

Electronic supplementary information

Morphology of ammonium perchlorate in presence of ethylene glycol as an additive: A first principle study

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(001) surface of NH₄ClO₄ without additive:

O	6.71783233753724	0.56088054803285	3.38374616566160
O	7.17048503896003	0.65438086133092	16.61624708045723
H	6.30642770491733	4.54517547602600	7.75946943707652
H	5.48687184697637	4.44409294089729	23.18092129752765
O	1.31336608193937	10.61394765188176	10.26401540003733
O	1.06659004862800	10.90520124303131	23.32439918442535
H	1.39118596563720	7.66787008810471	1.86232694433333
H	2.24802817226686	6.87896935413531	14.30970639977529
O	9.76070095911999	6.35611058517639	8.81739676571877
O	9.91329036839921	5.97891512791503	21.55975536579173
H	10.51647319729967	10.11342312702632	4.21647448049930
H	10.78246269784375	10.27582553447330	17.56766561233026
O	15.89265270567090	5.11047472341377	1.81777824586546
O	15.77055848339265	4.94747639083327	15.06861353863880
H	13.92052241982148	1.18764257827711	11.38880063237976
H	15.56131469182308	1.86916593120983	23.73073696052672
O	9.77938892753240	10.89231138711765	8.61043266793680
O	9.63425576338141	10.42782736364958	22.53346071531167
H	10.84089764056030	6.91194066250594	3.82275707969698
H	9.83280148276559	7.18872005135864	17.34597344833354
O	15.79569618344570	0.55424785310879	1.73130993796001
O	15.51355105521109	0.40358998014508	15.12944681970798
H	15.30863182628952	4.06216685663819	10.98442150638434
H	13.55714040322010	4.27518963558512	24.74815062840949
O	8.15672544642393	4.82755612082757	3.98350820288197
O	6.95010245516793	5.15858018124616	17.09408511814923
H	6.74820339787769	1.38734649946494	7.89158791567522
H	7.02914395420900	1.76897116484820	22.09985529293696
O	1.32916077194003	6.06534517453562	10.25272521429602
O	1.32019476602903	6.36308205319260	23.59527427139914
H	3.45633685402841	10.14671011792558	1.32665580012162
H	1.77471657099562	10.02468953071552	14.70718263969503
C]	7.69362229118881	2.83333880862581	2.06195027815056
C]	7.11528637317501	3.05874722109254	15.22288453771789
O	5.79583337945210	3.77157554835504	0.26584700574562
O	4.83029557364302	3.14768452798988	13.61708633693112
O	10.04837212653452	2.17935261281664	0.77416559073031
O	9.39280175630723	3.36081048787296	13.69636152517398
N	5.48667025288308	2.84574518188983	8.31973440493443
N	5.44690733873909	2.95711391961553	21.88184921171212
H	3.79811165329949	2.57784206908254	7.35292213381159
H	5.54045320577513	3.76511301004045	20.07921915030434
H	5.14156184066723	2.88107830965573	10.27351875146170
H	3.79861931310516	1.89063834303728	22.11443917493810
C]	1.43709572989797	8.33005728333606	8.66156667644615
C]	1.22515345288562	8.51943322953090	21.86875587764824
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O	3.57071090257918	8.58404779021523	20.33180169594711
O	-0.63692678581237	8.34095941759705	6.82365497097102
O	-0.98434832862988	8.30425527463020	20.20075587691956
N	3.23700054356158	8.34308641395485	2.09898030060821
N	3.01933104145686	8.52727005983153	15.06152517405422
H	4.46751248306024	7.00884896269989	1.30637902557235
H	4.76016857980688	8.88282296755324	14.23417094551873
H	3.58695132417067	8.45420219483118	4.06104436876857
H	3.24874055781996	8.33428330243582	17.02510053367551
C]	9.79493635631824	8.69754138323902	10.32897180083931
C]	9.50855986294866	7.84093794728471	23.57515385089973
O	12.17235301055788	8.75668411153733	11.81391104796231
O	11.55864939412844	7.54073704150527	25.48826985502528
O	7.61646692023420	8.79085943245234	12.02404446401001
O	7.05174276374942	7.43789717068443	24.78499581864458
N	11.81887346876654	8.63170351212713	4.01682357935736
N	11.31267693850583	8.46137681974418	17.01992753879945
H	12.95584653321583	8.55721016623946	5.61770823521639
H	12.88906143121460	7.91872573209458	18.05507245022125
H	13.01592069996224	8.99579753217899	2.50333150967959
H	11.76321867222783	8.48941215213798	15.08420156063153
C]	15.98414382624808	2.79896558614236	3.37016332072175
C]	15.61926283920010	2.70391305180522	16.72362625862346

O	13.81179248809783	2.80998906538702	5.12297046749542
O	13.26029844783331	2.85448450570351	18.21173110314145
O	18.38580023370878	2.72030882967117	4.76933830764278
O	17.81299133375303	2.59161923644955	18.39964722645611
N	13.86372708852866	2.86749849772631	10.36368812199802
N	13.89652046784627	2.89455539607300	23.39218033650061
H	12.12431131964385	3.74967197283546	10.61668456490530
H	12.35544775088792	1.64518832109918	23.21540700406897
H	14.08517276798799	2.51701225188135	8.42330347004429
H	14.06278233476792	3.80521409067452	21.65176930177810
O	23.83370921422151	0.49653226298762	3.67990459199117
O	23.91559762157467	0.70197960988988	17.03183576513911
H	23.57761816904002	4.27693219550867	7.93892029221905
H	23.99867230261307	3.98084886878503	22.01825131960123
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O	17.52045836778125	10.29579628866361	23.87972067031425
H	18.62234856089536	7.23186396899917	1.96595687752168
H	18.84659521887332	6.81737110437183	14.78912545604279
O	26.66534702367043	6.14212208248028	8.34001882531560
O	26.73569476586387	6.03715402477419	21.73760523362281
H	27.19135053311710	9.97648358858616	4.37538982735044
H	27.00594388105876	9.77500327948741	17.14873953525136
O	32.57763922588028	5.27295169567419	1.61641603520089
O	32.63688793001968	5.15680013860491	14.86430382765077
H	32.28492790188764	1.52669784244609	10.71353346344823
H	32.53250617685141	2.13077358772760	23.67662295785320
O	26.68449673721286	10.65841674185717	8.79616007076925
O	26.75390404397211	10.59818533477935	21.50847350511036
H	27.57245861351820	6.96431402143820	3.27254220638483
H	27.94973992670661	6.80322200866780	17.90001472981043
O	32.48568144121598	0.71823142652990	1.75015730855052
O	32.45132708953762	0.61585828026742	15.10722213625606
H	31.02905010436251	4.42875631484015	11.31722001018567
H	30.77572853029596	4.82639044137764	24.36464554569212
O	24.56514305925587	4.97818995647497	3.12454318563788
O	24.15758907053826	5.22715141647593	16.83724920529023
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H	20.26495075021851	10.02922144167286	1.47069398892565
H	19.09903424170662	9.99373396863598	14.53136039697347
C]	24.43898417592249	2.48664205136628	1.78982632220337
C]	24.07406704219319	2.92937339205613	15.29127298729849
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O	21.76842770040165	2.94105942439802	13.72047363873365
O	26.91165402506785	1.92030703375105	0.68142742854489
O	26.33178417289469	2.69322634632247	13.72200917727049
N	22.49618525144545	2.69804599831796	8.42589995374003
N	22.47196558790283	2.70727999951883	21.94457466043245
H	20.83302307998786	2.65124351231793	7.37957818723210
H	22.41743590595304	1.95236014309481	20.12116679571871
H	22.07935781349411	2.77186174888845	10.36435782770863
H	20.78812901139393	3.65695928415820	22.36835438190038
C]	18.27231563200189	8.31885909135224	8.96099629806658
C]	17.90726601524315	8.12048355125424	22.18125401933881
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O	20.15875201026325	8.56718493630187	20.59146689920155
O	16.18689163701983	8.14941468375115	7.13911327792954
O	15.65314350267935	7.78175613567069	20.59340601709827
N	20.25017416717523	8.28635985735461	2.38998571969494
N	19.93336953428759	8.38654766007546	15.30314492333765
H	21.86060394685462	7.20285479648248	2.00895611395063
H	21.76740497117417	8.18097362782351	14.64301141253908
H	20.27235299453300	8.62646319575786	4.35434805765071
H	19.97146379758650	8.53697290208401	17.28412346059405
C]	26.69897616271271	8.23408415001986	10.18458815687155
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O	29.08283305838839	8.07749941940622	11.65138699317548
O	29.13526910331566	8.47666926967370	24.72884550190081

