

This dataset was generated using an iterative active learning strategy with the ArcaNN software package (https://github.com/arcann-chem/arcann_training) to train machine-learning interatomic potentials (MLIPs) for aqueous nitric acid solutions. Each active-learning cycle consisted of three stages: (1) training, (2) exploration, and (3) labeling.

The initial training set comprised approximately 800 randomly selected configurations from a previous study by Lewis et al. (<https://doi.org/10.1021/jp205510q>), which investigated nitric acid solutions at 2, 3, 4, and 5 mol/L. For all configurations, single-point calculations of atomic forces and total energies were performed at the quantum density functional theory BLYP-D2 and PBE-D3 levels of theory using the CP2K Quickstep module. Valence electrons were treated explicitly, while core electrons on all atoms were represented by norm-conserving Goedecker–Teter–Hutter (GTH) pseudopotentials. Long-range dispersion interactions were accounted for using Grimme dispersion corrections. Wave functions were expanded in a mixed Gaussian-and-plane-wave scheme using TZV2P-MOLOPT basis sets for all elements and an 800 Ry auxiliary plane-wave cutoff for the electron density. Self-consistent field convergence was accelerated using orbital transformation and Direct Inversion in the Iterative Subspace, with a convergence threshold of 10^{-6} . All single-point calculations were carried out in periodic orthorhombic cells whose dimensions match those of the molecular configurations sampled from earlier trajectories. The CELL_REF keyword in CP2K was used to define a fixed reference cell, ensuring consistency in the reference data used for MLIP training, particularly when cell fluctuations are present in NpT simulations. The resulting high-fidelity energies and forces constitute the ground-truth labels used to train the MLIPs contained in this dataset.

Below we provide some examples of the dataset.

Example of dataset obtained at BLYP-D2 level of theory:

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Lattice="13.745143556437252 0.0 0.0 0.0 13.745143556437252 0.0 0.0 0.0 13.745143556437252"

Properties=species:S:1:pos:R:3:forces:R:3 energy=-43210.327253523166 pbc="T T T"

N	11.68575700	4.12682000	7.40437100	-1.09873994	1.20213687	1.46276859
O	10.81868600	4.58527200	6.58836800	0.15381780	-0.04809712	-0.52811080
O	12.40092400	3.11899600	7.08543300	0.72828406	-0.67402606	-0.54523127
O	11.81940100	4.68210000	8.56417800	0.21972444	-0.51910320	-0.29086430
H	9.38614600	6.55853400	10.26096500	-0.31668023	-0.75761109	0.30710853
N	5.84102900	7.12470600	12.72010100	-0.30322925	0.79138150	1.74523566
O	5.87035700	6.19889400	11.91077600	0.28443808	0.36493367	0.04568542
O	5.40833200	8.27244900	12.57501100	-0.16937401	-0.19460270	-1.01575964
O	6.35775400	6.98187700	0.32443900	0.44380072	-0.59026723	-0.24968242
H	8.59708700	2.99618800	5.60889100	-0.52926112	0.13817829	-0.18844542
N	10.47275100	12.01393500	13.37689700	-0.68791825	0.11857209	0.03565863
O	10.23251300	13.25051700	13.02078500	0.29173796	-0.58873691	-1.09790793
O	10.13465500	11.09628400	12.56003500	0.15729805	-0.32213148	0.07530145
O	10.94763100	11.74611100	0.79356500	-0.02323352	0.36032523	-0.50328783
H	6.06915400	0.34432800	10.34618400	-0.03148265	-1.71128938	-0.27450128
O	1.03614600	5.43730800	3.60108400	-0.55417716	-0.43690194	-0.63024223
H	1.54288500	5.71413000	4.39267100	-0.46120195	-0.40121554	0.17397937
H	0.28798700	4.79973200	3.79118600	0.71334389	0.56425589	0.30001794
O	12.37770100	10.56940900	10.53441400	-0.52555873	-0.61638090	0.97462764
H	11.97371400	10.28846400	11.40850300	0.31980464	0.29580647	-0.85962733
H	13.34748200	10.42020700	10.64012400	0.12491757	0.38369964	-0.20603588
O	11.73982000	9.89482600	6.04046500	1.10666048	-1.11501246	-0.33581438
H	11.94814900	9.96119900	5.05051800	0.15885716	0.15147604	0.60348167
H	10.59628500	4.96804000	1.88207900	-0.99019362	0.26925057	-1.10713562
O	9.53020600	5.57055700	10.37901100	1.69670917	1.08470275	-0.86654823
H	6.20288700	0.34513300	3.40381800	0.22548474	-0.16812496	0.10198179
H	10.42846100	5.47283600	9.89292000	-1.54255095	-0.16336842	0.50671871
O	6.08193200	12.39126900	12.58057300	0.59242181	0.41635882	1.46159411
H	6.49140800	12.99498100	13.28930800	0.27327795	-0.07585526	-1.07620988
H	3.43255900	7.31078200	9.65050300	-0.06632213	0.53702585	-0.08704779
O	1.22723100	10.13541300	7.58988700	-0.15427803	0.09316393	-0.76620937
H	0.49431000	10.78333600	7.46893600	0.01851914	0.28474918	-0.13838964
H	1.22264000	10.01375100	8.54228100	0.22649004	-0.33915990	1.21542330
O	0.29673000	0.39288300	5.49559000	-0.26679260	0.44925044	0.51790044
H	1.14739300	13.72256500	5.75367900	0.01925191	-0.14454846	-0.01151854
H	0.15882600	1.14652900	6.11927000	0.06545566	-0.48588197	-0.40934794
O	4.09480300	10.36567900	4.98979200	-0.90325535	0.67135160	-0.55720541
H	3.41973000	10.07196900	4.32981500	0.56987478	0.25734482	0.28022044
H	4.70834100	9.62879800	5.01820400	0.29931140	-0.74405212	-0.01462186
O	3.02159900	7.65453300	10.49608700	0.79646766	0.09624617	0.51160535
H	3.15776300	8.62474800	10.67681000	0.12655845	-0.90778667	-0.58293290
H	3.18647800	8.65959900	1.19766500	0.50889746	-0.82508250	0.09387356
O	2.38121200	12.37198000	6.25750400	-0.14684291	0.77468836	0.28803248
H	2.69209600	11.45698000	6.31678600	-0.19143767	-0.66997812	0.16473779
H	3.13005400	12.79697200	5.82095500	0.78001826	0.42029570	-0.33754731
O	9.64507600	13.02702100	5.47901800	-0.58960234	0.91307954	0.87700130
H	9.52424400	0.14171500	5.97756100	0.00859726	-0.70335361	-0.36402504
H	9.44477200	12.27265100	6.11240700	0.16591073	-0.05145652	-0.46958169
O	3.68161500	2.01173000	13.49884200	-1.38078073	1.00634374	-0.52951514
H	5.16457400	11.45612100	3.59073100	-0.44138337	0.66350151	-0.72539208
H	2.47670000	2.52124100	13.71754300	-0.46131559	0.07033665	0.83767371
O	0.64922400	6.88107700	10.82216200	-1.51766113	-0.59637463	-0.16332574
H	1.55348900	7.24088600	10.78904000	0.67135777	0.83976761	-0.32389012
H	0.09942600	7.50237500	11.33623700	0.39200122	0.03599031	0.12574341
O	13.59528900	13.41941200	1.48850900	1.00641574	-0.14933894	2.02050159
H	13.50601800	13.48406800	0.54776900	-0.37999674	0.32229809	-1.76200491
H	12.79499500	13.01870200	1.84464200	-0.60019889	-0.12741823	0.11127633
O	5.24063200	12.06013900	2.79395700	0.61428545	-0.49617101	0.50510868
H	12.31974900	7.35201700	12.83541300	-0.30659739	1.42759538	0.22982733
H	4.33322500	12.38476700	2.53431700	-0.12625763	0.01736780	0.35886432
O	5.65267000	4.52325300	9.08576500	-0.37050679	-1.51249321	0.56623512
H	6.35789400	4.01022600	9.51393600	-0.04320071	-0.19793485	-0.01939023
H	6.05469100	5.35463100	8.85809000	0.80242799	1.72971442	-0.53027259
O	13.57820700	1.88028600	10.15658800	-0.12498596	-1.06172171	-0.11977999
H	0.61611600	1.30190700	10.03093500	0.29629035	0.43775606	0.00990235

H	12.94272200	1.28243600	9.69263900	-0.19266872	0.24257178	0.15807555
O	3.04171500	9.55821900	0.86673300	-0.50317213	-0.26898266	0.47064356
H	2.48189700	9.86162900	1.65212600	0.11134215	0.52222709	0.00708082
H	3.55259700	1.04316600	13.41181300	0.41919064	-1.37729894	-0.14836501
O	5.14309500	8.49650100	6.92116500	-0.96038321	-2.40482703	0.37337615
H	5.33900500	9.39954200	7.02506600	0.68467969	2.71866722	0.19552830
H	4.30927200	8.39175800	7.44379600	0.67157066	-0.11099916	-0.38854977
O	1.64114700	10.31237100	3.03954800	-0.46523293	-0.48357004	0.85440799
H	1.48289400	9.79636400	3.90765600	-0.01543331	0.50633407	-1.29359358
H	0.68406500	10.50128700	2.78226700	0.41374195	-0.03552751	0.58082614
O	12.76467600	10.48400100	3.40476200	-0.20538642	-1.07313792	-0.78850238
H	6.37459000	3.37477300	1.12160100	-0.53866004	-0.92323643	0.23150112
H	12.36528400	11.38615500	3.32044000	-0.33893107	-0.07627024	0.33777408
O	8.16228900	12.87986800	10.54976200	0.12279538	-0.31927447	0.71251034
H	7.48125100	12.58336300	11.21058100	0.14243296	0.08461141	-0.13517062
H	8.98323300	12.89496100	11.10861000	-0.30415587	0.03543443	-0.25629118
O	8.27780900	3.13612800	11.39372000	-0.98606237	0.34119724	-0.34880771
H	8.24698400	4.04984400	11.04059000	0.48658800	0.16086674	0.11876749
H	8.92788200	2.70095400	10.80626400	0.51064581	-0.41032804	-0.12017131
O	3.19636500	2.44820100	3.69309500	-0.90587891	0.74684588	0.33971320
H	3.15286100	2.44168000	4.69394800	0.21791130	-0.38232204	-0.48676026
H	3.51634000	4.66133200	3.71623700	0.45366656	-0.06292210	0.24211361
O	9.30196800	10.53416000	6.58480100	-0.01280615	-1.40727132	-0.50607491
H	10.23369000	10.13042600	6.36765200	-0.74734982	0.57179076	0.36327428
H	8.69009600	9.95940100	6.02041700	0.45535526	1.14592175	0.55249566
O	2.96348100	13.35174600	2.07593500	-1.37340886	-0.71281578	-0.31792002
H	2.82803300	13.11204900	1.10574900	0.52091788	0.24939394	0.70184129
H	2.11563600	13.01895900	2.48944800	0.86893730	0.32503477	-0.34199069
O	1.31337300	2.81528400	0.22300900	1.93472495	-0.59279308	-1.55809173
H	0.96631900	2.71910700	1.15770700	-0.28945687	-0.36661157	0.71333309
H	0.94957900	3.50846000	13.36659000	-0.26628095	0.64109691	0.16528081
O	3.20109900	12.44510000	10.54629800	0.91434864	-1.54891443	0.33739355
H	2.82458500	12.96494600	9.80699100	-0.22809955	0.40321534	-0.44316669
H	3.82355800	11.75296900	10.16817700	-0.60477596	0.88664037	0.49452705
O	8.79960500	6.93133400	5.96268100	-0.27798050	0.14690925	0.60046988
H	8.39210400	6.96153100	6.88526100	-0.00921689	-0.02762136	-0.75582057
H	9.31213200	6.10667800	5.96880800	0.14594817	-0.09711829	-0.00371730
O	6.03104700	1.15614500	3.93063600	0.41925594	0.79797330	-0.06200421
H	6.87309700	1.65631300	4.13247400	-0.32394720	-0.53848726	-0.02786356
H	4.00069000	2.00378400	3.39457800	0.30154260	-0.27388113	0.14763584
O	6.41370300	11.49902800	6.86171000	-0.08792916	-0.49078661	0.76214909
H	6.90108400	11.22183000	7.69455700	-0.39119595	0.59066523	-0.61376351
H	5.95943500	12.37090500	6.96366700	0.16666252	-0.17395108	-0.28641989
O	4.48840200	8.13408400	3.08121100	-1.61309637	3.84669101	-1.77307865
H	5.29865100	8.37293200	2.63372800	0.77232140	-0.47188283	-0.03795000
H	4.49556600	7.36106800	3.55769900	0.71447003	-3.35542000	1.59820917
O	5.22817100	3.77577500	12.23130000	2.28986375	-2.17465569	-1.21407913
H	4.12363500	4.55409800	11.95647800	-0.41497814	0.12123729	-0.38148386
H	5.22363800	2.75602600	12.09299900	-0.71501562	1.57441926	0.20704633
O	7.50965300	0.26001100	0.64971900	1.20488846	0.32925190	0.53209344
H	8.42583800	0.67017200	0.72422200	-0.76782197	-0.73374868	-0.48856672
H	6.98443700	0.99551400	1.01214500	-0.54827648	0.31994245	-0.18914476
O	11.26304300	9.12948600	1.56873500	0.06780822	-1.70898979	0.34079821
H	10.96219800	9.95563900	1.18573700	-0.50603582	1.19371445	-0.46158813
H	10.42282200	8.51541400	1.70881500	0.89526796	0.73864663	-0.14090521
O	8.12820200	3.33049900	4.78872400	1.33843414	-0.44056011	0.41937473
H	8.99761900	3.43583200	4.18519100	-1.28582525	-0.49694697	-0.01945400
H	12.67720800	13.10526400	4.65860700	-2.77393258	-0.46169406	-2.04666565
O	4.45029300	5.41166300	1.17229300	0.74927454	-0.47019979	0.46856148
H	3.48137500	5.63557700	1.11359700	-0.33845645	0.44936613	-0.39091827
H	5.83995900	6.22228000	0.78606500	-0.54817981	0.02853256	-0.88021415
O	5.89280000	2.53882600	1.40278600	0.70655515	0.88224224	-0.35840872
H	6.26420400	2.38540900	2.29583000	-0.54807079	-0.00036561	0.01637227
H	4.47202400	2.17628400	0.30504400	0.20110399	0.31343653	0.90607226
O	2.01098200	6.27176100	1.04302100	-1.53662559	-0.54479521	-1.58836133
H	1.51008800	5.94491400	0.19053200	0.84163578	0.51572940	1.56466501
H	1.41478400	5.99147200	1.78157400	0.38795019	0.10684889	0.16318176
O	9.09471600	7.67910400	1.67676800	-0.09333002	0.08662304	0.22322679
H	8.60500200	8.24213800	1.00656100	0.01590947	-0.40225941	0.04392370
H	8.52682200	7.71262100	2.54994100	0.33660988	0.29347859	-1.10857647

