59793	0.284547
Al	28.728	22.18814	0.093552
N	26.8929	22.19598	0.256416
N	29.6319	23.78354	0.012504
Al	28.7198	25.36966	-0.00156
N	26.8871	12.68713	-0.06444
Al	25.9783	14.27866	-0.00773
Al	28.7267	15.86586	-0.09898
N	26.8942	15.86409	0.071026
N	29.6181	17.44731	-0.1775
Al	28.8048	18.98888	0.450343
Al	31.4457	20.61154	-0.06623
N	29.6232	20.60853	0.042277
N	32.3807	22.19474	-0.07425
Al	31.4641	23.78096	-0.04434
N	29.633	11.09852	-0.07109
Al	28.7188	12.68656	-0.10286
Al	31.4628	14.27336	-0.16376
N	29.6309	14.26815	-0.18104
N	32.3822	15.85714	-0.18915
Al	31.4435	17.43966	-0.15112
Al	34.2033	19.02543	-0.08206
N	32.3719	19.02699	-0.078
N	35.1272	20.61192	-0.06601
Al	34.2129	22.19988	-0.07171
N	32.3813	12.68483	-0.10109
N	35.137	14.26718	-0.04558
Al	34.2105	15.85328	-0.10543
Al	36.9576	17.4385	-0.02073
N	35.1279	17.43946	-0.07195
N	37.8732	19.02504	-0.04273
Al	36.9589	20.61435	-0.0494
N	37.8766	15.85275	0.068715

N	40.6187	17.4399	0.046037
Al	39.7049	19.02808	-0.02379
C	30.5927	20.54872	6.627411
C	29.5733	20.12613	5.764574
C	29.8832	19.96002	4.403345
C	31.1997	20.22815	3.984543
C	32.1294	20.67257	4.929824
N	31.8484	20.83196	6.234713
C	28.9437	19.47932	3.353538
O	29.4374	18.87743	2.34823
N	27.6117	19.66828	3.386122
N	26.9855	20.52544	4.312171
H	30.3846	20.67117	7.696898
H	28.5678	19.93319	6.141309
H	31.4818	20.08408	2.9373
H	33.1565	20.9056	4.623745
H	27.1266	19.37311	2.492163
H	26.7455	21.40431	3.833915
H	26.1117	20.08167	4.611599