O	24.52006896401291	8.08448807259181	11.86910896730551
O	24.55707311234046	8.48467860362365	24.89544322795694
N	28.52577669053317	8.59841453890516	3.86111936096247
N	28.45639568120268	8.44560755033935	16.94090394491342
H	29.63657813663354	8.13898771545511	5.41250360095817
H	30.10973135617880	9.16187380531845	17.71929145025835
H	29.72185692619399	9.34764489483945	2.48473809749329
H	28.74698198738077	8.06254972989098	15.019144481348258
C]	32.67600356194325	3.04225402217567	3.27578005367876
C]	32.55406103742969	2.97959852544731	16.60002454134406
O	30.49941546348995	3.13990725807726	5.02862838136415
O	30.21781358049367	3.14281916918861	18.13337046864377
O	35.06796579721494	3.03267582814812	4.69302012693552
O	34.77056237018134	2.96911945362255	18.25154006235221
N	30.82953999159632	2.78614752470365	10.25349320655212
N	30.92493262750309	3.20223410497631	23.26528263450305
H	29.09289513568750	1.93979413521638	10.61214381569888
H	29.31868086410043	2.04194474544065	23.36081736458633
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O	7.42231341758302	11.93137050526969	3.91305697172702
O	6.89886510320599	12.04209644698479	16.87601981857681
H	5.84829458419300	15.76839921240236	7.47350174815956
H	5.36173487650878	15.69430131060360	21.72956542405964
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O	1.34018448551073	21.96212747603075	23.47805571259872
H	2.82132433054504	17.84615726690701	1.19101937524328
H	2.72423986630227	18.05148488643117	14.17456045709215
O	9.81092212408630	17.36710962119157	8.88543325758805
O	9.32653940924396	17.50617716888272	21.69433521833741
H	11.36659906027835	21.12710315151009	2.26171198716330
H	11.28960700701437	21.31347400797782	18.33800470229925
O	15.55149465442551	16.22334626054913	2.18896915883589
O	15.55366868795628	16.20303316735347	15.68756429523854
H	14.24780126415829	12.44673618888956	11.49579873215508
H	12.93763302401079	13.49907630980695	25.09512361638533
O	9.91573083441635	21.86785575385175	8.30389427646909
O	9.79096699604132	22.03564370878989	22.08619293588067
H	9.81794037038301	18.48918793991270	3.42660997486780
H	10.08994805148174	18.41684230745033	17.61560586085617
O	16.00506076252972	11.68988098457244	2.00102630156574
O	15.56420454983055	11.67216967386457	15.27344450223252
H	15.30552283753033	15.41705051256149	10.80999019846680
H	15.54172569065591	13.65122079629813	23.11163490489451
O	7.01811086759672	16.48584738524798	3.66874339706543
O	7.09589719920720	16.57223011501613	16.95817837928708
H	6.81932373947952	12.78809997839763	8.18448690647961
H	6.79208255693085	12.91686816532878	22.65724074147904
O	1.23053848070209	17.31406943460158	10.53988599125063
O	0.97424642346295	17.44536299294467	24.00508864468280
H	1.20517079720017	20.61434700581403	1.87689812359546
H	1.54952090767549	20.93924667551084	14.96620341988469
C]	7.17533106397332	14.10315598004962	2.15580122635168
C]	7.03722560041884	14.34980466660716	15.28300186580899
O	4.78928486200033	13.81611778773902	0.74197990953997
O	4.72632826387013	14.46822860989312	13.70760517829919
O	9.34688757386678	14.23702070164810	0.48420549821606
O	9.28049761548802	14.24550045457097	13.68891017443641
N	5.38385473685255	14.12257072957081	8.44717643498339
N	5.28482257535645	13.72571067075892	21.67940850600213
H	3.69082677057717	13.41790600594019	7.74688172191409
H	5.50389298057051	13.11473811487121	19.80482095809860
H	5.16352948357163	14.49792996452295	10.38094467767281
H	3.56632836880284	13.01030291646868	22.37604001332402
C]	1.31477352161137	19.53072097601373	8.86503460137290
C]	1.13756986452600	19.50240932030703	22.14777681994615
O	3.64903027112747	19.39430470273759	7.30769236482018
O	3.44985767856502	19.15426065245061	20.61218790867855
O	-0.90173228034256	19.58928155339224	7.21037337422695
O	-1.10720906161895	19.50223266681914	20.52643010756048

N	2.82456795284201	19.51929249444542	2.21436693244690
N	3.00797644818003	19.64153422118608	15.29772734498868
H	4.43888790571478	20.62234263358039	1.90861786824324
H	4.74439076883996	20.46837511695808	14.88953478757782
H	2.88604946477412	19.06869424090475	4.15179081064086
H	3.02253566736552	19.13343280730713	17.21159051091926
C]	9.72542758260443	19.80326283544484	10.21040382073838
C]	9.47377116527936	19.58736177495269	23.54185451441969
O	11.93515041105394	20.00280463702841	11.92279966943731
O	11.70698412283177	19.26732792892978	25.14627612342372
O	7.37822262432167	20.06769382594130	11.63386836461250
O	7.16419069760893	19.74793210425985	25.01353785056082
N	11.44232136687470	19.63324082738448	3.55092969925756
N	11.53034790703803	19.71116255409236	17.22167888375740
H	11.46779031702020	20.43469869885788	5.35797470702417
H	13.27958997398306	18.89195050536367	17.59056095013531
H	13.05311093718021	18.51783818540812	3.24412266432393
H	11.48483893290138	20.18863732028273	15.30084788186423
C]	15.76181991168997	13.88092479246274	3.68631658391136
C]	15.32163279809933	13.79651871055215	17.06059332629144
O	13.44051771286142	13.59336767001985	5.23092739540930
O	12.79042446436357	13.67721643768111	18.25743837946847
O	17.97672377202076	14.05697275730076	5.35248554773931
O	17.28314179133581	13.61400087904163	19.02050662155990
N	13.86727692960583	14.08927146679008	10.48193077440817
N	13.75237759766355	14.39069774468829	23.43057323510879
H	12.13206959780892	14.83215494320754	11.01785267960749
H	13.86846130222659	16.33473648824032	23.68129990529063
H	13.78726909454431	13.70050872568679	8.53462155744066
H	12.69892444506607	14.02921525811104	21.80983278843798
O	24.15246522554897	11.77647364023636	4.13936552688750
O	24.01099934706410	11.63621011322659	16.89155712598952
H	22.99251209364438	15.60052126303698	7.90855196064312
H	23.26289074011651	15.61714168965494	21.31296962684698
O	18.32557016266733	21.83565383613455	10.51026880313267
O	18.25222951192138	21.99739423094597	23.72892375886116
H	20.02736772994836	17.68510650118873	1.33612544828055
H	19.74343682564344	17.81654932899843	14.42726757537080
O	26.61758364028173	17.11234880714179	8.64478121626624
O	26.34538952636242	17.56231682379169	21.86973762060579
H	28.18812599743194	21.13036961681646	2.37090480352182
H	26.96808094291426	21.17562154662613	17.40882124737183
O	32.43486284689416	16.31994517856134	2.00528650581111
O	32.42462974371156	16.48267425351492	15.12246948976133
H	32.14581780134361	12.63071129215000	10.72037117853904
H	30.63210974163893	12.30993903942320	24.10744364201558
O	26.87816588038148	21.63335935176292	8.65120481866374
O	27.14371658840906	22.05327322081271	21.88953305356512
H	26.81552801101842	18.41600775715037	3.59931271061456
H	27.62074844059025	18.10191902542149	17.98378701269650
O	32.58114491539627	11.76822611386726	1.80156080901283
O	32.67245021542413	11.94431012334139	14.98992637458453
H	31.24926760923923	15.66854567199741	11.26691418548896
H	32.11608645864989	15.21221183510573	23.75791738271130
O	24.07917868333116	16.33740129309438	3.83910430860905
O	24.21243371692075	16.18410717848698	17.02028665479333
H	23.62152993342774	12.51394175117414	8.46276250677876
H	23.59377332996820	12.44791216545715	21.11080440919093
O	18.11262155736053	17.29830652034572	10.77180067974311
O	18.09063624551687	17.47759124210570	24.23273497854114
H	18.28032196128730	20.39563164234434	1.96446503701176
H	18.50719567872971	20.76424863494896	14.81297996024737
C]	24.07163037263584	13.94399397291657	2.35336560528997
C]	23.99652591955496	13.97356712474664	15.35588383089153
O	21.67272673111115	13.81256226614511	0.93455169441700
O	21.53090382666947	14.11201528068525	14.00788412976759
O	26.24740638963283	13.86878911868667	0.68292471335578
O	26.06604597002045	13.91004701028595	13.52805583252075
N	22.27842638797173	13.94404086269091	8.69476074951185
N	22.34998498162839	13.89542044882028	21.60406726834806