O	12.35741500	7.24711900	6.79117100	1.57399812	-0.45123018	-3.07831779
H	12.05490400	7.54048000	7.61404900	-0.90920694	0.86604120	3.31901935
H	11.94933500	6.38796800	6.65798300	-0.56692418	-0.37273440	-0.28863155
O	7.93764100	10.53677100	9.03648800	-0.12141830	-0.39470293	-0.05593693
H	8.23032300	11.31222600	9.57365100	-0.13962017	0.40098003	0.25691853
H	8.61950400	10.42581200	8.33329800	0.29574014	-0.08079178	-0.49757278
O	11.84447800	12.82992000	4.01798600	2.74637703	1.35899063	1.67891868
H	12.32071300	9.88391400	2.71089800	0.01803320	0.58901973	0.68209881
H	11.00721700	13.14026100	4.46726700	0.56363060	-0.56746257	0.08357886
O	0.61078500	2.00524300	2.57515500	-0.06783496	1.48933940	0.23175463
H	0.31592100	1.10095400	2.34319400	-0.01650237	-0.88542630	-0.39999581
H	1.49384200	2.02038100	3.01616500	0.17884184	-0.33691430	0.10873196
O	1.39142600	10.28029900	10.42998900	-0.19546813	0.06361681	-0.97007010
H	1.33780500	9.94813800	11.35172800	0.16536103	-0.92305696	1.06962580
H	1.89345200	11.09846600	10.55492700	0.29305385	0.83138633	-0.22479568
O	8.60260700	2.97450800	0.37072400	-0.05874406	-0.24389281	0.39721542
H	6.07587900	3.99135100	11.70141100	-1.63261413	0.12945608	1.03702215
H	9.17448500	3.75512600	0.48674000	-0.00016095	0.71847067	0.24421111
O	12.51475800	3.47209900	4.05107200	-0.86393444	1.91733966	-0.68375100
H	12.34735200	3.37899400	4.99031500	0.11915933	-0.70612577	0.92026475
H	13.01105700	2.77252200	3.61584200	0.89264647	-1.16396112	-0.07870199
O	3.68991800	13.12317200	13.22454300	0.12887347	-0.98452999	-0.35536608
H	4.60129300	12.62821800	13.11481600	-1.33330479	1.52432594	-0.03595328
H	3.28700100	12.86413800	12.35618800	-0.02691534	0.25287419	0.12324378
O	11.82228700	13.26915600	9.52213700	-0.13199942	0.29888614	0.40270575
H	11.86639300	12.47523600	10.09902200	0.06982037	-0.06822628	0.22671990
H	12.18634400	12.89629900	8.68964200	0.07001526	0.00122127	-0.51622099
O	0.95350300	8.70752000	5.40571700	0.68320182	-0.48770951	-0.66963770
H	0.95198300	9.02250500	6.33416200	0.25967321	0.66069592	0.64414778
H	0.33086100	7.97725200	5.42005600	-0.94007201	-0.34948751	-0.22702123
O	5.28583600	9.61480600	10.05079600	0.10349822	1.16376520	-1.96725609
H	5.65180200	9.06875100	10.73562200	0.51019021	-0.77362906	1.01043848
H	6.04951400	9.80174200	9.42791800	-0.78117525	-0.13170940	0.89072123
O	12.51338400	8.36066400	12.91481400	-0.37312829	-0.77176296	0.87238206
H	12.17179400	8.62987400	0.09621000	-0.03717044	-0.42284469	-0.86499939
H	12.15795100	9.01143800	6.34995700	-0.87908544	1.14658921	-0.76671280
O	12.05249700	7.87581500	9.39368200	-1.01608360	1.06353845	0.07458205
H	12.80378900	7.30814100	9.54026100	1.05030961	-0.63603544	0.30943692
H	12.25724100	8.73670800	9.85362800	-0.27220014	-0.29683183	-0.37419581
O	12.90733100	12.07590600	7.29149700	1.03865326	1.04720321	0.37493732
H	12.37925500	11.41540200	6.83322000	-0.78656171	-0.93746286	-0.72597778
H	13.28036200	12.67651100	6.60323800	-0.17072898	-0.10798634	0.24375243
O	5.07341100	13.74915500	6.13504100	1.14606830	-1.29349331	-2.41744961
H	4.63037000	0.46464100	6.80930700	-0.97107438	1.86613768	1.15039804
H	5.36372400	0.57284800	5.32024200	-0.45375449	-0.47596009	1.48532848
O	4.13695400	5.36126400	4.04445600	-0.15215481	0.04694938	-0.04829561
H	5.06688100	5.03460800	3.97572900	0.12991477	-0.25927675	0.02835567
H	4.57503100	5.44715200	2.14361800	0.09283689	-0.12330292	-0.26580838
O	9.93618900	3.39592600	3.04264500	2.15283319	-2.07123923	-1.07451347
H	10.85710600	3.50969200	3.40909500	0.05786114	0.43780028	0.47899553
H	10.20916200	2.49404300	2.54805600	-1.25578242	1.46004990	0.83149483
O	5.75660600	3.17676700	6.59766000	2.26797286	0.44536601	-0.58391095
H	6.05295400	3.81057200	7.30400500	-0.84354714	-0.36640794	-0.05388930
H	6.64088400	3.10290500	6.07901000	-1.94819753	0.03095506	0.39911546
O	7.17592900	10.16688100	4.69456900	0.34725785	0.15925774	-1.63347854
H	7.44194500	10.85481300	3.99921500	0.03577947	-0.59750900	0.42787634
H	6.58582100	10.65279400	5.28721700	-0.22566163	0.46315188	0.96947361
O	6.82625600	4.96737500	3.02961500	-0.47428784	1.03789170	-0.05185350
H	7.02208900	5.96471500	3.06951700	0.09385864	-1.57459307	0.40173439
H	7.36721900	4.43204100	3.67147900	-0.16746470	0.90078864	-0.02961243
O	1.27985200	9.12457600	12.68819100	0.41830258	-0.30186091	1.02450139
H	1.91545600	9.06055100	13.49264500	-0.95940414	0.60773273	-1.13656036
H	5.83744400	11.64690700	13.20214400	0.47871425	-1.07191048	-0.41072348
O	3.83657800	6.29293000	8.25472200	-0.64186002	-0.27339519	0.24171457
H	3.17362500	6.40580200	7.51097000	0.33717707	-0.39187729	0.25864066
H	3.78907300	5.35290700	8.56602600	0.07425244	0.73420839	-0.39015362
O	8.00902200	9.17475800	13.39352600	-2.56466842	0.46882322	0.44856087
H	7.05088200	9.51241200	13.62904600	1.13046633	-1.06312039	-0.18421133
H	8.43121100	10.02536600	13.49432900	1.39561857	0.84571303	-0.31818176
O	3.03887700	2.27531800	6.53003100	1.70807242	-0.41497300	-0.41047100

H	3.89286800	2.79326700	6.61751000	-0.36342649	-0.52807841	-0.03920881
H	2.35375700	2.86154300	6.86190300	-0.92205629	0.85416168	0.33104704
O	1.72494100	4.00614200	9.85839200	0.10295675	-0.18933914	1.49144667
H	1.41417400	4.26080400	8.95640900	-0.13445534	0.03336418	-0.03316415
H	0.95008400	3.85930500	10.47338300	0.46856199	0.13539533	-1.10539704
O	7.13250700	6.91180800	8.20673300	-0.92727563	0.93302359	0.30418570
H	6.41132800	7.56229000	7.83811700	1.00410380	-1.03130453	0.72991259
H	7.36751100	7.16853300	9.15276600	-0.31963340	0.13830531	-0.99025892
O	5.88028500	1.24405900	10.55483200	1.13903633	2.09502347	0.72728235
H	0.33069900	8.94589700	12.96295200	0.42356768	-0.27542842	-0.06247010
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O	8.41947500	12.03187700	3.13387000	0.31978715	0.04938884	1.65810405
H	8.79374600	12.41843700	3.99072200	-0.15323005	-0.36271121	-0.70176673
H	8.51190200	12.75959500	2.51781800	-0.18324768	0.41604309	-0.86742651
O	5.55658100	10.39240900	0.61891500	1.19382192	1.08012618	0.66151045
H	5.64631100	11.01930400	1.42852600	-0.46329894	-0.73583025	-0.56396947
H	4.63638700	10.03651700	0.63546900	-0.34796079	0.11941747	0.15181954
O	8.10174900	8.16558900	10.61729100	-0.04634157	0.84715542	-0.31765005
H	8.07522800	9.03191500	10.07764500	0.23562517	-0.88058234	0.68317713
H	8.11960600	8.45261900	11.56781800	0.05770687	0.01586782	-0.26362500
O	10.39552800	2.09030600	9.70767600	-0.24177628	1.79189861	0.11276139
H	10.97478900	2.88222800	9.88590100	-0.32839418	-0.82583943	-0.28593343
H	10.93079800	1.30568800	9.85592500	0.39043953	-1.01887067	0.07102107
O	2.48590000	6.35422000	5.85368200	1.08005419	-0.98435721	-0.10721193
H	2.05578900	7.18821900	5.56912900	0.44462862	0.76237792	-0.11899786
H	3.35758200	6.10903900	5.33339500	-1.44101602	0.57503653	0.38491680
O	2.12118600	0.28908100	8.67432800	0.44515775	-0.88686200	-0.88696073
H	2.39007300	13.47764600	7.85445200	-0.58967536	0.76302995	0.83352189
H	2.74010700	1.04093100	8.71179500	-0.01360165	0.08031304	-0.36613181
O	3.21895000	5.14248500	11.64398700	1.43400308	0.21134933	0.20299273
H	2.78107300	4.64641600	10.84947900	-0.38873386	0.38165099	-0.37305682
H	3.50433000	6.09464800	11.38469900	-0.62212268	-0.69199293	-0.05167764
O	11.50644100	5.84867100	12.64202000	1.48168419	-0.08310783	-0.21838386
H	10.73934100	5.87756100	12.04921000	-0.39781860	-0.10896336	-0.30458730
H	11.22502100	5.44808600	13.50233200	-0.61267439	0.27686412	0.07217550
O	0.59786800	5.03880200	12.58852700	1.33886146	-0.57848746	0.25493570
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O	10.17390100	5.26164100	1.01658300	1.31870504	-1.58830065	0.80704981
H	8.28721900	3.01531200	13.19914200	0.20970022	-0.04509150	-0.56920732
H	9.70638800	6.09202400	1.19374600	-0.56969891	1.19640845	0.34139213
O	7.46087200	7.78604900	3.60700500	-0.63056053	0.64017440	0.71844599
H	7.16318200	8.70118400	3.99852200	0.35615027	-0.70454197	-0.52554896
H	7.94203800	7.42116500	4.38086700	0.20034449	-0.35717305	0.72939683
O	10.69222400	1.40804900	1.31129600	0.06115832	-0.32964014	-1.23079696
H	10.25230900	2.06815300	0.72049600	-0.15464056	-0.17922545	0.20361390
H	10.85232400	0.68492400	0.61390200	-0.12876548	0.26527513	1.06746658
O	1.22637500	4.19248300	7.19091700	-1.50686815	-1.23479913	0.83599221
H	0.25024500	3.89433500	7.13273600	1.15236596	0.11489850	0.10019178
H	1.38229800	4.83754100	6.50188900	0.30825833	1.03465468	-0.63322111
O	9.31597700	1.93519700	6.92569500	-2.16328421	-1.13988994	1.47601594
H	10.09481600	2.28900400	7.34200300	1.26457765	0.42453956	0.30020100
H	8.78893500	1.69062300	7.77322200	0.82520283	0.35302946	-1.77984271
O	13.00139100	0.30506000	12.64907600	-0.19891033	1.02143098	-2.38953668
H	12.10853200	0.02169200	12.35555300	-0.14282993	-0.34896660	0.72398569
H	13.20504300	0.85460900	11.80216800	0.34066040	-0.56792897	1.56518952

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O	2.26766600	6.55082000	13.13419500	0.48366105	0.33106504	-0.11356512
O	3.52280800	5.24804800	11.83491100	0.37411302	0.07676595	0.87932918
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H	4.89394600	0.47859300	12.40741700	-0.13008498	0.18185106	0.56504933
O	8.64297400	5.10696000	12.87614600	0.21024478	-0.47073149	-0.79790902
H	9.16838700	4.45713400	12.26362000	-0.51719853	0.58615758	0.88582173
H	8.05806700	4.48830700	13.39845600	0.39761805	0.37395516	0.20541265
O	4.30045500	13.43853000	9.16141500	-0.58536259	-0.79243926	-1.25869137
H	8.22160600	10.64527600	11.23624800	2.38635726	-0.59743032	0.48027594
H	4.28924600	12.43054500	9.05448300	-0.12581077	0.66565764	-0.15323622
O	8.80271800	4.94087300	5.15261000	-1.45016709	-0.17360141	0.60236787
H	9.66641400	5.22302700	4.82786000	0.50049253	0.24317650	0.63405158
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O	4.05011700	10.93636200	8.41035000	-0.06657409	-0.48692790	1.16028547
H	3.24651400	8.16452200	13.56461500	-0.46656270	0.36845248	-0.16390681
H	1.76351000	0.24189500	6.09137700	-0.26904951	0.05502933	0.33673330
O	5.79040100	1.54906600	5.30619000	-0.96954406	-0.63406392	1.10550914
H	6.02104400	1.34716800	6.27857800	0.24173308	0.22899841	-0.88872348
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O	11.39276100	0.63650600	0.14490000	0.54010500	0.23965100	-1.11993406
H	11.34283100	13.41074900	0.65891300	-0.16329592	-0.48210811	0.46040748
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H	9.86620000	0.14685100	8.29832500	0.78897495	1.05028184	-0.22749174
H	8.17464600	3.17129900	4.19192300	0.13170631	-0.20657684	-0.00745826
O	1.87470300	4.76988800	5.49449100	-1.39243348	1.78711431	-0.00945652
H	2.44050800	4.27099600	4.88094000	0.28732029	-0.45339403	-0.31832574
H	0.61148600	12.23838500	12.06085200	0.01522299	0.51606004	0.47764364
O	7.34972800	10.74765000	10.90230800	-2.92549501	1.45564406	-0.46229519
H	13.46069200	10.86408700	12.22614100	0.91525675	0.58743336	0.35879336
H	6.72628500	2.27324100	9.00629800	-0.21055280	-0.23402543	-0.52673783
O	0.39201700	7.76217700	7.07651100	-0.32550683	-0.62787579	-0.67266183
H	2.36457400	2.34371000	3.96227100	-1.19654112	0.71692749	-0.28342198
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O	7.73254600	8.30268500	7.17772400	-0.82695221	-1.02210204	0.36990464
H	7.99602500	8.64719000	6.29507500	0.32429738	0.92740933	-0.61179353
H	8.91654700	13.14756900	3.21704300	0.55169039	-0.21684737	0.17612110
O	5.05727100	4.66929400	2.32472300	-0.07492195	1.30218570	-0.01595832
H	4.29735300	4.88609900	1.69447600	0.65171197	-0.18806593	0.42545950
H	10.54313300	2.43793700	2.38826200	0.28252158	0.40031103	-0.33915887
O	0.20337000	0.16122800	11.77121400	-0.45668350	-0.21368286	0.09373934
H	0.62864700	1.00476600	12.00852200	0.22564157	0.45772325	-0.07552616
H	13.66752400	0.14405400	10.79532200	-0.03286950	0.40529999	-0.33200298
O	11.02407000	6.78548500	10.79094300	-0.42325658	-1.19392219	0.57101841
H	13.03391600	7.49619800	6.82145100	0.98513266	0.42654605	0.43782599
H	11.58622600	7.55008200	10.66169300	0.73685097	1.21108276	-0.48080970
O	11.29314500	7.52542300	6.52808800	1.06722284	-1.24488249	-1.46077290
H	7.06831600	7.52637000	6.91142700	0.34449494	0.31775187	0.16137068
H	11.18792200	8.50338800	6.51926000	-0.19182848	0.60509632	-0.03383264
O	8.72317600	12.89719500	2.28399900	-2.92568115	0.93986324	1.18423942
H	9.46523700	12.61764400	1.80275300	2.58452762	-0.83323958	-1.21461032
H	10.93614100	8.86344900	3.14993000	0.36969381	-1.94783449	-0.05376846
O	8.84060500	0.92915900	12.29768000	-1.00244904	-0.01456170	0.20402322
H	9.67013600	0.54384700	12.64648200	0.23442446	-0.24154642	0.20171797
H	1.22125300	10.39422400	9.32940000	-1.32240280	0.07830964	-1.77749581
O	6.86103700	3.24264000	9.12376200	-0.64266734	-0.33748920	1.53915658
H	9.78824400	6.28881000	0.13184700	0.65213929	1.68178443	-0.29321429
H	5.45336100	5.54921500	2.65403000	-0.57940740	-0.90292317	-0.16552146
O	4.73324800	13.10617500	0.19169400	0.60186188	-1.13508815	0.03768569
H	4.07159300	13.03646000	0.96577500	0.39075938	0.23778490	-0.66967730
H	6.82044900	7.45642600	10.87386100	-0.71735070	0.15157734	0.41650178
O	10.48521300	3.07011200	1.60796300	-0.21033323	0.46308657	0.69887680
H	2.32244800	1.82145300	7.45554700	-0.05474033	-0.59901669	0.42923337
H	4.30308500	13.69068500	10.08476200	0.13936717	0.47955037	1.24367973
O	11.16270100	10.17845600	6.52273500	-0.23947720	-1.75846142	0.23571876
H	1.00815300	7.32352500	6.43816200	-0.45039201	0.24503901	0.42255518
H	11.44154100	10.75726900	5.83671200	0.27473936	1.26555519	-1.17870589
O	1.81580300	10.40083600	10.06017500	2.24879140	-1.13281581	-0.36875999
H	1.32139900	10.78827800	10.77410700	-0.50905790	0.63560658	1.86481254
H	5.34356100	1.88516400	11.65789700	-0.46044913	-0.68072636	0.23237992