H	20.62171336422940	13.45114778514192	7.76470820009092
H	20.76177958493446	13.80179707655695	20.45749385850159
H	21.90717298931725	14.21006507939363	10.62454379790914
H	21.80427256789192	13.70729828110731	23.58406136600771
C]	18.22958643743621	19.49621244158083	9.02820210223611
C]	18.04565219950322	19.55705000098995	22.39345978086477
O	20.58437671481071	19.27397715139852	7.51651780126129
O	20.21877084015954	19.29134758196960	20.65238027253308
O	16.03330895745369	19.48330655889991	7.34721632309567
O	15.65964697813098	19.47431023800241	20.96861837686681
N	19.89863115246610	19.33508590540384	2.39352224576183
N	19.93925557763267	19.52379044324484	15.38613884693010
H	21.49657562313150	20.48883943548689	2.21566632513798
H	21.69024720971601	20.31915685247419	14.98964678960434
H	19.84938295834867	18.84315349658667	4.31818294772266
H	19.82346513399779	19.25538137516484	17.35173740970177
C]	26.69782012464547	19.33947439559693	10.28959478766730
C]	26.49806958958332	19.84772972955849	23.51225043155241
O	28.99888221906022	19.23955561806669	11.87853202615656
O	28.47535028808160	19.45509699942657	25.39141478085738
O	24.43920026988433	19.51216601597462	11.86471808282943
O	24.03659919097937	20.32484917810448	24.68604175197032
N	28.37929720612224	19.64467751981280	3.66367869483468
N	28.30579010829920	19.74360024348955	17.14273293304867
H	28.43451364478147	20.43789260812968	5.46944974373413
H	29.99879752758242	20.26128601379294	17.98467534460197
H	30.02498251763339	18.60559771482888	3.29617248324632
H	28.59892060567171	19.45012476149511	15.20267785122087
C]	32.53733141865678	13.96557420873726	3.50223728115240
C]	32.51565844452650	14.18031014913842	16.66595912674930
O	30.24523096677541	13.83410240953634	5.10634910546303
O	30.12212528937574	13.97423333824337	18.12818196478540
O	34.81235991464960	13.99165759577340	5.09071779929341
O	34.66890671702372	14.23483925283201	18.39732481163000
N	30.76627472938032	13.99524780706977	10.34965804880424
N	30.54792339141298	14.09611737195392	23.28173263806016
H	29.02137902307414	13.36523907805442	10.98751340446046
H	28.90006633293967	15.06103326889526	23.75231817144609
H	30.64156593116840	14.27398155446039	8.38639548798952
H	30.52048116468132	13.86933829766503	21.29641452617143
O	54.68122398403178	13.45013665127395	26.39437786613013
H	53.48059603174431	12.02741788025615	26.18711408802036
H	53.63607310127951	14.98722875085686	26.55978440899254
O	46.01075569409233	12.11684337333145	27.63356714453585
H	45.71074044634577	10.30986077377012	27.14785656449890
H	44.47924790339440	12.69491196501843	28.50115634080136

(011) surface of NH_4ClO_4 without additive:

O	6.89578699824085	1.08591653282133	3.65839749990987
O	6.79141749238760	7.64059580511323	11.67727854844349
H	6.98106815751787	16.49297937038070	9.31633300222232
H	5.77154487318674	6.71888502837243	16.16753814297099
O	1.19875003884049	12.67303288223915	7.34058052146187
O	1.37974363048667	1.08433823734119	15.51624839359012
H	2.68564464794598	8.05030917253552	6.40438550041959
H	1.17658820956921	12.69429698955585	16.36998287946681
O	9.81966588497692	11.36412139878190	3.06270979158349
O	9.61863421953695	-0.19985450779355	11.11923388028107
H	9.70348383717661	17.39249129055653	2.79921892282667
H	11.17300007886129	4.41061352863535	12.13431097361988
O	15.23344897036144	4.91732222758826	6.79025439619328
O	15.34335784363297	11.46256479531677	14.81457849658404
H	14.20659182891630	5.72803378364985	2.33003797940574
H	15.57109824994754	13.75000458164099	9.22139245872453
O	10.11989194490081	13.78146128397107	6.89161446594933
O	9.91453618924438	2.51171165891787	14.75175039416115
H	11.11025722765308	14.48636434741947	2.39304658090919
H	9.86467995117979	4.82785206327710	9.20033441659313
O	15.45056229772168	2.55010242402525	2.92137057199214
O	15.63533541909662	8.64534506140906	11.26180837037663

H	15.64034030771606	8.61045417490983	2.83695026800274
H	14.22732396321100	13.35313617779853	12.13906411859413
O	7.19432892668325	3.83368577216893	7.26678068049562
O	7.26321685166568	9.76339276627065	15.62662696773865
H	5.62602685875149	16.80815975342829	6.39530695942812
H	7.08928308596013	3.79248012393810	15.64707975326892
O	1.52774021726636	9.88567884866292	3.76442812227015
O	1.59807439122622	-1.26570199043046	11.63930262735343
H	1.36286188309151	7.59861802612608	9.32971678341217
H	2.16212577119544	15.76540118647150	16.23737164155293
C]	7.33703129643541	3.77107278482976	4.46839755518814
C]	7.45007600391547	10.09339730054755	12.83510946310767
O	5.41591398402677	5.39064060730712	3.38368948143675
O	5.65564398828794	12.05054253443675	12.01946372630906
O	9.88429260982831	4.48182283854314	3.63245645460437
O	10.02215186474542	10.78900851260921	12.13610446355223
N	5.46773114742756	15.94661890341556	8.16972355151920
N	5.37373204847770	4.80412969061290	15.85813469237175
H	3.77497976902674	16.47368304621632	9.03841978336381
H	4.35259598484584	4.64753713653309	14.16278713641083
H	5.46919899597460	13.99256152358857	7.96364831287629
H	4.23787362197571	4.03170783710552	17.24349287681003
C]	1.06801531975572	12.57768602683750	4.54311082173307
C]	0.96547167484333	1.22001486425311	12.75238405636950
O	2.98919007605911	14.19180829735006	3.44670559838100
O	2.65560496053017	3.16463814544903	11.68088498114893
O	-1.47645149687916	13.26281859982168	3.68454183817245
O	-1.66409982899437	1.81872600209865	12.19073919915676
N	2.87318138039515	7.11132169941888	8.13940813983367
N	2.75780330712609	13.87976968603048	16.26445804230389
H	4.57245444364854	7.61470708821386	9.00247622303693
H	3.61537203597204	13.51809943815517	14.52433684810525
H	2.88203265725365	5.16878271999842	7.85090595590705
H	4.20711892077572	13.61074519273308	17.68075740044699
C]	9.50717890022939	11.26103481665655	5.84031271930201
C]	9.48667879028777	-0.16524104820729	13.91821073675004
O	11.27433021913498	9.36947107095641	6.87709921880105
O	11.42243343560100	-1.78475711108608	14.98349541170377
O	6.90952820222998	10.61583183732976	6.50411313404201
O	6.94778199620837	-0.90225671335732	14.75371950390121
N	11.44919239405765	16.42371998949279	2.62831177649799
N	11.36838568294597	5.32742732956708	10.39031712209932
H	12.44738331804216	16.67325716022690	4.32648369444862
H	13.07093190680539	4.81620667327498	9.53789201044710
H	12.57069215800780	17.17747211611404	1.22155346981545
H	11.38727017720620	7.27416391038584	10.64634283755895
C]	15.78866475064009	2.40579239433869	5.69407985737847
C]	15.72577873000120	8.75009576659570	14.06096923136812
O	13.97821544283328	0.54367015458784	6.72281950241535
O	13.73008693064452	7.21079874779823	15.13206899989957
O	18.36925829119624	1.68923738542824	6.33254707233889
O	18.22836040391330	7.97495069491001	14.96177211605651
N	13.88717224970868	7.65853695565077	2.63482996535723
N	14.08515294665066	14.31116027757709	10.41018980706264
H	12.89753067914995	7.85304189822832	4.34413949067211
H	12.36742836129707	13.89671811052223	9.53045226640739
H	12.76864325050031	8.47115236354014	1.25904597250657
H	14.19367006119758	16.25084770940782	10.69794203805876
O	23.73277756805471	1.02401737629779	3.78325456225410
O	23.70236641150534	7.53559925411663	11.76000333913094
H	23.93435219527409	16.50010325614725	9.38046716429006
H	22.59850763588476	6.79744995927175	16.15696372690432
O	18.16735978759575	12.68638100807647	7.30965538397293
O	18.22612639047532	1.11940785413732	15.61527576085104
H	19.65753558864330	7.99184777176349	6.43259863336503
H	18.13076287146869	12.72586113037504	15.86052292635879
O	26.77692615594398	11.29029150928054	3.01953028851030
O	26.53059459188638	-0.11738191050611	11.20185108886023
H	26.55057183539621	17.36333641259670	2.83224050736087
H	28.08680050399479	4.46817149481071	12.22221350428570