O	7.15663100	0.89913000	0.80343300	-1.54100572	-0.64934193	0.03334053
H	6.23892500	0.40157700	0.75331200	1.49473717	0.66496601	-0.04243349
H	7.68373900	0.50716000	1.55327200	-0.01156585	-0.24278878	-0.29951092
O	5.66246700	10.43179600	13.16755400	-0.93185682	1.17371280	1.09543042
H	4.90917400	9.82115800	13.24714100	-0.40988376	-0.44385266	-0.17327488
H	6.30130300	10.20440100	12.50238900	0.75334203	-0.39916586	-1.53051253
O	1.18371100	4.50935800	9.80504600	-0.40574942	0.67129349	-0.50818938
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H	1.57222300	4.11230000	10.59348000	0.26417419	-0.66964439	0.81178321
O	8.67117100	5.34177400	2.35996200	0.08690484	0.47678232	0.45660019
H	5.98654900	6.58171900	5.38129900	0.33895473	-0.09948010	0.37927940
H	8.73970600	4.40316500	2.08505900	0.02291316	0.09578234	-0.05674888
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H	3.93929200	8.73170800	1.17698000	-0.00960256	0.59659368	0.30530156
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O	3.13091300	13.13176600	2.22176800	-2.25806794	-0.70591032	0.38758252
H	2.36708100	0.19620800	2.12375300	0.80891746	-0.42262717	-0.20715843
H	2.59547100	12.25583200	2.15182400	0.69299361	0.94053533	-0.22311161
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H	7.07062300	13.65214300	8.15298900	0.91247122	-0.95091847	0.41155600
H	5.53381700	0.37509000	8.28550400	-0.26659360	-0.44715447	0.62924156
O	3.42093200	9.03940400	0.39444100	0.54934195	-1.00167359	0.06907269
H	11.59978400	6.05499800	11.11800300	-0.17668725	0.16296836	0.03019401
H	11.54710200	7.28032800	5.57836400	-0.97381877	0.29331404	1.01676597
O	3.35326300	7.26686900	5.17760400	-0.59165408	0.83075127	-0.55034931
H	3.99784600	6.95023300	5.79525400	1.52743441	0.32590278	1.11420256
H	2.82407000	6.47112000	5.14922000	-1.26227806	-1.07760239	-0.46717720
O	10.95905100	1.88289800	4.06801500	0.49698246	0.29104890	1.27644330
H	11.41582900	1.05217400	4.36275300	-0.38293911	0.36728572	-0.08124790
H	11.06106800	2.47699500	4.90529400	-0.18095631	-0.60925226	-1.35436778
O	2.61189200	3.58041100	7.71114100	-0.42920868	-0.21197050	-0.97445486
H	2.20153200	3.91722400	6.84918200	0.40882858	-0.01811291	0.03248023
H	1.93807600	3.93818100	8.33303100	0.19806752	-0.01554798	0.92817140
O	7.82857800	8.27681900	1.51085300	-2.08060267	-0.22732565	0.44262933
H	8.23630400	5.89612400	11.04023600	-0.27028673	-0.36089138	0.39039531
H	7.63423700	9.24539600	1.44280900	0.41444387	0.22913159	0.10015836
O	11.16895900	11.78304500	1.25817300	0.01456839	0.06770178	0.20510771
H	10.94949700	11.10244800	1.92590500	-0.06010571	-0.32252692	0.41371676
H	7.68146000	12.50837100	5.04647000	-0.41094099	0.79931079	-0.09407924
O	4.33826700	7.15545300	9.54435500	-2.62217269	-1.41837540	-3.42609706
H	5.03343500	7.39301200	10.30660300	1.13535606	0.06933494	1.19079933
H	3.36802400	6.94836900	9.80257900	0.24655493	0.76606848	0.17273032
O	5.69658500	6.82336300	13.56337000	0.68539085	-2.58442272	0.74969004
H	6.36549000	7.36288500	0.42704600	0.62022572	0.54703052	0.39848451
H	6.11174400	5.87372400	13.67486700	-0.93429012	2.11657909	-0.47368569
O	10.96397100	6.89494000	3.57279700	0.21947298	0.09434047	0.22765423
H	10.27517400	6.38163500	3.09662800	-0.26557287	-0.04022131	-0.20146395
H	11.78815600	6.62848200	3.12627700	-0.02814073	-0.09639221	0.02842920
O	0.76829700	11.30046800	12.34790800	-1.31056287	-1.22712233	-0.54767484
H	5.60388800	10.18388800	8.60458700	-0.67885614	-0.12211198	-0.68982858
H	1.73283500	11.35955200	6.70902400	0.01027567	-0.22084955	0.44401258
O	12.14410500	5.25717800	1.48074400	1.94721794	-2.09806252	0.79312111
H	8.70229200	8.05028500	1.21911800	1.58441263	-0.13959446	-0.73527900
H	11.56464800	5.90500100	1.14550400	-1.58673485	2.34777888	-1.18786827
O	10.35149800	7.16873400	0.21988300	-0.35471096	-1.56929557	-1.69182047
H	11.56909700	4.45335100	1.58340800	-0.28174665	-0.34956259	0.23229919
H	7.19742900	11.77376400	10.76133000	0.35163798	-1.36722433	-0.10233249
O	13.39317100	0.27973400	8.98179600	0.94591922	-0.75359965	-0.17740048
H	5.37762100	4.44466300	11.81688600	-1.10850448	0.78317351	0.29732856
H	13.01767400	1.17758800	8.90856600	-0.36890243	0.69367958	-0.00305139
O	5.86012800	7.69718100	11.15942300	1.68583032	0.12622523	1.47939231
H	5.71180300	7.36861200	12.14819400	0.44108770	0.06971547	-1.32931289
H	11.44285100	11.24944700	0.46085700	-0.23534440	0.24941400	-0.07482991
O	2.58941000	11.46575600	6.23077500	0.21956966	-0.02690043	-0.41572325
H	6.58462900	3.39178200	10.10071800	0.53812577	0.03643871	-0.94770870
H	2.53038200	10.71240700	5.57852500	0.30647912	0.14041464	-0.29429415
O	5.95558900	6.68131000	6.37045300	-0.31221063	-0.50712803	-0.16751098
H	12.15977100	9.80976500	9.43530100	-0.25220467	1.13809479	-0.30277673
H	5.74333700	5.81397100	6.85236900	0.03157006	0.28483917	-0.35494699
O	0.58570300	10.35693200	7.59467600	-1.23409157	0.92355010	-1.08457676

H	13.36706100	10.80567600	7.19388100	1.08384760	-1.05381557	0.93105412
H	0.61305800	9.42424400	7.20722800	-0.32146505	0.19123764	0.18485462
O	1.45110300	10.82400200	1.26817300	0.65470268	0.02131290	1.82653138
H	2.09229000	10.10086300	1.10888200	0.14222418	-0.23557066	0.05300535
H	1.12367200	11.00374600	0.38006600	-0.50773430	0.65395294	-1.35868929
O	10.61687700	9.74881100	3.17968500	-0.65527243	2.27874989	0.32589712
H	10.64251500	7.35928500	12.84407000	-0.73182652	-0.38993765	1.99666849
H	8.26916200	5.32152300	3.25687600	0.11347719	-0.12629003	-0.16415415
O	7.90085700	2.36547900	3.69674500	-0.17767198	0.10179410	0.02419974
H	3.62189800	10.95648800	7.51830700	-0.29261985	0.28589024	-0.15698540
H	7.06621800	2.08402400	4.15085900	-0.14896562	0.16403691	0.10368077
O	2.21141700	0.81367600	7.53364700	-1.57753698	1.59234705	-1.30362500
H	6.75210900	9.97693700	9.65271200	0.64345770	-0.27394644	-0.70949700
H	2.93512100	0.51792200	8.05386700	1.95760006	-0.87645520	1.50461175
O	8.63845700	12.14236000	7.76732300	-0.81165311	-1.03024421	1.27768154
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H	7.94965900	11.74309300	7.17746100	0.42176945	0.30821976	0.09832054
O	13.59726500	11.05330800	3.64327700	0.40265639	0.10836944	1.03087773
H	9.77566600	9.72763800	3.71689800	0.26505608	-0.17160110	-0.12718991
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O	7.32284500	11.76454500	5.05027500	0.02281906	-1.14352239	0.35930758
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H	2.17447300	6.23965200	1.57138900	-0.06284754	-0.00816737	-1.51275546
O	8.79769700	0.14716800	4.85682700	0.63465219	-2.38265898	1.28116796
H	9.53807900	0.19125700	5.52089500	-0.61361747	0.38348470	-0.98726256
H	8.59534500	0.97280000	4.40636700	0.20268933	1.96469476	-0.10945290
O	8.22542800	9.45579700	4.63998900	0.39141912	-1.14581119	-0.04146418
H	7.73950700	8.80801900	4.06703000	0.09475647	0.77879493	0.26933748
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H	13.23695000	3.55411000	9.33318400	-0.42805529	-0.29678760	-0.12229042
H	11.70934700	2.99587400	9.29879600	0.90204334	0.01125475	-0.26541860
O	1.05177800	3.02581500	12.20315700	-0.86471246	-0.38365285	-3.53093740
H	0.18245800	3.49307000	12.09669600	-0.02637746	-0.13307311	0.07148799
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H	8.45986200	11.67969200	8.65422200	0.30405920	0.74848984	-1.38050459
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O	1.81796300	7.34323900	10.23508400	0.02201224	-0.15241295	0.75280261
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H	5.64638100	7.73845700	3.29310000	-1.14526817	0.98360285	0.45787803
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O	5.00840100	4.81260800	7.99049800	-1.07834955	2.02570036	-0.93652029
H	5.50355400	4.12349700	8.42318000	1.21426065	-1.21344458	0.70609543
H	5.20233200	0.72563000	5.09786400	0.95806048	0.90719223	-0.23452988
O	1.13597600	0.13281300	5.32124200	-0.24602888	-1.05698522	-0.28678241
H	8.15397200	0.86284200	13.05801100	0.67090886	0.13602680	-0.42898654
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H	12.14311200	4.10425200	5.40386600	0.87908338	0.02078891	-0.29364006
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O	5.95447200	3.68975900	11.74397600	1.12683130	-1.51287528	-0.43012605
H	4.97852900	12.17012400	13.49561700	-0.29701849	0.92158526	0.30621995
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O	5.11674500	0.91702200	11.55660400	0.43278869	0.66363418	-0.90851737
H	4.10510200	4.46093200	7.78476500	-0.22696466	-0.39662355	0.12054258
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H	11.49519700	3.95320800	12.01535000	-0.85970035	-0.65575220	-0.47559499
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O	11.82285900	11.66275400	9.00530900	-0.61729621	1.77016405	0.41849644
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O	4.51079900	12.98034400	4.63443800	-0.99692116	-0.19920498	0.71641687
H	3.78128900	12.86225500	5.31728300	0.53173914	-0.28469622	-0.86776950
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O	4.88169600	9.18653200	2.88005000	1.02967342	0.21569603	-0.95886215
H	5.55770800	9.87178100	2.63806500	0.06364406	-0.10894074	-0.03569823
H	4.21944000	9.63764800	3.40639900	-1.06175616	0.24059306	0.62098111
O	7.07009000	3.59427200	0.83221300	-1.02782017	0.92858278	-0.33259690
H	6.29612900	4.03533000	1.37096800	1.14591198	-1.39487397	-0.34316671
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H	1.20255700	1.46900900	4.48725800	-0.42629151	0.53565391	-0.68421894
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H	9.23388600	6.96471300	10.74899800	0.14675395	0.26374584	-0.14769241
H	7.09852400	8.98568200	7.83326900	0.43432209	0.15140508	-0.18140163
O	6.98933800	10.89875900	1.69434100	0.03994929	-0.70236631	1.13510203
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H	10.72065400	2.60179300	0.80200000	0.10300406	-0.80321578	-0.25005163
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H	9.68156000	4.20752600	8.33757400	-0.10717593	0.54343612	-0.12097093
H	8.56595400	3.16883300	8.78044100	-0.04718746	0.47720810	0.13552800
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O	13.22071300	4.34874100	3.99685300	0.08738615	1.03815035	-2.38230108
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H	4.36607600	2.73987600	4.96485700	0.10016196	0.19303793	-0.45388099
H	4.17244700	3.80661100	3.76986200	0.36186069	-0.26148841	-0.22066855
O	2.42610300	9.70917400	4.15243000	-1.24505681	1.95999273	-0.92461865
H	2.33693300	8.81663100	4.46853800	0.06852710	-1.37568069	0.52397698
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H	4.94426700	0.50143900	4.66193300	-0.12670295	-0.03557996	-0.01413130
O	12.85765800	11.96067000	3.73722200	1.00933497	0.19646572	-1.19737107
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H	1.53972600	8.58995000	9.69421600	0.44643148	-0.22761927	-0.03885503

O	2.13093300	7.28058100	6.87767100	-0.87693703	-0.92441348	0.68337048
H	2.54094900	6.38643300	6.88718400	0.01259224	-0.41188202	-0.26587214
H	0.45745100	6.20341200	7.11215200	0.54320318	1.21545621	0.00727777
O	6.92072000	0.32258900	10.15031300	-0.55984542	-0.97813051	-1.01445969
H	10.87816700	10.13421100	7.15133400	0.86781938	0.02457821	0.46280426
H	7.11483400	6.11939200	9.92630100	-0.86464510	-1.03552577	1.25937220
O	0.97580700	12.66239100	8.08637700	-0.34578821	-0.03652098	1.56619379
H	6.00332900	9.86649300	10.21863500	0.08573961	-0.18566914	-0.20513548
H	3.76807900	12.94093700	8.98654100	-0.12915784	-0.97730467	-0.30034138
O	5.94428600	7.47648700	4.51536900	0.80078609	1.14266827	0.07182737
H	9.57641600	6.94282900	4.55433500	-0.06174505	-0.04689950	1.46272025
H	6.39747000	8.07753900	3.86373900	0.20330537	-0.28643531	0.41356044
O	5.23443200	0.07491000	5.50971100	-0.27847364	0.38855388	0.23702951
H	5.99520900	13.49897400	5.23109700	0.53544410	-0.41975011	-0.03891108
H	9.85548700	11.20376500	3.50837900	-0.32086959	0.62714919	-0.10671313
O	11.23268000	5.75058500	7.57449900	-0.31602203	0.37470644	0.35103789
H	0.76386400	4.27930600	8.29376700	-0.98520722	0.93964984	-1.42401383
H	6.96448100	2.77856100	6.11682300	-0.13983923	0.36717310	-0.02814998
O	11.83455900	2.78544200	5.42076500	-0.88634161	1.26684897	1.08762404
H	10.96550200	4.83210800	7.90645700	-0.24112322	0.06635298	-0.38386368
H	10.83850300	2.75479200	7.67558300	0.75593062	-1.15561378	-0.59801088
O	12.56134400	7.85586800	11.68622900	-0.58366052	-0.44228172	-0.64513869
H	4.21952300	1.75160200	9.08041200	-0.41985861	1.25903281	-1.00263364
H	10.57071600	9.84364000	3.24028700	0.03360792	0.62095437	0.91662149
O	7.18426900	6.41141700	1.32392300	1.54151685	-0.51744792	0.97857274
H	7.52702500	6.62121100	0.43924700	-0.21690754	0.23101107	-0.89302339
H	6.21378700	6.49242000	1.41229100	-1.04980876	0.22503685	0.18574679
O	6.61315000	1.91043400	6.75259900	0.69595500	-0.68824272	0.67476808
H	5.99232900	1.19636600	6.32507500	0.08354183	0.02007209	-0.19043391
H	9.82066300	8.16399300	5.92405300	-0.03804102	-2.01597799	0.59531636
O	4.24311400	0.87524200	9.46475900	0.25985473	-0.73248884	0.99201704
H	13.67762500	11.31701100	11.27523700	0.04456905	0.66641868	1.83527621
H	5.06457000	0.93454900	10.00743600	0.15310201	-0.64859322	-0.27810237
O	6.45249700	11.35500000	2.56002000	1.19696432	0.71186088	-0.83277473
H	7.76300600	5.15717000	1.80639300	-0.57004241	-0.29656186	-0.56817836
H	6.79405000	11.56203200	3.48246600	-0.14794540	0.31617064	-0.64013172
O	4.15235900	4.78577900	11.12546200	-0.05779069	-1.13622457	-0.01267091
H	2.00745900	5.06462600	1.02039100	1.58161733	-0.15879906	1.23249645
H	4.01907000	5.70422600	11.36586400	0.03760342	1.51079577	0.03939907
O	10.39357800	10.53572800	3.98323600	0.89601616	-1.51584284	-0.58180624
H	10.31739700	9.18983400	1.13035200	0.36096646	-0.43260408	0.68487509
H	13.34750000	7.28002400	11.65263500	0.69373151	-0.13318110	0.09283637
O	10.05768600	11.45478100	11.68951600	0.18184437	-1.60517686	1.96855090
H	9.57909000	6.44111000	9.78338700	-0.25748880	0.52513501	-0.21163060
H	10.52382300	11.66942800	10.88780800	0.65245913	0.08092754	-1.30277139
O	2.75812000	4.67353600	1.64439200	-1.66155087	0.06856567	-0.46003210
H	12.38182200	10.56854100	12.97833700	-0.16306452	-0.77789915	-0.46904742
H	2.32152100	4.31481500	2.46843400	0.24242728	0.69161498	0.07998805
O	5.55977900	12.95228000	12.19918000	2.39772102	1.84230150	0.55682746
H	11.23919000	6.25461600	8.42454500	-0.23977596	0.00324936	-0.09368329
H	4.62554400	5.30645200	5.99918000	0.03881749	-0.04392267	0.51318092
O	3.56087200	11.96138100	8.82887300	0.53024533	1.45550882	0.44327159
H	8.07569700	9.11775800	1.87611700	-0.17258583	-1.16043923	0.69071972
H	4.44223800	11.57060600	8.53750200	-0.36326400	-0.19321585	-0.11597219
O	6.26956900	6.13948000	6.92461500	0.38178520	-0.76153408	0.50459601
H	6.76510100	6.50633400	7.69969100	-0.07682663	-0.30977630	0.43692302
H	6.38452700	6.77715900	6.22419000	0.15659665	0.60058764	-1.02130705
O	9.10067500	12.13520900	2.39010700	-0.13719562	0.60117693	-0.66054422
H	7.31225700	1.10870200	10.51520300	0.84645043	1.42159185	0.50490300
H	5.29679300	7.06509400	3.94066100	-0.91764633	-0.72031055	-0.84341087
O	7.99783000	8.77946300	2.83134500	-0.00603541	0.01524973	-1.78166511
H	8.03064100	9.63867100	3.24839600	0.12961755	0.79500059	0.97620270
H	9.66477800	12.55090000	1.69309800	0.36765287	-0.73176327	-0.29173487
O	13.74156200	10.92235400	1.19883800	-0.45798962	0.84308022	1.14041033
H	12.01207900	11.49867600	3.86930600	-0.68333346	-0.72546356	0.04615388
H	0.67581500	10.64386100	1.04073800	0.26705537	-0.15377409	-0.58107656
O	6.81173600	4.91826800	11.17455100	0.53241432	0.57505401	0.10981234
H	5.85128400	4.68401700	11.29628800	0.13643354	-0.04365168	-0.06820212
H	8.12868600	3.85081300	5.01006400	-0.15302436	-0.25090781	0.33788926
O	7.91842400	4.07350900	1.79684200	-0.34188116	0.63190933	0.37032219

H	7.09205200	3.67853700	1.32451900	-0.00398572	-0.53590330	-0.36993190
H	12.21757600	1.96403500	5.15502600	0.62566104	-1.47364847	-0.69576217
O	7.34227500	12.50423000	4.89345600	-0.31826197	0.16765291	-0.57414127
H	8.13559500	13.06970800	4.68928200	-0.18007751	-0.42890118	0.46560420
H	7.61982100	11.98518800	5.67112400	0.24898771	-0.28226241	0.61871237
O	10.84789800	8.82427300	1.90696200	0.25036428	-0.22075288	-0.90190295
H	11.66945200	8.43914100	1.48282200	-0.46959403	0.46373809	0.47632827
H	8.79233900	12.96890400	2.79141300	-0.34172329	0.35282172	0.62585284
O	4.61291300	6.67694000	2.12800400	-0.08643381	0.97705579	-0.82557615
H	4.18952900	7.38194800	1.49951400	0.59075677	-1.00678906	0.63545283
H	11.96960400	7.43680800	11.00812000	-0.08097844	0.50829685	0.44044492
O	2.84041700	2.13957400	0.94254900	-0.11955116	0.39601574	0.20407927
H	3.67794400	1.94069400	0.45457300	-0.20612844	-0.12197520	0.22630286
H	2.90297100	3.09465400	1.28334000	0.18566400	-0.62591660	-0.72532780
O	6.34925400	9.19669100	10.84817600	0.20971616	0.33322477	0.14112426
H	10.44530700	5.57737600	10.90247600	0.28986362	-0.12580049	0.17281980
H	2.70980000	12.02640500	11.96336700	-0.22361555	0.60345647	-0.58782365
O	5.83786500	10.61816900	8.21600200	-0.17016179	1.01802324	1.04670801
H	0.15510500	12.23469400	4.93598000	0.89381323	0.25650767	0.28690171
H	5.70923800	9.83018500	7.68691300	-0.27008258	-0.63395079	-0.69614835
O	12.33568300	1.00690000	0.62524400	-0.90484173	1.06133810	-0.17787767
H	2.14188800	7.67593300	8.53711800	0.20727001	0.06613495	1.15750663
H	11.82394300	0.18526300	0.46799300	-0.11173604	-0.35581757	0.13186881
O	-0.13628100	1.11934800	9.12735200	0.42976559	-1.42853589	-1.12244500
H	0.07209600	0.23878300	8.62208400	-0.11906008	1.40706203	0.70734293
H	12.58941300	4.96597400	3.15552800	-0.39817187	0.28293964	0.01137919
O	1.77375400	3.35253800	12.55886400	0.01774473	-0.11720066	0.14621659
H	1.84742100	2.66289000	11.83324400	-0.18173947	0.05243920	-0.01560763
H	2.03774100	2.84037300	13.36982900	-0.00711836	0.25524372	-0.10468299
O	11.80006600	5.27453900	2.59189600	-0.24621297	0.15908342	0.18220381
H	9.56343100	0.11796100	8.34549500	-0.38544439	0.06419377	0.13390923
H	6.68268600	11.07096000	7.94470400	0.07713619	-0.59956279	-0.09855913
O	3.55829800	8.17090700	0.08635300	-0.34698377	0.78076850	1.05505227
H	0.85327900	12.46216400	7.16037800	-0.60361537	0.09453484	-1.80667269
H	4.02134000	8.09883300	13.20416200	-0.01923802	-0.33400330	-0.59085550
O	10.62671200	4.89369200	12.36098400	-1.53173175	0.73849237	0.78083947
H	11.46568900	4.39837100	12.41275500	0.29481660	-0.83927705	0.35085122
H	9.94199300	4.45166400	12.95460700	1.45496323	-0.20342570	-0.99699881
O	7.35211600	6.80091300	9.30282300	0.94826046	1.57284266	-1.64842282
H	6.87740800	9.77490700	11.50011800	-0.44382335	-0.32097603	-0.42493808
H	6.91015100	7.65630000	9.50574300	0.23120647	-0.35831205	0.65261648
O	10.93086100	12.65897900	0.49041200	0.16440561	0.41721706	0.26440199
H	8.07942100	13.80815800	8.79891700	-0.73510982	0.18007648	1.62057108
H	10.60005400	12.70373200	13.55781100	0.17872614	-0.88755928	-0.14648296
O	9.65153400	7.12871500	5.78044300	0.39687500	2.77873900	1.07008243
H	10.36325800	6.60982000	6.25206400	-0.11470926	0.08623275	0.54239945
H	4.85625700	12.03618900	2.36969600	-0.49412699	-0.71058767	-0.28113678
O	11.79174300	9.83431100	13.35967000	-0.42271973	3.23895107	1.19494652
H	10.88012300	2.64395100	0.97670100	-0.42394461	0.52997640	0.25422042
H	11.96175200	9.03248500	12.90529700	0.93469738	-1.93802676	-1.41330313
O	13.55107300	4.59898600	4.40220100	-0.42931513	-0.55062030	-1.04318149
H	0.49628800	4.26800400	4.43837800	0.48569325	0.02075806	0.03019195
H	13.13054000	10.46910100	0.59652800	0.09379899	-0.60963946	-0.13659964
O	3.78042000	4.90215200	6.26730800	-0.40161200	0.38377112	-0.61398309
H	3.87878800	4.54014200	7.20611000	0.18125919	-0.29909183	-0.50877713
H	7.17776100	11.72961300	1.94038400	-1.14280197	-0.67105078	1.34674446
O	10.18929600	9.80847100	6.55741600	-0.64965612	-0.76526167	-0.07901361
H	6.63139000	13.77115400	10.89736600	-0.49934016	-0.57779378	0.68562122
H	10.39262100	10.10165100	5.63821500	0.04085895	0.63023760	-0.54326643
O	7.24510300	3.89327200	5.50491700	0.20583739	0.36523758	-0.06613186
H	7.24217400	4.67328400	6.12746200	-0.40395171	0.04929217	-0.13061154
H	1.88368400	12.34950100	8.22397600	1.01043643	0.03608389	0.41062629
O	9.89998900	13.22356400	5.16390300	-0.42326944	-0.35076226	0.85009008
H	10.39353900	12.85512600	5.94101200	0.01096113	0.36831827	-0.66068666
H	10.53852700	13.63838300	4.57206900	0.46285157	0.44830324	-0.27575392
O	4.33953000	8.63060100	6.44717300	0.41975165	0.61869078	-1.24389930
H	13.75230900	3.26021000	12.61836100	1.64671149	0.00107009	0.22371633
H	4.93788400	8.24111400	5.72824300	-0.35195268	0.04906025	0.55610909
O	10.33049100	3.38272900	8.16873500	-1.03303745	1.21909124	0.63985867
H	1.17962700	1.08141300	10.20980300	0.17656641	0.03948546	-0.57226848

H	2.73490200	3.56055500	8.61331800	-0.36854144	-0.14205089	0.09637627
O	13.45259100	11.73727600	12.23947000	0.84039805	-2.08170310	-1.43696345
H	3.97836800	9.41729100	5.96334400	0.18048529	0.09515294	0.52225589
H	1.15025200	6.58955000	10.45774900	0.63464859	0.33231717	-0.68287323
O	1.73029100	0.88823500	3.99279700	-0.66205655	0.37657871	-0.80212100
H	1.27570800	0.74646300	3.08839500	0.88391089	0.00172675	1.03295466
H	2.08389400	2.80293800	4.29764600	-0.01410662	0.57448374	0.03923709
O	8.34139000	6.82972200	12.75377600	0.53467637	-0.48758456	0.62501980
H	7.89606500	6.26822200	12.08808300	-0.79565262	-0.13652199	-0.33993021
H	9.12868800	6.28126000	12.95978400	0.12465892	0.49503922	-0.16717468
O	3.49987900	11.58736400	11.58315000	0.28659935	-0.59990784	0.56110577
H	3.52455900	11.65773700	10.59896000	-0.45920729	0.06197593	-0.17146997
H	10.00921800	2.99401700	9.00985100	0.33127844	-0.47064664	-0.07566089
O	0.27856700	10.53928100	9.92253900	-0.91233855	0.20851546	-0.79250970
H	0.52007800	11.23681400	9.22544000	-0.23652608	-0.43209860	0.56813826
H	5.54931600	13.62192600	12.95014800	-0.42555360	-0.71215501	-0.35671334
O	12.81471000	3.10508000	12.69286700	-1.65677633	0.61444640	-0.87039305
H	9.50744100	3.10537000	3.44961700	0.68839647	0.06240325	-0.97200563
H	12.61821800	2.53647400	13.44529500	0.12619490	-0.46241140	0.56604898
O	1.09591300	3.70925400	8.97254300	-0.75605557	-2.80077952	1.50260783
H	0.48043200	2.84971700	8.98645000	1.51385230	1.81344960	-0.23096119
H	2.92876900	7.77834900	6.62896500	0.85231460	0.99855587	-0.28660346
O	1.90594800	1.30142800	10.83662200	0.19370641	0.14673801	1.54002304
H	2.83519900	1.12595200	10.54940000	-0.41174935	-0.29846191	-0.76507809
H	0.83504000	12.54683600	12.82991400	0.82866096	0.89239553	-0.03396582
O	8.19628900	11.40055100	7.34717800	0.55666394	0.19628574	-0.12479622
H	8.99692800	10.77998500	7.25082600	-0.77735819	0.47879756	-0.19178220
H	2.86368800	11.10738800	1.18628900	0.31775084	-0.03458494	0.49249794
O	7.39484000	11.09078900	12.41959900	1.05329209	-0.55964487	0.26814808
H	6.72449100	11.79574000	12.30970100	-0.91437692	0.62467476	0.24732986
H	2.70329500	0.71892900	3.82977700	-0.64220557	0.23717709	-0.08987240
O	9.45445400	3.19308700	4.39713400	-1.50068928	0.27372224	0.51969918
H	10.25219600	2.86538300	4.85787300	1.23376812	0.01117916	0.00390139
H	3.28577400	9.12931400	0.18620900	-0.07068477	-0.36403841	-0.03047169
O	11.93190200	0.52569000	3.67427100	0.27316122	0.62436726	-1.08532136
H	12.19418400	0.74556600	2.73492700	-0.63105264	0.18514155	0.80780314
H	12.28521800	13.60548900	3.73143000	0.54286122	-0.76142815	0.22456994
O	1.01004800	12.62176200	5.31810800	-1.30123387	-1.09116290	-0.00136731
H	1.00772300	13.54410600	4.98291500	0.51262402	0.30850207	-0.14663568
H	4.11282300	5.84961000	1.94169200	-0.42605086	-0.03402804	0.03626130
O	2.38196400	10.67455400	0.43954400	0.40909751	0.36491773	-0.11248834
H	12.13740700	5.99627100	2.00093700	0.33396062	-0.08923683	0.06120357
H	7.38541700	1.44365000	7.20337500	-0.42710449	0.13223545	-0.21363504
O	10.37603700	3.39988300	1.37862500	-0.47052014	-1.16929616	-0.75207088
H	8.79051700	3.84433000	1.33920400	0.29860229	-0.42941232	0.13333382
H	11.00767800	4.01475900	1.79867300	0.69239094	0.65560822	0.38307486
O	4.26475800	7.62371500	11.62197200	-1.88415289	0.20970433	-0.61960609
H	8.23450500	11.50497200	12.12160800	0.29591034	-0.38987646	-0.20169432
H	5.00019300	8.18045700	11.28666800	0.70460831	0.40762221	-0.15431454
O	12.82713100	7.12235800	0.81498000	-0.31729370	0.60274634	1.44543472
H	12.33703400	6.79021300	0.08161500	-0.86827549	-0.42060989	-1.57146404
H	13.75748300	6.94893100	0.59122700	1.23187682	-0.02765787	-0.07569585
O	1.44005500	6.51415100	0.15923400	-0.28424731	-0.06580739	1.16135094
H	2.19203000	7.18813800	0.15828800	-0.07266298	-0.19875863	-0.32541993
H	1.30659200	6.19115100	13.25396300	0.16670366	-0.03227095	-1.23693469
O	0.83767200	-0.02704400	1.48223100	-1.01451523	0.57686767	1.13844344
H	1.46950600	0.28915500	0.82575600	0.59693821	-0.21324988	-0.48140620
H	11.45389500	11.84639600	0.67569800	-0.34359197	0.27247371	-0.68409810
O	3.62889700	11.54127200	5.42381100	1.10495430	-0.30512981	-0.35088311
H	12.55551300	0.76715400	12.28258300	-0.00837974	0.96626024	0.73558342
H	4.13341000	12.34430400	5.66978400	0.18867425	0.01412050	0.05067439
O	8.41072500	0.71065800	3.15058400	-0.49618438	-0.86819733	-0.93117034
H	8.20785400	1.11376400	2.28101900	0.00025762	0.09338350	0.30628680
H	8.68524600	1.38002500	3.77756600	0.30779553	0.76908747	0.50539973
O	2.12832300	3.80907800	4.31696900	-0.74045926	-1.28989634	-0.88055971
H	2.87650000	4.06714000	4.88998300	0.32218188	0.36712888	0.80394392
H	12.45444100	3.50168600	5.12377300	0.02821529	-0.32496124	-0.12524616
O	8.61287700	0.13613000	8.07325600	0.97143022	0.06440820	-1.77420634
H	2.58397200	11.31584700	13.70747700	-0.31646272	-0.46804674	0.16245517
H	0.88799000	12.99585300	1.56561000	0.11729682	-0.09811639	-0.45977345

O	10.48067800	6.51749100	10.15068100	-0.14344391	-0.25821643	0.04258519
H	8.50743200	12.31034000	7.58958500	0.06089555	-0.15980487	-0.14110678
H	10.52226700	10.61270500	12.08067900	-0.79647126	1.65130503	-0.59732028
O	3.83967200	12.00325800	2.41445900	0.73887392	0.91478881	-0.47040033
H	3.71468700	11.81713900	3.35319900	-0.45014569	-0.38763189	1.05207442
H	13.20582700	0.72310300	0.91798600	1.26783576	-0.55758490	0.24300475
O	1.65672600	13.17245300	12.92040300	-1.04742278	-0.81775948	-0.08947697
H	2.72054600	11.80535200	5.58664800	-1.28201642	0.29341380	-0.09826449
H	3.54595300	4.30684200	11.72754000	-0.27673146	-0.28645331	-0.02863284
O	4.25614500	0.77672700	3.15213500	0.02065522	-0.99364609	0.01238089
H	4.03619500	-0.09634800	2.71234300	0.30938395	0.22334661	0.08955204
H	4.14839900	1.42689100	2.44359000	-0.22589509	0.46250910	-0.44624996
O	-0.09492400	5.44052700	6.96994600	-1.05235621	-0.91895863	0.06122209
H	12.95596400	5.64248600	7.27821800	0.37597347	-0.06357207	-0.09274536
H	12.96168900	12.54438400	12.03235900	-0.54783837	1.08832235	-0.28674076
O	8.82771300	9.22926800	0.08271700	1.13415844	-0.29805362	1.94248197
H	8.75528500	8.54486300	13.41592800	-0.26737572	-1.17267768	-0.99252458
H	8.31115100	9.94662400	13.75456500	-1.22297514	1.78548423	-0.95837621
O	12.50946900	0.11205100	11.59244700	0.16899143	-0.88872811	-0.51860749
H	11.60146000	0.14188200	11.26565600	-0.58343375	0.31000925	-0.30021386
H	9.21685400	7.24555200	2.92044900	-0.03525343	-0.62423613	1.09685841
O	9.45090900	6.49810800	3.60057800	-0.10159561	0.32208675	-4.16234228
H	10.35247300	6.15613000	3.32269300	0.19769214	-0.42505790	-0.15037509
H	13.34148800	10.26944100	9.62919400	0.90504073	0.32071584	0.10436983

Example of dataset obtained at PBE-D3 level of theory:

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Lattice="13.773 0.0 0.0 0.0 13.773 0.0 0.0 0.0 13.773" Properties=species:S:1:pos:R:3:forces:R:3 energy=-43244.75170689696

pbcs="T T T"