O	32.08660013973527	4.79323487337146	6.83164213087462
O	32.13511246316127	11.35923994140376	14.88261573867459
H	31.12435049895766	5.65222011824399	2.36219907336947
H	32.33294679892515	13.75909519987213	9.32003794068148
O	27.00992245375053	13.71017124496322	6.85222546246506
O	26.87688625233594	2.55797803906487	14.85972052748119
H	27.97759933693653	14.47150979994545	2.35222488912215
H	26.74462189065984	4.79175809208903	9.28912787942757
O	32.30751754247690	2.46513493660827	2.94101245903464
O	32.51357118532966	8.67581631313893	11.23925260312816
H	32.51805256690015	8.56138557091469	2.86441842177683
H	31.02631372424174	13.27545942762658	12.24445163691845
O	24.07551474248029	3.81836155216380	7.34783888013947
O	23.68595001294791	10.04194826335481	15.54001556977102
H	22.59293503007367	16.85448605301126	6.44838179414660
H	24.08665927191134	3.91667768320306	15.76024045402826
O	18.44796054849307	9.87188435439707	3.75520894408101
O	18.47002940890818	-1.36010050945300	11.81913480277182
H	18.33232921979791	7.64509918120608	9.36759554612324
H	19.85952519216083	14.94227720813256	17.53295366210808
C]	24.22239822388058	3.71056314770538	4.55147749911380
C]	24.07989386341125	10.12881899221802	12.73760840307147
O	22.33181418968241	5.34865268427013	3.43771604648248
O	22.19840590875271	11.83254358692803	11.63757939743840
O	26.78386982230944	4.36252538636345	3.70999017896483
O	26.64668162614685	10.94664296907776	12.18088721971849
N	22.43164126825244	15.95699658576453	8.20586740769752
N	22.32112270697202	4.85007374017475	15.92084897470040
H	20.73570087119103	16.45249456762888	9.07989303760093
H	21.33943557759876	4.56112697361078	14.21700282146768
H	22.44402339066110	14.00643299773785	7.97467246486345
H	21.21233146648574	4.06883159564815	17.32296300731022
C]	18.01177068186777	12.57008164985778	4.51306028917903
C]	17.90094198062544	1.18139408735097	12.84763812621842
O	19.923784448433366	14.17155264049024	3.38816419794320
O	19.68674634580465	3.03106034474756	11.75016603719549
O	15.45678507136498	13.26453683897001	3.67903129663648
O	15.31126402391930	1.86024398993261	12.17181286069094
N	19.81435076001954	7.07779964926638	8.18104155780852
N	19.88057980065985	13.68436487099002	16.04453187650385
H	21.53713134730480	7.51986413584234	9.03142578225328
H	20.11429204199585	14.74473918898399	14.38514524556317
H	19.74618430223602	5.13105650164933	7.93377081498461
H	21.38060260738651	12.38345404575007	16.17384459179738
C]	26.40104262403736	11.19629617844458	5.79083223815956
C]	26.31902419785762	-0.08704531499073	13.99908760772356
O	28.13295451724695	9.29391140363900	6.87354210416803
O	28.12350510049591	-1.82608893255083	15.10140544963922
O	23.78777328859227	10.56819934582111	6.39942032817412
O	23.71648163008912	-0.67341880324224	14.75858397642093
N	28.29939732544506	16.40440007965664	2.63589241473813
N	28.25625926217607	5.33301061233078	10.44976606350864
H	29.30111068569849	16.61220165492433	4.33841305737499
H	29.95305230177535	4.80217664921409	9.59741155391418
H	29.41468500782234	17.20652632458374	1.25081381339032
H	28.26053362802902	7.28505724419227	10.64404996671107
C]	32.72742192510155	2.31625118766358	5.70302805262074
C]	32.65604976048602	8.71340306592054	14.04464038949124
O	31.05812653034226	0.35083350758687	6.76411252969248
O	30.78370196133926	7.01125339541927	15.10123812761893
O	35.36476564950366	1.73660393766904	6.25846870841854
O	35.22215355574794	8.04815240543235	14.86456550369648
N	30.78200329975359	7.57850227325020	2.67418548100484
N	30.82751930178170	14.22827432915598	10.51687380223064
H	29.79890944502480	7.75461743485950	4.38974949334685
H	29.13178558595630	13.72177279709869	9.64809458117352
H	29.63896812806588	8.38333982352212	1.31321628145972
H	30.80256365416407	16.17020986422267	10.81379650372502
O	6.88088394716638	18.65997772480039	3.67851519920366
O	6.80413737877466	25.35454397727439	11.57401318310890