N	8.81804200	6.63935900	6.13019200	-0.39540152	0.01848293	2.00635066
O	8.12562700	7.29010300	6.96895100	-0.36395670	0.49968541	0.03129989
O	8.38856500	5.47449200	5.80417900	0.85492711	0.05043231	-1.10860088
O	9.95175600	7.09059000	5.81858700	0.46652109	-0.33455067	-1.11342491
H	12.56041600	5.94855100	5.40567400	-0.74118217	0.42552840	0.34848554
N	6.33884000	5.37147600	2.86037800	-0.77285163	-1.48539166	1.09077265
O	7.24586200	6.21214500	2.75876700	0.36046870	1.57764504	0.29928698
O	5.39503600	5.50194800	3.76489100	1.09647429	-0.33253919	-1.47579932
O	6.42465400	4.31754700	2.13387100	-0.68328587	0.06813569	0.24211866
H	3.76304300	5.67285800	3.16547300	0.18274756	0.29256042	0.45508702
N	5.49127700	10.77348700	12.06914600	0.51460365	-1.38060546	-1.04202535
O	5.45138700	11.35705900	10.93528900	-0.65368863	1.09442298	0.06476051
O	4.58491500	10.75880000	12.90343400	-1.10674680	1.18146887	0.37080528
O	6.49628900	10.01452500	12.27390900	0.89687697	-0.78156372	0.57389181
H	3.48226100	12.48138600	12.08062600	0.05226179	-0.03419988	0.17047179
O	9.65499100	9.13063900	8.37874000	0.09621220	-0.37914917	-0.99399513
H	9.17166600	9.89033900	7.95522500	-0.11379965	0.74985481	0.31056973
H	9.29261500	8.44017200	7.75166900	-0.14535597	-0.48028070	0.24236921
O	12.80698200	7.19968400	10.78169700	-0.32098595	0.02439930	0.38061805
H	12.73731600	6.75101600	11.66714000	-0.12917596	0.07637232	-0.32437949
H	12.29590500	8.08436300	10.81641900	0.40535104	-0.55874801	0.31545264
O	8.69401300	4.12944400	13.76261600	0.62130732	-0.49921089	-0.82704243
H	8.98032300	4.45760600	0.93044800	0.04249172	-0.02382116	-0.27110805
H	9.10818200	4.77064600	13.03194900	-0.03989871	-0.27106892	1.25394680
O	12.95480300	5.21200100	5.89967900	-0.29733664	0.25966912	-0.80329340
H	0.01654300	3.50342000	2.74423800	-0.34249265	-0.59419219	-0.38383503
H	13.51838600	4.90830900	5.12025200	0.40432025	-0.70356219	0.54251619
O	0.42260500	9.64592000	0.15223400	0.71449529	-2.17942862	1.97184425
H	13.30304700	9.37307500	0.48850300	-0.04716102	0.22160725	-0.03043360
H	1.52651600	8.77203900	13.48828300	0.47235784	0.06579819	-0.52628229
O	10.90376500	11.90141400	7.57613800	0.87816620	-1.13264793	-0.84870995
H	11.59207400	11.20406800	7.42148400	-0.32343332	0.45900348	0.72990377
H	10.53025100	11.87066400	6.65640600	-0.75981142	0.63891111	-0.23286419
O	1.97178400	2.80751200	6.11482800	-0.11182852	-0.65587845	0.61362010
H	1.67166400	2.22833200	6.88132400	-0.46547163	-0.15824946	-0.72658337
H	2.71224900	3.28851400	6.53901400	0.50117209	0.83239745	-0.03599964
O	2.14918900	11.55196100	3.01040900	0.95629747	1.28408813	-2.40615339
H	1.29321400	11.65858700	3.56993700	0.02923315	-0.51450233	0.66787532
H	2.91976300	12.24093200	3.32946200	-0.32435616	-0.82117399	0.73973866
O	2.21193200	8.27426900	12.86312900	-0.53534338	-0.29207421	-0.30540680
H	1.84230700	8.16581900	11.76400800	0.13776770	-0.05902460	0.03696980
H	3.19662500	8.18736300	13.04058400	0.06883841	0.14533805	0.27816908
O	3.87037800	1.39327500	4.89127900	0.43535693	0.05954457	0.53246982
H	4.28617300	1.91293600	4.17264400	-0.14427398	0.24898367	-0.68416546
H	3.03236200	1.84636100	5.16028900	-0.24788599	0.20818938	0.30144367
O	9.26128300	9.62471600	3.88855900	0.19193001	-1.06026756	-0.64926965
H	8.80067500	9.30795100	2.98539300	1.21573874	0.32070464	1.13036832
H	9.74940000	8.89097200	4.35617700	-0.81336058	0.25222496	-0.72230991
O	5.11629600	8.71394900	2.17175900	0.18296887	2.19265813	-0.39980729
H	5.06436600	8.27620600	3.05727700	0.52407223	0.26821861	0.19598902
H	5.22004700	9.77654900	2.35922100	-0.41335031	-2.07259292	-0.39592351
O	9.41384500	1.58540100	7.95913500	0.97596919	1.10631517	-0.51335450
H	9.58304300	2.38552200	7.36227600	0.02986654	-0.64142275	0.67493584
H	8.97823900	1.92198700	8.77698900	-0.08968320	0.49367501	0.34866834
O	1.74330400	12.92000200	0.90141100	1.08541185	-0.18462017	-0.97785630
H	0.97887300	13.50259800	0.75979400	-0.99431807	0.38293123	0.29652083
H	1.92216500	11.98799400	2.04505700	0.24260529	-0.32933066	0.72635724
O	5.72203200	8.09253900	4.67577200	-1.39316704	-1.25052840	0.85841161
H	6.16036700	7.19982400	4.63110700	-0.13862926	0.79598239	-0.15551384
H	4.85283600	7.79916500	5.20451700	1.07767303	0.41827835	-0.20906503
O	6.81012300	6.16750900	9.55329100	0.08540735	-1.92922062	-0.99049411
H	7.10166800	5.56737100	8.75238300	-0.99419831	1.24791898	1.32427645
H	6.29041300	5.47066700	10.11616700	0.87642538	0.66010955	-0.44045655
O	12.41088700	5.46710600	13.17153900	1.48803851	0.55273420	2.09915131
H	12.66138900	5.74492400	0.37369900	-0.86713087	-0.71045590	-2.03019565

H	12.98915300	4.64848400	13.02873000	-0.37686801	0.30238157	-0.08377966
O	4.78983300	7.85218700	13.42605000	1.44888653	1.58818463	0.60270759
H	5.45527000	8.59243800	13.11641200	-1.24197985	-1.37643913	0.23935026
H	4.78824200	8.08671700	0.66868100	0.00039541	-0.12695944	-0.65030354
O	3.98525500	4.57662200	7.03187300	-0.04175673	0.05115821	-1.03122707
H	3.57746100	4.91140100	7.88292700	-0.11535106	0.04940300	0.03157493
H	3.72693000	5.30011600	6.38337400	0.45993198	-0.39316633	0.62856767
O	0.29501000	11.61139800	4.54494700	-1.26733787	0.21937859	0.71103868
H	13.47223800	10.84737700	4.87103900	0.99519951	-0.26429301	-0.12402844
H	13.37116600	12.21503900	4.16004700	-0.12098069	0.42249393	-0.04763698
O	12.76739900	0.52449000	10.70698800	0.25287579	-0.40235845	1.29927719
H	13.66530900	0.90436400	10.84724200	-0.39753613	-0.28238029	-0.54360733
H	12.59874700	0.34256900	9.75364700	0.10198237	0.39836112	-0.39376768
O	5.08717500	0.11533000	0.74755300	0.01019166	0.00435618	0.20029876
H	6.59620400	0.30173700	0.10378800	-0.51539928	0.04421444	0.15740571
H	4.36187300	0.27648300	0.10834000	0.07004243	-0.07786228	0.07090370
O	9.64532200	6.10220400	9.88607600	2.11734161	0.35744606	-0.52630547
H	8.81105600	6.49311900	9.64078500	-1.62703530	0.27832828	-0.02699811
H	10.30976100	6.69067300	9.43767200	-0.42794369	-0.76304394	0.52134848
O	10.50026800	3.79337000	6.45367600	-1.28735659	-1.68799396	0.11572866
H	11.36732700	4.17023900	6.42209200	1.92123217	0.65517154	-0.10386570
H	9.90434600	4.51664500	6.23832900	-0.86701484	0.84447922	-0.22359039
O	10.04430000	11.99161500	4.97223100	-0.03005498	1.27728257	0.08324928
H	9.17582500	12.37715900	4.59549300	0.34316896	-0.27064948	0.32519666
H	10.03844400	11.08030700	4.65947900	-0.47945473	-0.97211155	-0.55425811
O	8.35395800	11.94629100	1.29463500	-0.22017711	-0.69246762	0.26632694
H	7.88329900	12.54321800	0.65416700	0.27222163	0.59374954	-0.36083789
H	8.02921900	11.02279400	1.11715500	0.19339674	0.27041149	0.59779785
O	11.95902300	0.49249000	8.15139400	-1.10700348	1.12016748	0.11799407
H	11.07312700	1.03490900	8.22865900	1.47340517	-0.91181423	-0.25201546
H	11.66789700	13.41329200	7.74935900	-0.15864243	-0.11415574	0.14582136
O	1.60472500	12.13160400	7.03265700	-1.03200989	0.18058575	0.27330001
H	2.55767200	12.03494300	6.86521000	0.95797891	-0.26146778	0.02668682
H	1.22928000	12.01618300	6.13473200	-0.39141906	-0.17773575	-0.18767606
O	5.83021100	4.14276000	11.05548000	-0.49503361	0.37545539	0.00640206
H	5.73016300	4.58490000	11.96674000	0.55280663	-0.45877110	-0.17412616
H	6.69544900	3.67993000	10.99877500	-0.17092696	0.03558847	0.52144109
O	13.29043000	3.20341800	1.91776700	0.33800219	0.64611493	0.16250573
H	2.28255600	13.06435000	0.03088200	-0.01823675	-0.26478636	0.91763860
H	12.59684200	2.54425600	2.15067400	0.11144815	-0.09392236	-0.02874990
O	3.97066900	11.31413500	6.19011600	1.72773823	0.42729970	1.90796138
H	3.42388000	10.62680100	5.83543700	-1.21289290	-1.63070372	-0.85426513
H	4.48797000	10.85845200	6.97257000	-0.42974798	0.82453854	-0.76035492
O	6.76469300	4.05461800	7.40602900	-2.97641252	-0.46165620	0.20348804
H	5.74433200	4.18789600	7.10625800	2.18436874	0.23687132	0.81397702
H	7.27816000	4.50934800	6.72278500	0.41630430	0.58960756	-0.52346527
O	13.22444000	0.35900700	0.20476700	2.33588230	0.28534329	-1.40030315
H	12.39534400	0.19435300	0.61717700	-1.66014293	0.28345607	0.22419631
H	13.25615300	1.10516200	13.32106400	-0.72044629	-0.44142676	0.86916485
O	4.67698700	2.11172100	2.46511500	1.32593163	0.20171833	0.90700917
H	5.47693900	2.71153600	2.63563200	-0.85109986	-0.46972563	-0.57626292
H	4.97918600	0.77841100	1.50191900	-0.14875054	-0.01734737	-0.41656560
O	12.58798800	8.01461600	3.15242800	-0.86634892	-0.23748078	0.01288262
H	12.09571600	8.62471200	2.54963000	0.36186430	0.44581350	-0.11469692
H	12.21349700	7.14803500	2.81314600	0.50826997	-0.60735940	0.46503804
O	2.78521700	5.78041500	3.10153200	-0.87421426	-0.25443031	-0.33541584
H	2.49682900	6.72534900	3.02089500	0.39776659	-0.14119940	-0.16890800
H	2.93714500	4.46919000	1.46925200	-0.21103823	0.01953806	0.19329823
O	3.33413300	3.81625200	0.85913700	-0.95942635	-0.32410332	0.57613879
H	4.07887900	2.65984400	1.90943000	-0.17035877	0.59642146	-0.43779297
H	3.91350000	4.37975300	0.33785600	0.96120455	0.38912596	-0.70297474
O	5.56559500	11.39207600	2.41960600	-0.32992795	1.26872995	-1.85168739
H	5.12813100	12.02599600	3.07566800	0.05894342	-0.49066692	-0.47601198
H	5.47882900	11.90063300	1.51578500	-0.02990696	-1.03776250	2.09351538
O	2.29563500	1.07018900	10.43782700	-0.97992946	-2.21659118	-0.48422407
H	2.68876600	1.90504400	10.65098500	0.46982094	2.03250648	0.23156443
H	2.03023700	1.06363700	9.48955900	-0.08186683	-0.08848336	0.14775283
O	7.52440000	0.10050500	13.58993100	0.88994212	0.33686483	0.52732892
H	8.86550500	1.14891300	13.68202800	0.64776172	0.47656282	0.17299122
H	7.50601000	0.02200100	12.60494500	-0.41382238	-0.21602114	-0.55539626

O	9.44867900	12.11051100	10.02275800	-0.27589565	-0.52850946	0.54859461
H	9.69565600	12.12888300	9.07719200	0.29528332	0.15453941	-0.13269727
H	9.04971300	11.17809200	10.13672400	-0.10415135	0.56091602	0.31362023
O	4.56229500	7.52850200	8.88848300	-0.94788773	0.73166929	-0.58319060
H	4.77701600	8.46581100	8.65085600	0.22629384	-0.22150722	0.37170472
H	5.39527600	7.11100500	9.18319200	0.89100999	-0.26677604	-0.11545441
O	1.43083700	8.22018100	2.88227300	0.29649043	-0.22746057	0.14216826
H	0.50118400	7.90493900	3.07510900	0.07972555	0.58240810	-0.36811205
H	1.32788300	8.99864000	2.30025000	0.04348341	-0.21832147	-0.03238211
O	7.87860400	13.53078100	7.24968200	0.85124986	-0.47752078	-0.09983849
H	7.01989000	0.17607100	7.31495400	-1.22202492	0.61691513	0.00086941
H	8.53624100	0.45706000	7.58076700	-0.30859531	-0.34925663	-0.47629225
O	4.04749500	12.82414000	4.11449500	0.02484761	-0.52401323	-1.07629606
H	4.14184800	12.33168500	4.97956800	0.02683508	0.03653737	0.14659802
H	3.96410300	0.04292900	4.28028000	-0.14809209	-0.04259177	0.49617437
O	9.61846100	2.82398000	3.92681400	-1.08146963	-0.65762859	-1.65800789
H	8.61827800	2.41731800	3.93786600	1.29235470	0.37290048	0.62258882
H	9.96706500	3.11888100	4.77495800	0.07323885	0.07102203	1.24053383
O	2.15971000	9.30565000	5.31992700	-0.80347793	-0.16683986	0.02890325
H	1.14474600	9.33659600	5.44348100	0.86315640	-0.05473959	0.20142669
H	2.16164100	8.93078500	4.40387700	0.13521227	0.11742369	-0.08580608
O	0.97765700	0.79362900	7.82152700	0.66409778	0.97726284	0.18394273
H	1.21493900	13.72829100	7.37730400	0.54736798	-0.76840707	-0.06322904
H	0.01206700	0.76530100	7.80120500	-1.01536360	0.36900409	0.22375248
O	0.73266900	4.21411300	4.02864500	1.70338761	1.46693873	-0.82888862
H	1.25795100	3.65415400	4.63300900	-0.11170274	-0.53880873	0.64730917
H	1.49724300	4.86150900	3.69223000	-1.06373997	-0.80227925	0.33651381
O	12.46804300	9.04524700	7.82906700	0.18231419	-0.47591643	-0.59471119
H	12.88763900	9.76530500	8.36299200	-0.10551027	-0.27958068	0.62497861
H	11.49033300	9.01009400	7.89655700	-0.44975968	0.30080387	0.53551589
O	3.73250500	7.29584100	6.22799800	0.47337644	0.10322667	0.85967979
H	4.16477800	7.34418400	7.18053200	-1.10571896	0.13999648	-1.23074066
H	2.99820400	7.97918500	6.08538700	0.51724572	-0.37653812	0.48145382
O	8.12729900	9.32177100	1.58295700	-0.75103166	0.70930067	1.65746825
H	7.20875500	9.01894600	1.63552100	-0.76708012	-0.39038514	0.11643318
H	8.48019200	9.12657300	0.71856500	0.91695687	-0.96946688	-1.62738572
O	11.91618300	5.60043100	2.31245700	0.51547223	1.43526402	-0.00382379
H	12.32122500	4.72118700	2.27038200	0.52171214	-0.85476824	-0.17311250
H	10.94204000	5.45864600	2.42878200	-0.42405862	-0.27798355	-0.15814356
O	11.49326500	11.93707100	11.93314200	0.70242022	0.60377109	0.01157353
H	12.08160100	12.71826900	11.63128800	-1.38149256	-0.14124617	-0.24883433
H	10.70320600	11.95737500	11.33201000	-0.13039042	0.62642782	-0.34944509
O	7.28385100	1.76436700	4.03757800	0.52350212	-1.67720317	-1.60406691
H	6.96935200	1.92248900	4.90609800	-0.71725685	0.57296595	2.01859308
H	7.36630800	0.73488300	4.02844000	0.05914623	0.83465508	-0.34347221
O	5.55037100	5.21304500	13.43620000	-0.60479616	0.59772495	-0.61544884
H	5.48213200	6.22278900	13.38771100	0.00031785	-0.62309278	0.42796347
H	6.09836900	4.89666800	0.41050000	0.26055340	0.21627934	0.22495414
O	13.22643900	9.34724300	5.44082600	-1.22484551	-1.15157480	0.67883072
H	12.86884800	9.07040000	6.43353800	0.53097340	0.75769754	-1.48072454
H	12.79898000	8.72051400	4.76386600	0.56133887	0.64737621	0.48250575
O	7.06244700	10.30499800	5.18596200	-0.51247294	-0.66607751	-0.46349181
H	7.76969100	9.89236000	4.58171500	-0.49988514	0.51782397	0.99568969
H	6.34863800	9.57105700	5.22583800	1.06050244	0.62667539	-0.30423490
O	5.32391100	10.25505400	8.30050000	-1.15996740	-0.50909493	0.03651408
H	6.25464300	10.46421100	8.09562000	1.35689078	0.29272637	-0.45408774
H	5.26058800	10.60950200	9.20467700	-0.36853338	0.22711190	0.43716208
O	0.56884400	6.57270600	7.73655200	1.20329049	0.99235663	0.96324825
H	13.70066000	6.09085900	7.22729000	-0.89692309	-1.12371298	-1.14852623
H	0.13478100	7.40270700	7.97585900	-0.09953335	0.17947963	0.24472602
O	0.49670300	11.63330700	12.18070400	-1.87889417	2.49448276	0.95173495
H	13.36432100	12.17125100	12.24542800	2.76096894	-1.69841833	-0.04198864
H	0.26892900	10.36045700	13.33288700	-0.06838828	1.88038518	-1.64448350
O	0.37310900	3.22664900	12.89330300	0.63070532	0.44145722	-0.87922692
H	0.55698400	3.13260100	0.06982800	0.09033050	0.07357947	0.44687226
H	1.22732500	3.53206900	12.44975400	-0.82217225	-0.51885261	0.50723380
O	1.39865400	7.96735400	10.56782600	-0.37875552	-0.77757329	0.78984503
H	1.27951000	8.82568600	10.14270000	0.03368738	0.75394725	-0.44974630
H	0.36425600	7.61595100	10.67609000	0.76332334	0.00172157	-0.18396987
O	2.74161100	3.63552100	11.02729600	-0.15129756	0.24498086	-0.22721095

H	3.67939700	3.80052900	11.20344500	0.53070773	-0.04438490	0.19384159
H	2.58157000	4.20438700	10.21142500	-0.28678582	-0.24376117	0.30907867
O	7.90039300	2.49762600	10.07248900	-0.79801860	-0.91041490	-0.11916420
H	7.52753400	1.58590800	10.32255200	0.23890565	0.86092318	-0.11842918
H	7.23183000	2.87255900	9.45005800	0.41818306	-0.22348934	-0.07667117
O	11.60852100	9.46200800	10.82557900	0.09806377	-0.10970008	-0.03846243
H	10.76641800	9.43266200	10.35562700	-0.41543536	0.09548354	-0.23356958
H	11.74654600	10.39149100	11.11722900	-0.03442157	0.05562015	0.35376318
O	3.02054000	13.27964300	12.41066000	-0.03557159	0.05770971	-0.31611771
H	1.06491700	12.23287800	12.77515200	-0.52964188	-1.10903357	-1.06156146
H	2.65354500	13.75504000	11.58838400	0.26834794	0.04271809	0.23204033
O	10.95310500	12.12005600	1.02705400	0.33636248	-0.52307033	0.22060840
H	9.99933100	11.98387700	1.36212400	0.17883166	0.46969361	-1.29280082
H	11.03653000	12.05071100	0.02950800	-0.47866696	0.14470479	0.65922408
O	7.69407100	12.80442000	3.78505300	-0.08889266	-0.27558419	-0.07508080
H	7.77279900	12.47822100	2.83088300	0.17830199	0.21871697	0.29627746
H	7.09330800	12.11419700	4.17025400	0.25560956	0.14066830	0.20018898
O	8.52953400	9.70873000	10.68827900	-1.77050773	-0.23005003	0.36070549
H	7.51770900	9.69986400	11.02508300	1.98960431	0.35066698	-0.29480607
H	8.57009100	9.31512500	9.77809200	0.04599982	-0.14537376	0.32160777
O	9.67450800	1.78801400	13.65989700	-1.35728695	0.09376631	-0.38080617
H	10.16736100	1.67059600	0.73742800	0.18077925	-0.22130513	0.25788644
H	9.12205800	3.04567200	13.64067600	0.06007655	0.48019071	0.29566834
O	12.08572300	12.88171000	3.46268800	-0.24849332	-0.09308369	-0.73906054
H	11.86493100	12.37437400	2.64272500	0.34336690	0.21108530	-0.34385328
H	11.31098100	12.59605100	4.01544900	-0.38925563	0.17619147	0.77272142
O	7.77417900	11.03528500	7.65791700	0.42531573	0.78225063	0.86323793
H	7.83289400	12.08922900	7.57095400	0.00895877	-0.87913254	0.19200014
H	7.57468100	10.78412600	6.73851000	-0.14722532	-0.48890411	-1.23162469
O	2.52962400	5.38243500	9.02059800	1.07895354	0.47862930	1.49505649
H	1.77452800	5.84247400	8.58001100	-0.72772414	0.29914311	-0.32248462
H	2.92168600	6.08653700	9.61872900	-0.40282918	-0.45464706	-0.97187581
O	9.54906800	8.59717400	13.29564600	0.21275412	1.85011786	0.54350826
H	9.41042500	8.99740600	12.41181100	-0.11304740	-0.15406259	-0.29329239
H	9.54624700	7.64399100	13.17899500	-0.04619462	-1.47046411	-0.71448545
O	11.15244600	1.45618700	2.14316600	-0.00839967	-0.11692909	1.11339404
H	10.68174000	1.85131200	2.94664600	-0.17172131	0.19797370	-0.54158287
H	11.51787400	0.62418900	2.55005900	-0.09090191	0.09874375	-0.18472344
O	9.50185500	4.92136300	2.40115200	-0.98395237	-0.25456034	0.53180941
H	9.50519300	4.11998700	3.07023300	0.06507460	0.34580736	-0.51086371
H	8.73738800	5.50730500	2.71396000	0.34579453	-0.38395640	-0.43042150
O	11.79463200	9.46462300	1.01346300	-2.09772890	-0.48849744	-0.78507928
H	11.30541900	10.32473700	1.11763400	0.78492496	0.53252971	0.31857039
H	11.11413100	9.05899800	0.36871300	0.69100498	-0.16476324	0.53460072
O	9.93868700	6.06927900	12.49103900	-1.82317260	-0.01712160	0.16677102
H	9.96776900	5.98765900	11.49697500	0.03929174	0.30014721	-0.24302690
H	10.82295900	6.03736400	12.87050200	1.30208848	-0.80383309	0.00213235
O	5.47141200	1.32436600	7.22498200	0.38065720	-0.49461174	0.43498556
H	5.57359900	2.23460600	7.55399700	0.00215396	-0.06007812	-0.42856536
H	4.95430900	1.33218900	6.39452400	-0.32265790	0.34681069	-0.11390521
O	7.26079300	13.60621800	11.04582600	1.26344512	-0.87459803	-1.05066322
H	6.58248100	12.90259000	10.83862700	0.24143533	0.36687510	0.16996617
H	8.14203700	13.16751100	10.72008000	-1.18381770	0.40499408	0.09794185
O	0.35268200	10.30458500	9.43512100	0.44428925	0.20140778	-1.30477059
H	0.13917700	10.79067700	10.23234700	-0.05335951	0.57887834	0.98380570
H	0.82197900	10.96034700	8.86588500	0.09702994	-0.14765007	0.05182788

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H	0.75125500	4.85103400	8.22950200	-0.06207968	0.20192762	0.22851750
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O	8.39628300	6.88047100	4.65357400	-0.27352309	1.59625129	1.31868216
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O	6.51849000	7.94534900	5.35876000	1.82166674	0.02665824	-0.93124740
H	2.82924000	5.35377800	2.97772900	-0.08179171	0.42629004	-0.97219759
N	6.01550900	9.83619100	11.55930000	0.27467911	-0.05716620	0.37354989

O	5.03035900	9.92024600	10.80988100	-0.44651473	0.63109068	-0.95332404
O	7.05375700	10.58173900	11.45330100	-0.12894916	0.24295247	-0.32112316
O	5.98918500	8.97607900	12.48301200	0.36270488	-1.05167233	0.75638197
H	6.98407100	13.38017700	12.78192800	-0.30980527	0.53988989	0.15040463
O	13.19522800	10.97434900	11.10424200	0.00700631	0.18690282	0.43658189
H	13.01801200	10.29590700	10.41231300	0.18022522	-0.21892923	-0.31661609
H	12.62472500	10.59772000	11.81259400	0.20273956	-0.45387731	0.11526789
O	12.46434700	8.81730800	9.27795100	-0.46553769	1.10973028	-1.59583772
H	12.39773400	9.25872500	8.34899000	0.76277729	-0.54740189	1.14507584
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O	6.82012000	4.44633900	1.78082300	2.10883392	-2.05362655	1.30401222
H	7.34597100	3.91891700	1.11294700	0.04779773	-0.13008226	-0.08569390
H	8.07908200	5.19690700	2.55015200	-0.78584421	-0.24876082	-0.44689568
O	0.72909500	3.89312700	8.42226200	0.44771553	-1.02025457	-1.81478197
H	0.30366000	2.36896700	1.15006400	0.30957995	-0.11926107	1.13728425
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O	2.54353300	10.29709900	9.52982600	-0.18814938	-1.93849402	-0.59469660
H	2.52437600	10.78937500	10.37780600	0.07041329	0.61179968	0.82168081
H	12.90137300	4.29668100	12.00603800	0.21928026	-0.05977904	0.23030741
O	11.09817200	1.47119100	10.09016200	-0.20711368	0.68482893	2.85751498
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H	11.28171500	1.57870400	9.17541500	0.41465215	-0.25110129	-2.30382928
O	1.05490300	0.23749500	8.63004900	-0.98193730	-0.56778838	0.26298625
H	1.16776400	12.50635700	8.28413200	-0.75061553	-0.43785370	-0.53933595
H	0.74755900	0.44443400	9.56073300	-0.03168723	-0.20055031	-0.17080022
O	0.53269600	11.13560600	1.22663200	0.87140280	0.17832377	0.82015957
H	0.16512900	11.84549500	0.61959500	0.13553992	0.37129966	0.47056845
H	0.91852000	11.58217000	2.07778700	-0.71120993	-0.53486631	-1.09935624
O	12.38661800	4.95664500	12.53373900	-0.95854639	-0.73912459	0.07926762
H	1.07621900	7.04808100	9.88011600	-0.45044946	0.19564574	-0.00221365
H	11.91938200	4.47513300	13.29978900	0.61381993	0.18150712	-0.42590804
O	2.72429000	0.88343100	4.88828800	-0.22444185	-2.32442247	0.38461815
H	5.16172700	0.49960000	4.46894900	0.98002933	-0.17307644	1.47696731
H	2.45621200	13.48117400	4.85602700	-0.00294309	1.59163422	0.17530806
O	10.36799200	9.75206000	5.28802800	-0.82838004	-0.72699019	-0.44052249
H	10.36031200	9.23663400	4.42053100	0.21571028	0.58825140	0.40819571
H	8.51195200	10.33033300	5.28033300	2.09174083	-0.16583378	0.08943707
O	2.92668800	9.87623200	0.29348200	0.93512438	0.84934067	0.24111231
H	2.10524100	10.32543200	0.56408500	-1.02925314	0.33491705	0.72353658
H	2.62159600	9.16464000	13.32542200	-0.18565103	-1.23707065	-0.50848001
O	10.16568600	4.04419100	10.71620800	-1.13869290	-0.60842181	-1.42831461
H	10.77311000	4.36242800	11.36499100	1.35348032	0.83003323	1.32421851
H	10.46653600	3.12716800	10.47958500	0.45716406	-0.33470524	-0.05747582
O	4.34602400	13.36957700	0.81804900	0.63987737	-0.90850426	-0.17162228
H	4.70674200	13.59189600	11.41652600	-0.79094041	0.23930010	0.11104504
H	4.36115500	0.16255200	13.49670500	0.07757980	-0.20447293	0.24031042
O	5.29667400	6.28889900	0.82925100	1.82174460	0.59470700	-0.83298173
H	5.05657600	6.60401000	13.50593900	-0.77404311	-0.35759318	0.66750816
H	6.37409000	5.08924800	1.26466600	-1.81165749	2.12705550	-1.31778776
O	9.68086400	7.88403400	6.91614100	0.08780403	0.57898473	1.71369473
H	10.60372900	7.54340300	6.93328400	0.87174988	-0.10362175	0.23544760
H	2.94012000	9.13625700	5.82656600	-0.10351012	0.45574614	0.03607490
O	9.90742300	8.66381300	10.03058400	-0.48646005	0.58578941	-0.63803395
H	9.15832200	8.21703600	10.46399900	-0.57879012	-0.79097952	0.41294755
H	9.46928400	9.44433500	9.58831000	0.50803173	-0.00462187	0.24445516
O	1.57349600	7.95698000	11.15755000	1.63931242	-0.88984738	2.23577196
H	0.95751600	7.85419000	11.97293900	0.18215356	0.07003739	-1.21242723
H	2.48619500	7.51542700	11.48725200	-1.61367147	0.81929181	-0.73012098
O	4.66172200	3.90436800	7.91428000	-1.22512064	0.65303212	0.07738450
H	4.10128500	4.51477300	7.35563100	0.58258273	-0.48334422	0.72657256
H	3.77885700	2.09930800	8.70101000	-0.12403054	-0.05185346	0.22589824
O	1.20881500	11.82458300	3.89512900	1.30208268	-1.19677406	-0.00468008
H	1.21650600	10.88618600	4.26468500	-0.18928499	1.13757882	-0.38535573
H	0.34922700	12.20996400	4.16223300	-0.87714531	0.18462415	0.27726379
O	12.98298200	13.17555100	13.50373000	0.04999086	1.21940035	-0.28742278
H	13.27582100	13.59389900	12.58611700	-0.38322382	-0.45686095	0.74151320
H	12.92739300	0.42564100	0.49822500	0.20739473	-0.84303017	-0.19553262
O	5.57695100	3.42747900	3.85602200	-0.42231784	0.74776164	-0.30861983
H	4.86693400	4.12453700	4.03344200	0.27364559	-0.74251816	-0.09321778
H	6.11686300	3.80967100	3.08874800	-0.29623554	-0.11957817	0.43091136

O	7.71827300	10.86663100	5.39482600	-0.09126679	0.28826311	0.29968674
H	7.10586100	10.21839600	5.05646600	-1.51875040	-0.39262013	-0.50530312
H	9.30587200	7.34481000	6.23889400	-1.06900625	-1.11775853	-1.56197429
O	9.77302400	3.29161400	4.09230800	1.42143315	1.66303874	0.10949557
H	9.59242500	3.41798000	5.06081600	0.34965393	0.00926446	0.60170852
H	9.18256900	2.62591700	3.78949600	-1.71081004	-1.71353689	-0.68745530
O	11.08380800	12.29898700	6.63368500	-1.57837324	1.27187851	0.75510274
H	9.92783500	11.16593300	8.29525800	0.80442892	0.29747051	-1.48295391
H	11.13266400	13.15453300	7.16170500	0.85487519	-0.64106637	-0.15341130
O	7.23136800	8.60825400	1.76066900	0.07893765	-0.01199454	0.04544660
H	7.78945400	8.82769500	0.99007100	0.22269087	0.67546305	-0.13881319
H	6.70384600	7.85119200	1.45603300	-0.49617035	-0.49442323	0.06027349
O	9.79313300	3.29992700	6.79018400	-0.32138708	-0.00843457	-0.04460622
H	9.54392300	4.04667300	7.42043100	0.48370228	0.17208415	-0.34867823
H	9.20198500	2.54663900	7.05642200	-0.04833049	-0.17205219	-0.05471670
O	1.29062700	11.49673000	7.81146000	0.56825116	-0.15115910	0.52657040
H	0.53788200	10.97023400	7.42301200	-0.83657116	0.62287401	-0.31432518
H	1.71398400	10.84325100	8.53751900	0.37764746	0.67736121	-0.14814536
O	4.93088600	4.67145400	10.80709600	0.34514638	-0.30378732	0.25244957
H	4.84378400	4.65301800	9.84155800	-0.29546551	-0.37245804	-1.04192079
H	5.87846900	4.44430200	10.93537000	0.30674895	0.06068276	0.23624329
O	13.04269400	1.95300600	1.49904500	-0.49775287	-0.69361927	0.54049555
H	5.03830900	12.64524700	0.80947000	-0.81238655	0.95433387	0.01536774
H	13.01973700	1.77633100	2.50754600	0.43066714	0.73069662	-1.39198251
O	4.05649900	6.48235400	6.36064600	0.45979085	0.55033642	0.43417908
H	4.77591500	7.07323200	6.04099900	0.05309430	-0.38236847	-0.07242435
H	3.33730600	7.09435600	6.66897800	-0.44940069	-0.25014029	-0.20994597
O	6.79085000	3.58573300	6.20991800	-0.34678621	-0.22168678	-0.35631566
H	5.51350500	3.93271700	7.43854400	0.67466538	-0.17770449	-0.37893184
H	6.34584300	3.46813500	5.30418000	0.31309055	0.12615279	0.39688987
O	3.73687000	0.30886300	11.31366600	0.63880640	-0.74037826	0.53983079
H	4.02010400	0.98701400	1.95598100	0.20820496	0.27483370	-0.10870933
H	3.16929100	13.06577400	11.49784900	0.45644000	0.42596388	-0.06718291
O	3.85326700	1.79280000	2.52311000	0.60385177	-0.28878344	0.13976151
H	3.16298400	0.98880700	4.02656200	0.08968567	0.72965564	-0.73269007
H	4.74514900	2.22072700	2.71935400	-0.96067518	-0.06049946	0.12163335
O	11.45325500	5.92176000	2.75737300	1.37740343	0.34321524	-1.26453197
H	11.35860700	5.69329500	3.70873000	0.54238926	-0.22935970	0.95978213
H	12.42094600	6.21573600	2.66611500	-0.88353009	-0.12104956	0.08969987
O	2.76108900	5.78607000	2.04027600	0.19960120	-0.49839460	0.03272315
H	4.54316200	6.15147100	1.41870600	-1.40199082	0.10915437	0.05059369
H	2.47361400	5.10064000	1.37407500	0.07700392	0.29997740	1.07783714
O	1.85656000	3.09642400	1.06895100	0.57806280	-0.11508255	-0.32738774
H	2.54041800	2.71029100	1.69865500	-0.33611458	0.07103622	-0.34056758
H	2.28848000	2.99016300	0.17812300	-0.01185110	0.08976641	0.39640489
O	5.23235400	10.50565900	2.07156100	-0.52816569	0.15868582	0.25156372
H	4.33470400	10.26804700	1.70445400	0.70205061	-0.14618526	-0.03874900
H	5.91100200	9.82929500	1.78444500	0.06533985	-0.20885604	0.12157913
O	13.44965800	0.74778200	11.24003300	0.90470435	0.62602033	-0.02576700
H	0.13410400	1.75121300	11.32504100	-0.33162365	-1.01850263	-0.36338648
H	12.51810600	0.81256500	10.92584400	-0.46022402	0.06883943	-0.39033752
O	7.81624300	1.46838600	3.28131200	-0.39890024	-0.55913893	0.50661162
H	8.78328400	0.32312800	4.26423300	-0.10822224	-0.69738676	0.32895026
H	7.89797500	1.10136400	2.35612900	-0.55722101	-0.12280359	0.34484830
O	10.78693800	12.36202700	10.95719500	-0.90706432	0.06638167	-0.40903565
H	11.57821800	11.88144700	11.25640300	0.45859523	-0.18658969	-0.53678009
H	10.28542100	11.79159200	10.30548300	0.27102258	0.34065295	0.28339844
O	3.51341400	9.93082800	5.95502700	-0.68536503	-0.24263795	-0.59550331
H	7.19605400	10.88794500	6.98671400	-0.31160017	0.45623853	0.09053952
H	6.14980300	10.50286300	8.14436100	0.74566485	1.06655290	-0.53556355
O	13.01435500	7.38651700	13.07688800	1.62969988	0.95027136	0.77012566
H	12.27534900	8.00986100	12.92098900	-0.40962193	-0.07781706	-0.58908445
H	12.85903500	6.46826100	12.76022400	-0.62594198	-0.24281981	0.00365982
O	5.93554000	0.26588100	7.55625100	-0.13848375	0.40380969	-0.21499668
H	5.10906200	0.68131500	7.94319600	0.16298690	-0.79126391	0.20650849
H	5.87818500	0.20937200	5.92841900	-0.57211564	0.63337631	1.51616637
O	5.95311400	0.11437100	4.96671200	-0.91168915	-0.14101901	-3.39963564
H	5.13394800	12.12892200	4.75047400	0.42465779	-0.13571624	-0.27072750
H	7.05467700	1.03597200	3.82237400	1.08164573	0.52453884	-0.99739580
O	8.48564800	1.04413100	7.29010200	-1.44636386	0.19856838	-0.17052718