H	6.95197998689024	34.20305243802461	9.19995563610919
H	5.75504670995934	24.66896828619060	16.03401589265869
O	1.15213701300230	30.42092996722829	7.21028652808342
O	1.33236888628311	19.03756735058554	15.53184205452560
H	2.67982659505714	25.79140936807704	6.33845018558006
H	1.17694150709636	30.45284356565115	15.65906275229190
O	9.78461695123323	29.13860440567559	2.75897670043806
O	9.66711074966042	17.61758637698311	11.27891002520096
H	9.67178870810134	35.22543700024355	2.72674963046613
H	11.34275516499623	22.37398403098427	11.92149679209126
O	15.32107667437745	22.62407875218348	6.70192074340931
O	15.15361293219167	29.19609382014604	14.61956435785348
H	14.26365619673809	23.33832217439852	2.32521669468688
H	15.45370235735783	31.43630559950032	9.18847322364699
O	9.99234157118393	31.51181531379734	6.61904697994224
O	10.15610493670942	20.54167560913415	14.72115453389060
H	11.06060242305506	32.32534425875922	2.18282874134685
H	9.75126142941604	22.38898557269466	9.09545176505927
O	15.49785741264578	20.15505749175395	2.90779102084492
O	15.39788873689721	26.47334502334544	10.97782127695511
H	15.63370334390069	26.25713189915018	2.79786761557949
H	13.80488706411996	31.22881505236582	11.97203185568474
O	7.06702918545259	21.39670513377293	7.29616325155626
O	7.03666500560496	27.81381199267623	15.38035962980286
H	5.63967961410934	34.66096243878535	6.27765066257838
H	7.24677182186773	21.81245236458697	15.64323397541140
O	1.47701631901039	27.58686015962500	3.67278686295234
O	1.65599325918666	16.53963897040896	11.75845244845907
H	1.35254758026704	25.29300826421756	9.25205667605820
H	2.58020377887369	33.36478666061256	16.11691244622282
C]	7.31746769885654	21.33730207680365	4.50125325956308
C]	7.32530625069767	27.90652737421322	12.59865402162931
O	5.46080114378198	22.98289327995377	3.34841775654183
O	5.47034752427022	29.70714678592126	11.54952630284358
O	9.90724066721280	22.02803538606202	3.77832423277892
O	9.88435144645122	28.64725725448795	11.90393092604433
N	5.43778956703326	33.73035163403147	8.01371367937223
N	5.47875402951876	22.71994420134617	15.81292813488634
H	3.74501795533482	34.25597102640762	8.87688144184912
H	4.47074586493134	22.42691127242322	14.12241777324852
H	5.39976186177819	31.78658496568802	7.73811805086902
H	4.39193024107455	21.94010340212482	17.23381757353637
C]	0.97769561772670	30.28153150959539	4.41766179134183
C]	1.01806222188886	19.07312374193420	12.75646232156300
O	2.84490325031964	31.91942287625059	3.26618435511811
O	2.77688666860482	20.95545551599933	11.67638447366033
O	-1.59530551537500	30.90141195097739	3.58957249713823
O	-1.58070406270035	19.68207335545373	12.07161772961217
N	2.86581387113657	24.82907115583595	8.06013433487034
N	2.91821000693781	31.43577367939065	15.81818683640108
H	4.55708719646927	25.32141744491012	8.94667782998942
H	3.87125673061959	31.24534589651682	14.08825103169012
H	2.88519007402425	22.88878061413298	7.75269851057615
H	4.08204628603406	30.64783907735129	17.17051454514375
C]	9.39294891683948	29.00734588852404	5.52250278613094
C]	9.69238088549977	17.83840944648632	14.05926697552335
O	11.13170516374777	27.09406723000173	6.58181580180777
O	11.64558666402797	16.24405597702281	15.14122643317731
O	6.78454606647245	28.36296595673428	6.12361293885107
O	7.18451001367272	17.15454781069722	15.09220895005330
N	11.40940952251604	34.25042744112064	2.48981216520672
N	11.30921242990156	23.10937409891953	10.08965828654691
H	12.42968608957338	34.43427731412049	4.18330985125635
H	12.97606831673485	22.65386864615146	9.12905818770380
H	12.50641820533969	35.05919179314742	1.09451929368686
H	11.16682664029794	25.06545921723959	10.16036053569221
C]	15.88293362878128	20.07799032754568	5.67787357179970
C]	15.44343546587211	26.53263482713833	13.75914700482412
O	14.10746028105411	18.23270174166011	6.79113222878040
O	13.46082960419126	24.97793074652186	14.82492529513896

O	18.47809374333699	19.40630781978490	6.29563851391765
O	17.97370659371562	25.64265180559434	14.61272180128434
N	13.90482115599072	25.28005150066073	2.49702145714549
N	13.86421306750650	32.06782506250740	10.19003519605081
H	12.75716465528489	25.57585392715480	4.09257871238623
H	12.23048730540684	31.61844164586235	9.17445522202371
H	12.94087101870336	25.99534023244071	0.96088006176853
H	13.94961466280891	34.02049075919881	10.38891705613865
O	23.74444802338416	18.66704384919820	3.72242315390351
O	23.57962412654978	25.41011693544381	11.80016725504839
H	23.90117179437690	34.20567319525242	9.30775969273845
H	22.11168732551927	24.14236559561230	17.57669874698240
O	18.10829027673616	30.33280944909504	7.33052728997074
O	18.38840337868911	19.22561567536045	15.53391779395198
H	19.78829891251243	25.75302029616427	6.34591408598883
H	18.07958840014355	30.68035077409271	15.32512098308221
O	26.61684734062248	29.06902406047453	2.89220229965353
O	26.51928508180572	17.55839458005624	11.34363006850785
H	26.51397772551244	35.14452533941206	2.88129572264641
H	27.98039823297697	22.16633472228884	12.16584859591236
O	32.05752611370769	22.53496879234845	6.80060404823465
O	32.18155628481195	29.13965181283653	14.76314940923000
H	31.10734399940263	23.30274384521927	2.36801235847929
H	32.30621519425417	31.49472484993112	9.18478804605393
O	26.95442403582811	31.38816011348915	6.77637867960885
O	26.83864746656244	20.36268473033797	14.89879259743813
H	27.88469003170459	32.24172442574883	2.31656920211425
H	26.67470919365600	22.52552256356539	9.22294873700559
O	32.31994174341720	20.13743645137335	2.96200142411726
O	32.51497080342524	26.33668312346757	11.20071211313017
H	32.48484352153435	26.22786476767907	2.79014430301691
H	30.99173656818405	30.96339687272111	12.10016764198871
O	24.04941149064313	21.51242150581289	7.24998554680768
O	24.35282134035542	27.85245269107118	15.54491147032592
H	22.41427909767425	34.66350469867967	6.47076988032683
H	24.14278646407650	21.83711032931730	16.25438861019069
O	18.38213079942406	27.60767227279849	3.70609717496172
O	18.65455519347924	16.53440328197897	11.88243263063814
H	18.25054052573346	25.34208009397520	9.14605321851097
H	19.65682174082013	33.20843550392741	16.51264441034769
C]	24.22224330791231	21.36593308677683	4.45697508861808
C]	24.46167106370787	27.91301094517958	12.79345536774956
O	22.33918156288071	22.98808382282663	3.30663039202821
O	22.75468236395943	29.89599868649521	11.82274160586358
O	26.78836267451750	22.00912118908655	3.62470222990185
O	27.02826931147958	28.33349255031827	11.86435086368991
N	22.34990413158586	33.68647048320698	8.18962478457509
N	22.37763998963199	22.75398570697482	16.18384626967008
H	20.68724542663166	34.09934461221511	9.17041936795363
H	22.33821993038858	23.65950707717060	14.41600931844210
H	22.39885409101597	31.75107142009979	7.85886717365040
H	20.92056810659617	21.40817586394822	16.19956586951344
C]	17.92548137071061	30.28306185894429	4.53234677731893
C]	18.13961350393058	19.17442133545483	12.74966963486629
O	19.81414596095074	31.92654772577746	3.42743866701676
O	19.99991916696500	20.87374105982570	11.61582417108881
O	15.35788610532508	30.97671906017764	3.74114380890871
O	15.56778967209447	19.82706471455630	11.98858948103439
N	19.85986179962684	24.86268366717806	8.11075238767633
N	19.83506930340395	31.31356606787572	16.00896878418635
H	21.47265782821954	25.42039630668086	9.11030832320189
H	21.14936368306660	31.20108671920911	14.52462700799284
H	19.93828083611041	22.91357749074103	7.88525571555093
H	20.39924435838914	30.09624984591267	17.47578812779819
C]	26.27918765242488	28.91313846238671	5.66309567161731
C]	26.38878878190723	17.67199077764971	14.14548763104067
O	27.97502217002123	26.93936101565770	6.66691865030708
O	28.32001779015386	16.06567860348230	15.23957395256750
O	23.65912722332222	28.33392915831137	6.30181407653317
O	23.84896141676402	16.95584408375282	15.00553244913093

N	28.24472704598185	34.16570641178488	2.62197040553282
N	28.17623465957465	23.04821643502264	10.40335598669738
H	29.30142737734087	34.33463987901574	4.29362806566273
H	29.87903130427097	22.52042235149103	9.56414055954656
H	29.32299886183987	34.97227225832756	1.21069775478699
H	28.17997804829126	25.00337787033062	10.62834956459542
C]	32.69953608894149	20.03315132557103	5.73397254279492
C]	32.66606353071620	26.44928298374863	13.99547660943981
O	31.00311693732522	18.09806316209564	6.80944067593623
O	30.78393235863815	24.81345891889266	15.12010466192207
O	35.32539637853959	19.44094176778181	6.33446612512362
O	35.23298103259892	25.80453799844549	14.83265597763342
N	30.75403917224018	25.24444574588623	2.55538901222842
N	30.78837624615258	31.92560209548616	10.38032026113850
H	29.66115256224106	25.52416356437698	4.19380571518746
H	29.10371292202291	31.38978790467596	9.50588726108460
H	29.72169410361161	25.96093348999526	1.06480735281127
H	30.72944296942880	33.86320741573401	10.69486968730967
O	40.78309282135095	-21.79618280530836	18.98838707700449
H	41.40054042554019	-20.32748581848037	17.99692084170152
H	41.48484584551954	-23.24937960650364	18.02670861350706
O	53.91293007283828	-8.63543779047410	18.88720341129248
H	52.68721029548917	-9.10394310389301	17.50054583227340
H	53.00131943059102	-8.87372265502708	20.48299817865097