H	7.70062400	3.85948700	6.01826000	0.02394833	0.09489040	0.18150861
H	7.46324300	1.09596000	7.18700800	1.36029689	-0.17892983	0.26857137
O	13.64535500	9.08247500	4.47297100	0.34564294	0.27031565	0.35851270
H	0.25666100	8.44646600	3.75192400	-0.05028508	-0.23994288	-0.34051787
H	13.04920300	9.73605400	4.05383100	-0.34497211	-0.05776727	-0.24736753
O	11.81682700	1.23172900	7.42983100	1.32070583	1.04192710	-0.39546970
H	11.26630500	1.94613500	7.02217400	0.15909394	0.06697804	0.09026155
H	12.77227200	1.52291500	7.22248200	-1.59015713	-0.64016948	0.36477907
O	1.11481600	2.89332400	5.74905400	0.38996828	-0.84224884	-1.25598654
H	1.78565300	2.19454800	5.38228700	-1.06136327	0.66556233	0.75985804
H	0.32338500	2.77274100	5.13142900	0.65808199	0.19055216	0.87495239
O	1.76697100	7.79402400	6.76359700	-0.38683838	0.18394671	1.82036306
H	1.45171300	7.53245900	7.72482300	0.45035018	0.18830787	-1.03520889
H	0.94565100	7.54726400	6.29449100	0.21442637	-0.40188297	-0.63609430
O	3.19771700	4.96656300	4.51573000	-1.21503445	-1.55944957	0.70963745
H	2.47999900	4.38249300	4.94321700	0.79275784	0.60835389	-0.82363751
H	3.43607900	5.58316900	5.27763100	0.30114913	0.40229739	-0.35559507
O	7.94235000	7.16738700	11.29258700	-0.99124973	0.23066696	0.21191712
H	7.11319600	7.57884400	11.68325000	1.07825431	-0.18231574	-0.24656240
H	8.43187200	6.81337000	12.06809600	0.12500329	-0.00369412	0.13339696
O	0.42157800	7.34517100	2.24860000	-1.68954248	1.11926151	-1.52125281
H	0.18448300	7.60527100	1.26280900	0.53689888	-0.86232444	1.83044791
H	1.31588200	6.97874000	2.27665100	0.78168748	-0.62661936	-0.43826271
O	10.18744600	12.75797600	13.34101900	-0.41403643	-0.26506581	-0.81187583
H	11.17261800	12.90391100	13.49347200	-0.62436062	-0.17402590	-0.12896032
H	10.12487100	12.57809900	12.27839300	0.75073123	0.46535581	1.65497757
O	9.04595400	13.21155700	4.94087800	-0.46469382	-0.32455369	0.41031764
H	8.76840600	0.49018600	6.52022700	-0.08914296	-0.12348957	-0.26082966
H	8.36243800	12.46580200	4.98063000	0.55550049	0.93713586	-0.50072884
O	4.04480600	6.87479300	11.84369900	-1.72359117	-1.23328074	0.50967226
H	4.68104700	7.53920400	11.64366100	1.21615461	1.44767748	-0.52899852
H	4.22267600	6.05386100	11.29206500	0.47914430	0.41726440	0.40475627
O	9.39693700	11.16513600	9.08032300	-2.96001538	-0.53372372	0.38401606
H	8.39175600	11.17818100	8.76318800	1.67483253	0.19678478	0.41761437
H	10.05215000	9.02280200	5.91964600	0.38116622	0.78352203	-0.19209539
O	4.89479800	11.20603200	4.46942000	0.48038782	-0.97575848	-1.48678242
H	10.57242600	7.36477300	3.02455200	0.56143338	1.23727049	-0.62852938
H	4.22610000	10.59255500	5.08890800	-0.16215467	-0.00044334	0.17986757
O	6.79531500	11.23405300	7.84218400	-0.29735831	-1.10056427	0.72601837
H	8.38664200	0.73683900	8.94858400	0.31847450	-0.16626354	-0.00957005
H	4.41099400	9.58998100	8.88715500	0.32810203	-0.63236417	-0.63359650
O	0.47934000	3.23167500	11.12941800	0.30845678	1.01157357	-0.28148637
H	1.38843800	3.34112800	11.52659300	-0.18137320	0.06796432	-0.49688538
H	0.50616300	3.61903000	10.18313200	0.28227203	-0.69702112	0.44277457
O	2.46485100	11.52072200	11.79685900	0.18881384	0.29974033	0.25793189
H	1.50686300	11.54613500	11.98572800	-0.40369911	-0.02654342	-0.25536616
H	2.17940300	9.41312800	9.81602700	0.12792130	0.45965367	-0.05943598
O	9.44416100	6.59769000	0.09681600	0.02257787	1.16182875	-3.10281914
H	10.17226400	6.05075800	0.31261100	1.51639399	-1.00038928	0.51231365
H	8.89298700	6.59960800	0.83192100	-1.59632974	-0.12330675	2.43220601
O	0.68186500	6.73344900	9.01859000	-0.17908220	-0.32066115	-0.52752746
H	4.03577400	9.72519900	6.79390000	-0.06780589	-0.04490906	0.10991371
H	13.34008800	7.09958200	8.97969500	0.73606449	0.17916396	0.22667396
O	3.13480900	2.97437000	12.12087200	0.10517133	-1.22642726	-0.38725313
H	3.94305400	3.45306100	11.83595200	-0.14375516	0.56401602	-0.14178724
H	3.31931800	2.05126200	11.75888200	-0.36360385	0.57398276	0.61972706
O	7.67074800	3.43712100	11.15681600	-1.08603647	-1.29668350	-1.14161578
H	8.59005800	3.68579500	10.89133200	0.32335215	0.54096752	-0.25369618
H	7.52296200	2.59413600	10.60843000	0.38452677	0.97755539	1.00177869
O	4.71399200	9.29283800	7.97829000	0.57309911	0.18399333	0.90578968
H	6.05593400	12.88517300	7.77160700	-0.18721495	0.15516208	0.22699006
H	5.41513300	8.58606200	7.97507000	-0.25520600	-0.02769303	0.85083619
O	6.31301400	13.14233600	12.08518400	0.67824780	-1.18070723	-0.53198298
H	2.84430600	10.92045600	12.50591300	0.07010041	0.29314003	-0.07526605
H	6.62905900	12.21839500	11.79427600	-0.56436202	0.78137192	0.10889288
O	11.84637800	10.58988500	2.72392700	0.95330572	0.16722166	-0.62833062
H	11.43154700	9.72325900	2.52672100	-0.35599978	-0.06511335	0.06356630
H	12.59107400	10.69122800	2.05245200	-0.41530059	-0.01231282	0.42327003
O	10.35484300	8.35931800	2.85540300	-0.66363700	-1.45465153	0.23171501
H	9.45825800	8.27524800	2.46196700	0.26422952	0.55055583	0.11127228

H	10.26982500	12.56214200	6.10734400	0.60639713	-0.68656447	-0.22301752
O	8.86804100	10.24716400	13.60146000	0.91280339	1.13156299	0.59845404
H	9.23327900	11.22115600	13.66392100	-0.58052894	-1.61256562	-0.22068867
H	8.16527800	10.20172800	12.92479200	0.03595344	0.52163209	-0.40932041
O	8.43217000	3.34819700	13.62039700	-0.21117810	-0.53365057	0.69908570
H	9.33367900	3.44650100	0.39476800	0.63981794	0.09301495	-0.26010017
H	8.36494700	3.43830800	12.63408100	-0.16405103	-0.07146929	0.06833896
O	12.29334400	12.69015200	4.36989300	0.96906246	1.05803309	-0.85554274
H	11.90261200	11.98757000	3.80281100	-0.35614929	-0.25306822	0.20772162
H	12.01438600	12.60189900	5.30325300	-0.46469180	-0.58686183	0.32456257
O	8.58219800	0.79594700	9.92064700	0.07557706	0.90329845	-0.17205362
H	8.03031200	0.16782400	10.37083500	-0.79682008	-0.83328822	0.53248990
H	5.16627900	10.76762000	3.41216400	-0.55148384	1.09685549	0.71438303
O	11.18132200	3.70386500	1.08578400	-1.67007085	0.24158813	-1.74160476
H	11.24789700	4.41494900	1.72703000	0.42506526	0.98380976	1.14757754
H	11.90794300	3.06709000	1.21704500	0.77919135	-0.89285005	0.55531202
O	8.66901500	7.56974100	8.46133500	0.96580167	-0.13098615	-0.11578756
H	7.65848400	7.80385600	7.87491900	-0.94928729	-0.73933905	1.17670662
H	7.15332500	6.89883300	9.15884700	0.00936115	1.05000782	-1.16765750
O	12.34998400	2.02276100	4.37603400	-0.80482499	0.15611149	-0.47413726
H	11.44496300	2.43430800	4.28614500	0.63765562	0.30420884	-0.01750390
H	12.11804700	1.07260800	4.38830200	0.37494304	-0.66639405	0.08787464
O	8.97589900	5.47391600	2.90536000	0.31730699	-1.83821225	-0.55991558
H	9.35688700	4.56472100	3.24840700	0.17444219	0.22932879	0.06815577
H	8.72561600	5.99153000	3.81204200	-0.17943716	0.67244771	-0.07406747
O	11.27730000	9.28801200	12.17056400	1.22486280	-0.02029870	0.32050130
H	10.73137000	9.07454400	11.38035500	-0.21291138	-0.07459306	-0.32264135
H	10.66953900	9.70161000	12.78331300	-1.06912020	0.29318778	0.79087913
O	9.31521900	5.34199800	8.41100600	0.25063753	0.59190788	0.43784632
H	9.58486600	6.27940200	8.22084200	-0.15960085	-0.75500570	0.07251313
H	9.80068000	5.06436500	9.23403500	-0.23747681	0.17811183	-0.24238421
O	3.62281500	1.14457900	8.88898900	0.11070250	0.15353738	-0.14086603
H	3.64486300	0.93578400	9.89488200	0.17109129	0.18362299	-0.88715042
H	1.96696300	0.55355400	8.53309300	1.06953081	0.77883250	0.16174936
O	7.95560000	0.58827000	0.47363800	-0.72889942	0.92368626	0.20490997
H	8.19319700	1.49887500	0.13526800	-0.22684135	-0.28184865	0.26330536
H	8.78650200	13.67440400	0.40474700	1.18681720	-0.60664999	-0.29874999
O	12.80263000	10.14741900	6.84879300	0.01995302	0.29062998	1.16989448
H	11.93441900	10.41898600	6.49679800	-0.19759020	0.28896164	-0.36218300
H	13.08102700	9.41239800	6.29664600	0.33141377	-0.74616114	-0.93110360

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N	10.94090200	9.83493000	5.08202800	-1.00433284	1.30564209	-1.08957876
O	11.47549500	9.07049800	5.86241800	1.25655165	-0.94242039	0.77974059
O	11.60956800	10.73237600	4.38599200	0.15798023	-0.83874415	0.55309579
O	9.66894100	9.83767500	4.94921700	-0.32154621	0.03663717	-0.40954535
H	11.66664100	5.10441300	5.60749500	-1.69200234	1.07148939	0.93684723
N	4.62280100	4.23071900	6.65312100	0.76834978	0.67251813	-1.73561860
O	4.82043100	4.58629700	7.84698400	0.06989134	-0.25269720	1.17075715
O	3.65416700	4.74859700	6.01739200	-0.11958223	-0.52356683	-0.19519300
O	5.48813300	3.48498000	6.04645000	-0.75550332	-0.04023551	0.53009703
H	12.50302400	5.74781300	2.72203600	-0.34677341	1.22918600	-0.90341502
N	5.14031100	11.14986200	10.17841100	-0.37456930	0.77249080	-3.53560948
O	4.91325600	12.37827000	9.63088500	-0.09809685	0.05344008	0.28099487
O	5.21365600	11.13689100	11.39071100	0.08000970	-0.52830184	1.37420464
O	5.22996800	10.20051700	9.37225800	0.17568983	0.08536024	1.02843374
H	1.35020600	12.36924400	9.54697700	-0.10225077	0.52757077	-0.06261191
O	8.03769100	9.20789400	7.95268500	0.38919918	-0.65213440	0.44673827
H	7.42934700	8.71913900	8.55117800	-0.04273927	-0.15489634	-0.22084342
H	8.82290600	8.59800600	7.86758800	-0.25687122	0.42273637	-0.01011524
O	11.81403700	0.01152000	9.18590600	1.33301074	-0.81037487	-0.93685214
H	11.93338700	13.25651900	8.30422900	-0.72588323	0.80125635	1.44178385
H	12.71841200	13.70711100	9.60502300	-0.57944881	-0.00800727	-0.28276102
O	8.45480000	3.75484000	6.72490300	0.68147662	0.52158100	-1.29721145
H	7.71141500	4.00542000	6.13953300	-0.24280695	-0.52358415	0.96597569
H	8.28213000	3.34870700	7.61902900	-0.47922074	-0.05505902	0.33328383
O	13.43118200	1.35126900	4.04231900	-0.66978205	-1.48791232	2.65477858
H	12.85695300	7.69259800	2.29260000	-0.68495624	0.12080599	-0.32766565
H	0.45523600	1.72632300	3.59468200	0.75507390	0.43984915	-0.41093452

O	11.65333600	11.31474400	12.89254900	-0.99251683	-0.47620308	0.35272863
H	11.08006400	11.15155100	13.71850800	0.90074962	0.04958691	-1.05933818
H	3.57099900	6.04802200	0.82829000	-0.99415656	0.52553646	-1.45288341
O	12.13691900	0.28346600	2.18153500	0.01501154	-1.42835047	1.47196674
H	11.87491100	13.07610800	2.30371800	-0.04287407	1.53551082	-0.23899720
H	12.66542200	0.59194800	3.08783400	-0.40612630	-0.08077480	-1.51087392
O	12.36845400	4.81740500	2.98009300	0.01753083	-1.41894954	1.03584483
H	13.05199000	3.34793000	0.41869200	0.39071010	-0.41878054	0.11249537
H	12.32789900	4.17671600	2.15309900	-0.11741585	0.04832171	-0.27070709
O	1.39645900	10.64434100	1.40261300	-0.04421646	0.94192161	-0.05242614
H	3.16191100	9.88293100	1.30652600	-2.02391568	0.44885091	0.10272753
H	1.04341100	10.82119000	0.47326900	0.17879255	-0.21595581	0.30971081
O	2.53889800	6.35490600	13.11119800	-0.03677267	-0.02140416	-0.17390644
H	1.55820600	6.25022400	13.13841900	0.14919254	0.40538836	-0.14586847
H	4.81325300	1.39776100	12.38521000	-0.67281065	-0.06031417	0.15019921
O	4.30675800	0.83005200	6.04296400	0.45999264	1.27129169	0.65524169
H	4.95108300	1.63226400	6.05859000	-1.02718608	-1.04481398	-0.24357078
H	4.99848900	13.19502800	6.61012600	-0.01191784	0.84063663	-0.12225483
O	11.85885800	12.49120800	6.77147800	-1.20342434	-0.66654622	3.43374191
H	12.64339500	12.88963400	6.45946700	2.07117032	1.00103563	-1.72990701
H	11.25570500	12.08888100	6.17518800	-0.51809847	-0.35347785	-1.65127622
O	0.52685700	11.14866300	12.55645200	1.36366303	0.40626119	0.08287437
H	5.35441500	7.63008600	4.58384000	-0.19565631	-0.40934441	0.29305052
H	3.20197700	7.00304800	9.74669500	0.30706352	-0.14474242	0.42329497
O	12.80864100	4.50061200	9.73712200	0.23852804	0.50445962	0.09986683
H	12.89166100	5.39892000	9.31486300	0.13634144	0.01156564	0.25082500
H	2.27715300	3.63649900	11.19880300	-0.53687093	0.11812485	-0.16315575
O	2.44477500	13.04464300	2.18732200	0.74941202	-0.44206945	-0.04130307
H	1.64960400	11.57551700	1.73845300	-0.20817418	-1.11300588	-0.47983415
H	3.43351600	13.01595800	2.06836400	-0.97772257	0.17397324	-0.17605186
O	5.81244800	7.25954400	5.42907400	-0.14499479	0.64501305	-1.11465147
H	6.78717500	7.49639800	5.35185500	0.47445505	-0.26894357	-0.15532513
H	13.27332100	5.39796600	5.65411800	-0.22357494	0.00081752	0.52703611
O	11.33190100	2.49237700	8.27558400	0.14247322	-0.71091696	-0.20209420
H	10.95852500	2.34987900	7.36921500	0.30785038	0.25404838	0.16279604
H	11.64679400	1.55774800	8.56096700	-0.44315839	0.85617358	-0.07735395
O	12.19359100	3.52624300	0.90019600	-2.16638479	0.58425113	-1.96515541
H	11.52890100	3.81424100	0.14366600	1.57887337	-0.48655321	1.90384811
H	1.19288600	2.58775300	1.82496700	0.35779518	-0.60882412	0.49212506
O	4.90018900	2.35643200	12.16118400	-0.63680340	1.18578948	-0.26321903
H	5.25864500	2.60465400	8.90603700	0.63138000	-0.53159204	0.07703300
H	13.34707200	11.01011200	12.63197000	-1.28547002	-0.17492633	0.10983260
O	2.68807400	5.88364100	8.85828600	-1.44658026	1.00057525	-2.21823976
H	2.14796700	4.59587900	9.31891200	-0.81417376	-1.68530095	0.43143568
H	3.46626800	5.55186400	8.32975500	0.48143390	-0.37116414	-0.16718362
O	1.85737900	8.42481800	4.94469900	0.47845389	-0.07609629	0.61447877
H	1.13107700	8.88053900	4.43357600	-0.03694533	-0.12736464	-0.24351094
H	2.34788700	9.11057800	5.49779100	-0.77860078	-0.24004520	-0.23585728
O	2.39379900	3.73303500	12.19095200	0.85005599	-0.54361654	0.08153804
H	1.28286600	13.28303700	10.82763600	-0.09431245	0.31618624	-0.29983458
H	2.64734700	4.65519900	12.37763600	0.04912176	0.59873254	-0.02472610
O	5.27698500	12.14076800	0.85209200	0.23434719	0.52871561	-0.19327243
H	5.00393700	11.22021700	0.95773800	-0.77441040	-1.29124988	-0.01308310
H	5.66353800	12.28820700	1.71658300	0.46884599	0.59002377	0.67732309
O	10.55124600	2.13413000	5.36190900	-0.72702101	-0.20554471	0.84956671
H	9.98444200	2.78148900	4.87777200	0.56616073	-0.21227800	-0.02983251
H	11.42129300	1.99034500	4.97816500	0.50296818	0.36530975	-0.79760300
O	10.23228600	5.54541400	6.28391600	-0.40939457	-0.58905003	0.21387919
H	13.76695300	0.81678200	4.87658100	-0.69839852	1.05508109	-1.45052474
H	9.53334900	6.15537400	5.95392900	0.21372983	0.23712242	-0.15922715
O	8.38193700	10.71810100	2.34088700	-0.47670841	-0.07155903	1.05585602
H	8.87167900	10.18382600	3.02328500	-0.39768435	0.03218782	-0.47205572
H	8.37008700	10.20447100	1.50234700	0.14156824	-0.16821595	-0.20059762
O	4.10209700	9.77447800	1.36488800	1.88135961	-0.01529765	-0.83279059
H	4.26610100	9.26125300	2.17561900	-0.13985528	-0.27439537	0.52686539
H	0.88619100	10.57892800	11.83785700	0.05680546	-0.05166302	0.24844823
O	2.48385100	12.71509600	4.90997800	0.33873799	-0.24992359	1.66181405
H	3.23406200	13.35454000	4.96523300	-0.35063788	0.05089247	-0.29596118
H	2.17427900	12.65658600	3.99988800	0.19785459	0.35109063	-0.94727547
O	1.65811700	10.98222900	8.52696000	1.02450142	-1.25663978	1.00079639