(210) surface of NH₄ClO₄ without additive:

O	3.55554016046074	21.10932964046682	0.89902206725944
O	4.40324580583771	11.56688537805037	7.47068707857515
O	4.47350493877315	2.71841883898451	13.60971051854677
O	4.71235521127245	21.59592660221187	19.81229049556039
H	9.08797083443866	7.89858600048390	9.37748044459060
H	9.27373389073390	27.58927506331684	15.77441477379660
H	8.94255460821141	18.09189530767299	22.18080163969147
H	10.74504949750946	7.56272001008854	27.12627334669039
O	11.45062759947560	-0.11867957598752	8.91862505353377
O	11.33532719395028	18.85708084237856	15.37527255132507
O	11.17797784802111	9.86821629772270	21.57946211579374
O	10.50402383654576	0.23490432025989	28.09447032407995
H	2.37193087756454	13.73484399869020	1.66226805510046
H	2.11406928561558	3.34468896406980	6.82149828512608
H	2.30027412019460	22.00845040056286	13.13045990679688
H	2.23578014104458	13.47713676713003	19.73791696019877
O	9.59636253103740	17.60394835770959	6.37063684753826
O	9.62424505828700	8.52936197531354	12.78313563007275
O	9.62745955423521	27.60611205821791	19.14564074987940
O	8.67042431223306	17.52240508237699	25.47609515651500
H	4.26321196936926	24.35978661195967	1.68356826374504
H	5.33306733057069	15.12868644304816	9.21064694874423
H	5.70163037338417	6.64481070846598	16.16824357773345
H	5.13905458039048	25.03940455215083	21.36321996729493
O	1.97011580189538	3.73285560429504	3.54512364801935
O	2.65651474271688	21.80381727239717	9.79586803665129
O	2.68056145474510	12.90640148821768	16.34894757640988
O	2.73551235475842	3.89055397886004	22.81143569986858
H	11.73642740134417	24.53320925210183	7.57306040247189
H	12.39823718236356	15.08469535929607	12.98016957422612
H	12.32543417948716	6.20782066187949	19.87655345947108
H	11.09378856305049	24.96367867397210	27.22519512172462
O	9.31184117802527	13.85100465101132	8.90220160818762
O	9.42320199590878	4.89747036362738	15.49181730748863
O	9.39244603426146	23.79878768770289	21.58710824060302
O	10.34022270673339	14.07069608448074	27.97652444370909
H	4.60535447532919	27.72777307589981	1.52842988415404
H	4.79840010714233	17.30886715275003	6.86624984380374
H	4.51936156960446	7.76078283074846	13.36024392908342
H	4.76892285513365	27.68938532112615	19.69116233529231
O	3.40186786063312	7.17871145330887	0.91017833377945
O	2.59574588241131	25.60462705209149	7.33538223638107
O	2.56786041096840	16.64451697510629	13.78741943737536
O	2.40498136357009	7.63556918464335	20.26512632278306

H	11.69039916448344	21.87799586361174	9.29896943324680
H	11.56282923210116	13.57589416433728	15.72915684599621
H	11.70324656014079	4.25017126984713	22.39370422071849
H	11.20892387832209	21.59743107176149	27.46629170033034
O	4.98956271001986	17.71269755897054	3.59835148063409
O	4.29247973956780	7.79570207825737	9.97491292004066
O	4.30182396849354	-0.94010741174571	16.28026920882663
O	4.11075921752449	18.50119749147746	23.07291670883118
H	9.05876669131875	10.54715396107530	7.63188235542966
H	8.23610359261525	29.02230556146240	13.05267794801265
H	8.47932698427534	20.21159445969097	19.75499044676548
H	9.83747655370498	10.77777604666267	27.28962240299106
O	11.19365682442196	3.63967139115508	6.38987233574950
O	11.18000696790399	22.51056447799698	12.69276112976557
O	11.21097680308496	13.63599799600440	19.08127762292517
O	11.52646941235210	4.07187717464722	25.84144867902917
H	2.71769523072591	10.36627142485403	1.79195662747161
H	1.56260644283966	1.21183396395800	9.20835139259553
H	1.46800561918680	20.31409984898768	15.74989976306818
H	2.11908829993780	10.90372517039617	21.58506661073319
C]	2.75413624444766	18.95376839799466	2.46454386429144
C]	2.69787902589701	9.75356943885989	8.77950258095279
C]	2.76616584600661	0.99989752053019	14.96847118950044
C]	2.79783785995192	20.14290382211599	21.24764014119559
O	1.44232505373037	17.09755648645934	0.86761970211435
O	1.05930766019299	8.54632281152649	6.87097838643357
O	1.07900260318618	-0.29122314577195	13.15285228265540
O	1.28866479712735	18.59182854667255	19.47723745589537
O	1.08913315093198	19.84281053434964	4.50893769290036
O	1.19358950670821	11.05988342572820	10.68165905416575
O	1.26290693620323	2.41723454240634	16.81906503219356
O	1.14547486858631	21.92171838704585	22.57237422023919
N	9.44206900075373	8.60188165911093	7.56248078209947
N	9.47212111311880	27.68757863523627	13.80830107168326
N	9.45915205500380	18.60114283099812	20.32489918214747
N	9.58047223601262	8.99710066463807	26.43849028919671
H	8.30293569210520	7.65346295218804	6.25750555658660
H	9.12042235663108	25.92022467910857	13.02812507662131
H	9.02878797024719	17.12938856776634	19.10524642910416
H	7.73696581871020	8.33703406904158	26.58240073818387
H	11.36269712542957	8.32151819301286	7.17939496346882
H	11.33698962003751	28.16126812882018	13.35548501666504
H	11.41596264674216	18.90074735055087	20.23278624340941
H	9.98677250105042	9.22049440417815	24.49182016059714
C]	9.71078028328426	1.66437901524235	7.60568118176415
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C]	9.43195928534873	2.35970828772508	26.65530484329769
O	7.97900582418656	2.80146510232145	9.49777649230544
O	7.95667814688138	21.88682048021407	15.82515472338629
O	7.94494256214104	13.00880369468851	22.17653061487432
O	7.68463333266430	3.79041758235897	28.22627740415914
O	8.21668441357603	0.22927734702819	5.76104456273006
O	8.12334148800801	19.17261810776376	12.16561035058088
O	7.99657804160300	10.48886075915649	18.36607171973098
O	8.18805792193801	1.39983495109348	24.35431634615660
N	2.21191961806228	12.05802508644237	2.71868456282358
N	2.49487853795536	2.87473034543611	8.72023778012626
N	2.50237077669710	21.85628437308359	15.09348396716709
N	2.55045170966384	12.83987990096568	21.58567453184815
H	0.35524048875009	11.95231604444596	3.33805391265727
H	1.86247431840464	4.31488105383090	9.88716788292955
H	1.86693589564534	23.50119748013910	15.95510714876764
H	1.41978602000674	13.86177177756877	22.84368096601336
H	3.28715516938130	12.18523348965049	4.38818642716955
H	4.44656357639202	2.67747425641785	8.99052564415535
H	4.41301533841487	21.61877039584714	15.54762918373204
H	4.47966266993295	13.06345709133852	21.97824042614648
C]	11.06527389784564	15.63061685233101	7.60304381573342
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C]	10.98525157992310	16.35964660668641	26.53394299571753
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O	12.80874326910829	7.91405452753484	15.96474239740636
O	12.78949548822861	26.74016083309384	22.29487639530829
O	12.19772815847798	18.19434026919740	28.22739204966534
O	12.58215159517977	14.19358138579916	5.77942066586062
O	12.67034434053523	5.17953464937837	12.31328925928116
O	12.67575454517286	24.28913609217731	18.45326009454827
O	12.69437259560838	15.70870886792920	24.43276286303749
N	4.77437626457968	26.05758401075876	2.59147525254691
N	4.43458272031846	16.82241786554275	8.76596126085481
N	4.30912695683304	7.75318538906362	15.32706496135453
N	4.47932863249447	26.89555646110224	21.47643682126608
H	6.63407026862087	25.95873895671548	3.20329484793452
H	5.12842449110244	18.22817357425022	9.94094795776870
H	4.38935947655137	9.60495316742011	15.99364861764376
H	5.47543360497262	27.93412488163029	22.83195276254327
H	3.70649214661910	26.19854485804701	4.26604837269383
H	2.48158033112336	16.66350680459046	9.06208511275520
H	2.52823353631842	7.05170969354223	15.80281661290316
H	2.52584705221777	26.90430905268304	21.82065137790699
C]	4.20675422631031	5.00456835054621	2.44988456332065
C]	4.27643810015713	23.76189663759420	8.63179264672900
C]	4.25964690276870	14.84802081352215	15.05906019639952
C]	4.17584024387469	5.88898446758282	21.58643358947914
O	5.54229086427620	3.18423593195295	0.83342479418806
O	5.92231268663696	22.56373858569799	6.72768992946209
O	5.86743161767313	13.56010028502913	13.17714857648212
O	5.91885566890705	4.78134066502019	19.68219634260939
O	5.84935337884358	5.87646815194257	4.52050331000384
O	5.77064377429157	25.03120929938580	10.56784793424063
O	5.83402663605407	16.14133934847067	16.93128895035931
O	5.65491784779633	7.36573521960141	23.41342838492470
N	11.34420310338882	22.59101542548892	7.48636437689920
N	11.27213832013342	13.67871599772225	13.77589123306971
N	11.33201749926907	4.61712666406457	20.47657557024941
N	11.47118511551745	23.21397423072853	26.34650953680109
H	12.48625771130808	21.64374837246865	6.18295452491923
H	11.68681543116822	11.93978313134115	12.96489472331600
H	11.89203331618603	3.07340494792146	19.40561223049555
H	13.32216939830471	23.15044027213426	25.68975875103955
H	9.42343125748226	22.32330254574145	7.09555461453746
H	9.36590962318138	14.05702905980093	13.40918892987218
H	9.38328922648307	4.86870293243550	20.20836730824690
H	10.35757695368993	23.12315654240188	24.70161591282192
O	17.42950891074163	21.09971453252914	0.92220600781775
O	18.21051859816787	11.56183166646677	7.44630158022670
O	18.18340586597309	2.64867382493865	13.79910914334484
O	18.50667554295216	21.53048803400965	20.16532566447398
H	22.90002611352061	7.93113489270464	9.46156765222513
H	22.94351092641573	27.65287729393656	15.79369408664641
H	23.03993258811742	18.36970908536335	22.35689014860350
H	22.23201772656533	6.82938548607657	27.44565717605917
O	25.25621213505213	-0.13121263649096	8.93670482493121
O	25.18843890470878	18.78065127554431	15.42483527901765
O	24.88310351289224	9.98022622708151	22.18206865192540
O	24.63070964317498	0.22227112505881	28.26917140929909
H	16.24610008810304	13.69806752834565	1.62067475790097
H	15.93343023644812	3.33590817399576	6.90855259899261
H	16.16657506105892	21.75108192319759	13.33340282423213
H	15.96563282690782	13.40697143830972	19.67788848703006
O	23.39656618485657	17.58330658633873	6.49831249119997
O	23.31155771116968	8.53130339867614	12.87055069643600
O	23.17139868412489	27.71198260754732	19.15167426745128
O	23.32711255713055	18.29408555097211	25.83449622165778
H	18.04316087906634	24.31457356893420	1.77995142605638
H	19.17453090744474	15.12592114066905	9.26232220316166
H	19.21653699641897	6.22071882502919	15.98086715831036
H	18.63807104635051	24.79390872514119	21.44558558340699