H	1.72479900	10.19360300	9.21220900	-0.00349679	1.18999320	-0.31594810
H	0.70328000	10.89471400	8.34904000	-0.87206292	-0.17539637	-0.31578492
O	11.04053300	4.45500000	12.01493600	0.24223336	0.27396131	-0.14592642
H	11.49975000	4.76455100	11.18271600	-0.05624824	-0.70096719	0.44827802
H	10.92067700	3.47754100	11.87380700	-0.07052830	0.18613760	-0.37000131
O	12.25165000	7.04962600	1.82000900	-0.00863691	0.50532564	0.34482954
H	11.24575700	7.44400500	1.84898500	1.25873666	0.20946448	0.24119927
H	7.85596300	3.59369200	3.35755800	0.72418873	-0.27444071	-0.03999030
O	1.62092900	9.37359200	10.71599400	1.59267607	0.66724233	-0.77404667
H	0.82295600	8.87832000	10.84025300	-1.36454792	-0.91578196	0.16451155
H	2.39953900	8.67643300	10.60404800	-0.49621428	0.37930882	0.47691484
O	8.66915500	2.74709300	9.08863900	-0.17632342	-1.32486944	-0.19654908
H	7.13987600	6.89960700	10.35086100	-2.30938128	0.36550871	-1.73563336
H	9.67102100	2.85322100	9.01024700	-0.86226127	-0.68653833	0.06889393
O	12.72579900	8.12415000	11.60448600	-1.11863827	1.33706288	-1.50695686
H	11.74987400	8.36303000	11.57764900	1.36359725	-0.43295545	0.45842292
H	12.91178000	7.38975100	12.22809600	-0.31213224	-0.59837879	0.71694285
O	6.00194900	2.73512100	2.70735600	0.18130988	0.06037614	0.95212591
H	6.32682300	1.88261100	3.10813200	-0.12223183	0.12441156	-0.12920997
H	6.25360400	2.71764500	1.75792000	0.14651895	-0.20793410	-0.64542766
O	9.93838800	8.13219700	1.96009700	0.81991953	0.74649482	-0.34657509
H	9.88003500	8.65896800	1.12033700	-0.28288920	-0.67377136	0.49868460
H	9.45042900	7.22525900	2.01283800	-0.10818149	0.47186150	-0.39504551
O	13.61337900	9.18230100	3.29228300	0.04948446	0.46055654	-0.38866217
H	12.86712000	9.70830200	3.76204200	1.13099579	-0.09786729	-0.92302840
H	0.28773100	9.70460900	2.52451700	-0.75245017	-0.12985896	1.11661433
O	6.67991900	5.47103900	0.88037100	2.21004046	0.25483560	-0.48111067
H	6.83959200	4.54968600	0.55130900	-0.32631637	-0.16285427	-0.11329414
H	4.89560300	1.50255200	9.88774100	0.13950675	-0.13305878	0.19330756
O	4.03546000	8.08311800	3.51119900	1.11742918	0.93586846	1.40513710
H	3.25447100	8.04774300	4.14741800	-0.43784118	0.10850300	-0.66753732
H	3.97649100	7.37411100	2.87434100	-0.22778396	-1.39656322	-0.99260549
O	1.73170900	3.64843800	9.59618400	0.29547129	1.13766278	-0.32298361
H	0.75377400	3.85311900	9.65245900	0.34423044	-0.09576258	0.09004498
H	2.17863000	2.23125400	8.35998200	-0.24687871	0.29798176	0.73280871
O	4.79626400	8.66617900	12.53374000	1.15142019	-0.47587111	-1.34937978
H	5.02056300	9.45719200	11.98727400	-0.18179006	-0.15365614	0.49642853
H	4.37166400	8.99803700	13.32088100	-0.37967176	0.45958774	1.32165672
O	8.73800000	0.21788800	6.06487500	-0.57502960	-0.68306884	-0.33454711
H	9.53489600	0.69298800	5.78640700	1.03677344	0.64141503	0.26987769
H	8.20112500	0.41831900	5.24883100	-0.55531137	-0.26632328	0.18640441
O	6.80402600	4.27050600	10.75061100	-0.37486757	-0.10220857	0.141110881
H	6.30836800	3.53443400	11.17318700	0.07007742	0.28559571	-0.25585978
H	7.39311500	3.80864900	10.11820300	0.24941060	-0.04675068	0.07865199
O	4.20014800	5.98667700	1.54169000	-0.21536781	-1.15131202	2.15804845
H	3.79194700	5.22273700	2.11982500	0.98538443	0.74199519	-0.47350111
H	5.74045700	5.65924300	0.98430700	-1.48716115	-0.07746247	0.41496895
O	7.80255600	0.20516500	8.62569000	0.68718647	0.13058344	0.07374981
H	4.25188900	13.00762200	11.85134100	0.21714175	0.80623995	1.51494493
H	9.65914200	4.71471200	6.53449200	0.01654330	0.37605384	-0.08760336
O	3.18934400	10.10938300	6.52765000	0.21023712	1.50405503	-0.66273397
H	2.63411600	10.48864700	7.26396900	-0.65329285	-0.11194974	0.64248991
H	3.42570300	10.97542000	6.07053400	0.09563004	-1.03956702	0.12071453
O	8.85628000	3.66204400	3.39330800	-0.87349517	0.52162726	0.45229566
H	9.18188800	2.91766300	2.85672100	0.08837595	-0.88788057	-0.72837997
H	8.14115600	0.62018700	3.01135300	-0.84613081	-0.08817203	1.02370082
O	0.85863600	6.18757700	6.65197600	-0.49523435	0.09027191	0.87409869
H	0.38423100	6.83538000	7.23510300	0.00603212	-0.25181581	-0.42097060
H	1.21230300	6.69868700	5.90526200	0.42047426	0.76553741	-0.18681453
O	2.42599600	1.31398200	8.13481900	-0.08652553	-1.00671418	-0.51812610
H	3.66416400	1.05502300	6.79032500	0.34226221	-0.19726428	-0.36334672
H	2.05221300	0.68614900	8.82861800	0.09816534	0.65086658	-0.26012393
O	12.54234800	4.79520000	5.38616300	2.03830869	-1.31490499	-1.00943349
H	12.41390100	3.94201900	9.04812100	-0.50435647	-0.61025965	-0.35749701
H	12.49104500	4.65989600	4.06007100	0.10624584	-0.00760488	-0.13164276
O	12.81834200	10.34425900	8.43337600	-0.04345162	2.41134875	0.49446272
H	12.54801100	11.11206600	7.80653300	-0.16269019	-1.67322478	0.39790861
H	12.79833400	9.47975100	8.03942000	-0.28767165	-0.76707497	-1.07922961
O	6.32014400	7.16272800	9.76344100	1.17550195	-1.28863924	0.89146538
H	6.61708800	7.77823300	12.68115200	-0.20546867	0.09054360	-0.05206920

H	5.07371200	8.39883400	8.13668600	1.13809073	0.15108225	1.70568862
O	10.79617900	11.51304600	1.85707100	1.85709590	-0.59274489	1.13752757
H	9.85011200	11.47448900	2.11562800	-0.25583770	0.15126309	-0.16064932
H	11.25390900	11.05684400	2.66350300	-1.02233595	0.75334642	-1.38917227
O	13.20751600	6.16589500	13.26906200	1.99642022	1.36543157	-0.26984747
H	12.80755200	6.44164500	0.34183900	-0.38129944	0.38731380	1.01668400
H	12.69836500	5.45678300	12.93563100	-1.28198223	-1.83841342	-0.75737802
O	0.71728800	2.70143200	0.13200100	-0.63206826	-1.26009682	-0.30528265
H	1.37079500	3.22751800	13.39492900	0.25331482	0.05432796	-0.66080345
H	0.64508600	1.81618200	13.37944100	0.33230654	0.99759021	0.97560526
O	7.35732900	0.49627600	3.67643100	2.36000617	3.01480232	-0.94936470
H	8.18502600	0.28384700	7.69088900	-0.92174290	0.09828913	0.24427092
H	7.03579300	13.39533900	3.53465900	-1.00707385	-2.22332450	-0.06313657
O	6.75011900	2.82988700	0.13670300	1.23952494	0.29015816	1.03375075
H	7.46143900	2.22307300	13.58848500	0.21328138	-0.05553774	0.11002834
H	6.04838500	2.76134000	13.24301200	-1.10137998	-0.17868977	-0.86073715
O	12.16649800	0.20337600	13.33650000	-0.28112619	-1.07972947	0.11763572
H	12.14670300	0.18729900	0.58476700	0.30628761	0.49362967	-0.78371991
H	11.90608800	13.02551900	13.08639300	0.16910342	0.76356328	0.15390394
O	4.67123600	8.17794700	7.31827400	-1.89990862	0.53573550	-1.32350654
H	5.05168700	8.98843900	7.10967500	0.75000855	-0.50478634	-0.14693502
H	5.33214600	7.79972700	6.27258000	0.19589790	-0.40132415	0.47394816
O	7.49552000	7.35172000	12.81019600	-0.23870363	0.00573206	-0.01363941
H	8.34374000	11.87434200	6.02877100	-1.25035619	-1.04161357	0.58725464
H	7.26474000	6.60706800	13.44175000	0.05888254	-0.08430214	0.02025829
O	13.01580900	7.12912500	8.98245900	0.47320393	-0.32879110	-1.22134534
H	12.87993800	7.51391500	9.85876000	0.21590817	0.37125995	1.21345124
H	12.09788500	7.19319100	8.59306500	-0.32283330	0.15254438	-0.04591889
O	10.71843200	10.33818800	10.68211500	1.59659918	-1.34544625	0.41962437
H	11.44760900	10.07104500	10.06646900	-0.72278779	0.66404789	-0.04579754
H	11.23600000	10.87843700	12.04950700	0.06462489	0.63369915	1.03637356
O	1.57240400	2.22373400	2.69003900	0.02911877	0.26101116	-1.19444420
H	2.39612300	2.76043400	2.85996200	-0.07968502	0.07384120	0.22152931
H	2.09923900	0.11404600	1.83862000	0.11686534	0.42685506	0.18359577
O	3.36608500	7.56978600	10.56775700	1.14246236	0.39370798	0.56903190
H	4.33616200	7.69811300	10.83019600	-1.39891946	-0.30741906	-0.62577012
H	2.79887100	6.98121500	12.38103900	-0.37103715	-0.42965112	0.21990285
O	3.62925200	3.82556300	3.17962700	0.98402390	0.10905854	-0.04526699
H	3.62684900	4.10362800	4.12740000	-0.04588967	0.04359353	0.13536358
H	4.57715700	3.43156700	3.04840100	-0.73728013	0.03281450	0.06127642
O	5.28948000	12.42405200	7.15290500	-0.31513034	-0.99265524	0.47811315
H	6.09758600	11.97308400	6.77991200	0.21797150	0.23075735	0.34031682
H	4.99900300	12.36776700	8.50730800	0.45473339	-0.28762547	0.05705356
O	8.52934100	11.45898100	9.75048700	-0.35482020	-0.74897794	-0.47960910
H	8.12939200	10.71152200	9.18289900	0.64761082	1.54783419	0.34714216
H	8.52068000	12.35679000	9.31223100	-0.55753005	-0.57009159	-0.35342000
O	1.08308700	13.28615100	9.86171400	0.23307744	-0.41546763	0.22549853
H	9.93363200	10.66920000	10.21750400	-0.42842269	0.58004625	-0.64963482
H	4.01671900	2.86598100	12.25754800	0.77906101	-1.06534673	-0.01625376
O	9.55629400	1.27217400	1.99782600	1.63809210	0.56295581	1.27035682
H	9.36456600	1.04580400	1.07708900	-0.79953367	-0.16253681	-1.23033561
H	10.58144400	1.17718200	1.97866300	-1.08498253	-0.35987404	0.72225643
O	6.25110000	11.95303200	3.78052600	0.47658452	-1.24470736	-0.62153487
H	6.43185500	11.65965600	4.69540000	-0.04647367	0.08315981	0.30932211
H	6.90249700	11.34198000	3.31226500	-0.34080771	0.45503147	-0.10711197
O	10.53974100	7.28004300	8.19372900	-0.50626166	0.50590340	0.92644070
H	10.00962000	7.08826200	9.01557100	0.37829635	-0.31566989	-0.38693271
H	10.55849800	6.45771600	7.62804600	-0.61137942	-0.07509161	-0.25355021
O	7.76555300	12.15354600	12.27744600	3.92439093	0.51987910	1.13406138
H	6.86021200	12.04635500	12.28743900	-3.47217333	-0.34860885	-0.31106938
H	8.13075100	12.07474200	11.37727000	-0.45564762	-0.29679822	-0.48332445
O	1.19784000	0.19935800	12.84170400	-2.75392956	0.74169485	-1.36252330
H	0.51078300	13.26541500	12.66355100	0.81104072	0.51672334	0.74729534
H	1.99175900	13.57875400	13.11895500	2.14027259	-1.20719130	0.57901694
O	7.56502700	11.24353800	6.22705200	0.61843936	1.13028598	-0.41402771
H	9.44647900	0.94492400	12.61988800	-1.01225507	0.39151354	1.01828025
H	7.85603200	10.45486900	6.75410500	0.08744555	0.29406579	-0.22164445
O	5.59472900	1.73488500	9.25390300	-0.59236009	0.68607734	-0.46616562
H	5.94302100	6.25584500	9.53677200	0.74475102	0.92883479	0.32398689
H	2.01373500	6.15573400	8.09486200	1.29135666	-0.72218358	1.19823786

O	8.44334300	7.41103500	4.98910800	-1.31180543	-1.56000709	0.94372779
H	8.94465400	8.22062000	4.99016100	1.07658918	1.66097566	-0.11157194
H	8.70332400	6.86640100	4.22729300	-0.09477210	-0.03686502	-0.90921203
O	9.03106800	6.42826800	10.63765700	-0.35418416	0.59299904	1.03794446
H	9.54538500	6.11576200	11.40496700	0.96685225	-0.85252843	-0.41441891
H	8.32031700	6.73635600	11.27546700	0.09338007	0.25427278	-0.33733895
O	8.78309300	6.06839100	2.46495700	-0.11650117	-1.36682106	0.34166344
H	9.01373800	5.07305700	2.64460700	-0.03210034	0.92816596	0.18271247
H	7.96758800	5.98480900	1.90846300	-0.43092248	-0.07382582	-0.04816592
O	8.88842200	9.62037900	13.50479400	-0.33857338	-1.30396376	0.36765114
H	8.41606300	8.75696900	13.26692600	0.31813758	0.53897128	0.17925059
H	8.50016300	10.26835300	12.90470900	-0.12314626	0.83850444	-0.28031756
O	10.77756600	1.63252600	11.62733700	-0.27378390	0.43108248	0.64175357
H	11.43202800	1.20304000	12.25846300	0.08124575	-0.34322055	0.20888526
H	10.81438300	1.12210900	10.81193400	0.12095238	-0.23492551	-0.58366071
O	4.29733400	13.56494900	12.69191500	-0.70107124	-0.57668224	-1.46896652
H	8.39727900	1.71753300	8.99443000	1.07493086	1.94578564	0.33838509
H	4.51679200	12.95896100	13.44745600	0.37760816	0.13121788	-0.20228923
O	8.70801400	0.85289800	13.34451300	0.90099426	-0.06995893	-1.49432358
H	6.93317300	0.68132000	8.76176700	0.15677492	-0.30721708	-0.50846069
H	8.29712400	13.76010500	13.11044600	-0.07977851	-0.11054683	0.01401139
O	0.36977000	13.74221200	6.34321200	0.95544284	0.93552843	0.21084183
H	1.16472100	13.33328000	5.91729400	0.12846050	-0.74266526	-0.47964273
H	0.87115000	0.68096700	6.83605200	-0.65694412	-0.26040629	0.27907143