O	15.78374143960774	3.71430931620912	3.62804060495645
O	16.46948234944663	21.74049834006948	9.94012005174581
O	16.43386576843116	12.92998204638483	16.34482416565925
O	16.37312415797631	3.69195462715871	22.68717364047152
H	25.51709574678457	24.51681514853323	7.60996338242161
H	26.24940961081917	15.02071385119444	13.25529772983943
H	25.93178458356997	6.44540342703662	20.08595583496734
H	25.37974917645490	25.04995877838358	27.31095249954403
O	23.12244569168434	13.83316128624184	9.03472691269569
O	23.22474133838871	4.78257209749063	15.42761871898811
O	23.54576425950654	23.90317626278248	21.58775963864693
O	24.00191857241635	13.98457965680785	27.17809410246054
H	18.36378960142476	27.68606468871013	1.64440627494989
H	18.65154738065678	17.27326577836069	6.88185060444028
H	18.47918736941950	7.99709195640214	13.38158533564726
H	18.61725814894068	27.50666344076811	19.80016811789734
O	17.21134839920812	7.12554191874508	0.94687474776644
O	16.34801782548720	25.53042019246381	7.45763444543255
O	16.36347196227370	16.64340355036317	13.74267308111372
O	16.18066418441465	7.50143353301034	20.22414272871027
H	25.42279691081512	21.87434844841584	9.36085159735303
H	25.22141327254602	13.52636132455310	15.95256168578755
H	25.38215587495591	4.19225219779627	22.34572345268501
H	24.30941324467180	21.97348968301414	27.27559061770541
O	18.84376036134472	17.68783507485088	3.61121887904248
O	18.08533805250557	7.81167061739235	9.98582242045409
O	18.01738331396791	-1.09867585590290	16.34383133189907
O	18.19318771389541	17.78256607984676	22.70790540815935
H	22.84157704888073	10.55089599863774	7.68429463138173
H	22.13990175670656	28.90857159338578	12.90652321492602
H	22.41062994393031	20.29545248134106	19.83550538038400
H	22.42840546564217	9.84018164374058	28.84441839988624
O	24.95855124417236	3.63168189554999	6.42095314509715
O	24.96408277678612	22.44086094154983	12.75287184003578
O	24.98783642441769	13.54142910872306	19.36760056712556
O	25.37603606304053	3.87177669443206	25.64096061976522
H	16.56031739112829	10.32726841493832	1.78157495213133
H	15.41080592014035	1.16598034346040	9.26706251500580
H	15.02348001717840	20.64570049319289	16.15896115796981
H	15.90906916280984	10.83323537371047	21.51748718503204
C]	16.61587310365709	18.93457122587034	2.47048327917148
C]	16.50010340165616	9.75455076418797	8.75684867077802
C]	16.46920764940847	0.86678414459038	15.05986592837607
C]	16.75104938211372	19.82514580350103	21.55719675031780
O	15.31486332668807	17.08932432545336	0.85412757158740
O	14.87487786010304	8.53157015430567	6.84927034843504
O	14.85270655385525	-0.39995618798481	13.16844017236730
O	14.88943507806856	18.77989844834036	19.74324193062926
O	14.93734121892764	19.81439499094922	4.50902350347397
O	14.98026188810321	11.07873697383342	10.63580274458788
O	14.90343041053725	2.17543278415118	16.92949625600166
O	15.43019452341087	21.33542878184731	23.47318238671211
N	23.24025912682028	8.60931536169622	7.63311699854479
N	23.29614211912695	27.62013748268541	13.84505452705334
N	23.32260762579309	18.64694456528550	20.41386402991336
N	22.22685370032945	8.79685287649201	27.10427426252272
H	22.10261357309380	7.63820450221096	6.34476322199172
H	23.00173511364673	25.80453711405366	13.15510848525754
H	22.57759514612869	17.12355937116255	19.42843391055569
H	20.51107381134410	9.20581063692322	26.26112309143302
H	25.16187895708981	8.34159298985443	7.24333023564136
H	25.19474756262501	28.06488352086836	13.50925717151083
H	25.25817236118967	18.76308008991834	20.02299847527750
H	23.59657810116716	9.27793973322783	25.77330835615795
C]	23.49852109504335	1.64751007830060	7.64661325623359
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C]	23.43071225281117	2.17159317435973	26.70390697028860
O	21.78477306415403	2.77305684381524	9.56780616335642
O	21.79530217781631	21.77927258540968	15.93673717023946

O	21.58904781014428	13.11581165694447	22.33843624733811
O	21.71523509417159	3.68463521520946	28.28975755658146
O	21.98291554054958	0.21635902428019	5.81779283039375
O	21.92241026302337	19.08598452441142	12.26392402119672
O	21.86450920573165	10.27203872174005	18.77538999833286
O	22.02661433469273	0.98797308978900	24.61845321212007
N	16.05651229794040	12.03189556363261	2.68635359381958
N	16.32162392432339	2.84792526443393	8.80202983034431
N	16.40458215854824	21.75025320081301	15.29708048984637
N	16.26680467963947	12.78183406230690	21.53486951898799
H	14.19008659811319	11.94916263956392	3.27953748117076
H	15.67100633540737	4.26456889288249	9.98879751833788
H	16.33575361631956	23.60867399242885	15.95417662872643
H	15.07066181467541	13.76056162734512	22.76535371163795
H	17.11142243126998	12.16399702146811	4.36919526731819
H	18.27697550765351	2.66888075521033	9.06288329527587
H	18.19232203791645	21.05278890063646	15.75217529000967
H	18.17605817805184	13.10398175030405	21.96261700580398
C]	24.87163710452060	15.61323546134840	7.73178419345492
C]	24.89597291252059	6.58510805809629	14.14137475929264
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C]	25.22572051018490	16.42759121440231	26.68796166344660
O	26.58429290394529	16.75464309885206	9.63923592682423
O	26.53298599872359	7.86989560208778	15.99824993635194
O	26.70701056010026	27.14857545600110	21.93336946512361
O	26.38608599733751	17.33226349474534	29.05065188230513
O	26.38618578432554	14.17947899278659	5.90163053748799
O	26.44303519391089	5.28805114787456	12.24099476280773
O	26.38586973707977	24.67676796258589	18.10006754357382
O	27.14551856888090	16.14830621311404	24.70003199729628
N	18.53124327137029	26.01299471530455	2.70326007961944
N	18.25620537852534	16.79779371368197	8.77709861877521
N	18.23530245456292	7.80173321288461	15.33428634754050
N	18.23509232646645	26.73189073583590	21.57585567930886
H	20.38757330779597	25.92380075336381	3.32699669991155
H	18.89641715273957	18.22878791287510	9.95136289984769
H	18.89507489917024	9.40721600893248	16.24704957343564
H	19.36056111621200	27.63005467468252	22.92736559395312
H	17.45158976146899	26.13810006687461	4.37039892837350
H	16.30091929688216	16.61503140830267	9.03292553315676
H	16.30761765223016	7.60231769602879	15.74034913447561
H	16.31010308050099	26.98014400774343	21.94999347088286
C]	18.01887272617976	4.96687010392323	2.50780493739282
C]	18.05624346625775	23.70914590980341	8.75203843906726
C]	18.02377368364178	14.85737315882160	15.06576090445654
C]	17.89265387049808	5.65230838924101	21.48315849583446
O	19.33948659188934	3.12431980300237	0.90433139453707
O	19.69251938541719	22.51687510689755	6.83229117809924
O	19.67886776767447	13.54994699253969	13.23376111645660
O	19.57558155677100	4.50562868607946	19.55661615199700
O	19.67450995151585	5.85819015205407	4.55874964334348
O	19.56422284200150	25.00515006682899	10.65819733331570
O	19.56592698379293	16.18698151617379	16.94917799358868
O	19.44383510288535	7.00354851524532	23.34005466964074
N	25.10210945009954	22.57924668928317	7.53949219764851
N	25.04205476076030	13.64623421345566	13.98365835107123
N	25.09544794063153	4.70110033506379	20.44109948092269
N	25.63701859248698	23.22691399619887	26.56401166775264
H	26.24062735431765	21.61007840022426	6.24956405813536
H	25.43843011804922	11.89467695232804	13.18903954773254
H	25.91856407849678	3.36010805399559	19.27375112503616
H	27.51046838164407	22.41357540145982	26.92775499620967
H	23.17968504625559	22.33194089014991	7.14047449301080
H	23.17153248429345	14.08648171135490	13.51128267256818
H	23.15701035665234	4.77298589291404	20.05054051356363
H	25.31526330422995	23.33463503149029	24.61925986250351
O	2.33755420255146	20.81493629014759	27.70056802113520
H	3.12877339803991	20.05166916194041	26.17715871410689
H	1.47826028414450	19.35858524314214	28.52040761956410
O	22.39245132095926	11.69392981917127	31.24996605012530

H	23.55837190372069	11.37405024094057	32.65398889131451
H	23.10556092639657	13.15002624258890	30.28853784305861

(100) surface of NH_4ClO_4 without additive:

O	0.83504087474207	4.34099534544808	7.56833206204276
H	4.11152844944093	9.48571618269696	8.97915219330152
O	10.92411960307343	10.08130655689982	3.79272346964039
H	7.54178302003326	-0.04532538913333	3.43863252018940
O	6.09188676535501	9.81953850987719	11.68068649187566
H	9.60375158695326	6.36943348505967	12.18801439738795
O	4.98626481289885	4.25766195334427	16.19158294448609
H	1.57227965040705	13.91117002916861	15.65315522087105
O	10.59719618787484	10.02586412211386	12.03178783601541
H	7.43716272862595	4.50657986271695	10.64809314346989
O	0.54611103256527	3.40150667160968	15.87256206158604
H	4.42831523575505	12.80686503629759	14.67669377193822
O	5.31723163351312	3.73196976115888	7.96989570587154
H	2.09397492065998	7.55103660257623	7.35066438919293
O	6.42504949496967	10.49408187023915	3.50794960953371
H	10.37475733072517	0.98328060880282	4.56669885187732
Cl	2.83534696577678	2.44538398780192	8.01643500404496
O	2.75698908649979	0.58791423487355	5.92711133243684
O	2.42511196780358	1.19072272225673	10.44367768340790
N	2.89313564861475	9.35883823967576	7.42362423933771
H	3.91435983017582	9.75604910157631	5.77098205794466
H	1.44609234559275	10.66454569437781	7.59100979032561
Cl	8.52207691480579	8.69367246379537	4.08150850399395
O	8.24496395338724	7.77878435992543	6.67653242598783
O	8.41295015193425	6.58840205293285	2.28497243706323
N	8.50282272397510	1.51446803385283	4.20672984695357
H	7.64686470697124	1.98859109297078	5.92287146731376
H	8.45592343297487	3.15468970494071	3.09685529262025
Cl	8.27583417732470	11.55766712960648	11.63484648685480
O	8.01300213890466	13.34075973779633	13.77044903347905
O	8.42727074406357	12.93044747459106	9.24912562391094
N	8.47670879329560	4.75848520799528	12.30525054764887
H	7.21023585507738	4.86833032190735	13.83834110302922
H	9.62952903299894	3.20359183351287	12.62873363139923
Cl	2.50306811587284	5.37477274711090	15.57136471455924
O	2.52535160193259	6.29048165730269	12.94877213181759
O	1.95478073297256	7.48420027765867	17.29490693517220
N	2.54729193829448	12.30484453810119	15.00162251696119
H	1.72822165681969	11.71917915668488	13.30086930682314
H	2.43050978528647	10.73273908264834	16.21272901572956
O	11.45573119604946	4.01642144941741	8.03806430471476
H	15.00696655472828	7.56227229617500	8.03358876995691
O	21.37734479324634	10.27564356329609	3.44340263112479
H	17.15932546352958	0.89837766876109	4.60280011173905
O	17.83330499575625	9.27734192592709	11.94791867820926
H	20.75054911831815	4.02042858342984	9.90601141926575
O	16.47173786040901	3.25573765052242	15.47707755331780
H	13.99789423811673	12.58410928152539	13.56902296329954
O	22.20466214944568	9.98808321887017	10.92183684037060
H	18.92056959872392	6.09214108091746	11.59670053576691
O	11.96466485476249	3.07773764395071	15.93313120429637
H	16.45822918721957	12.27107649662981	15.51379417792570
O	15.98617912553539	4.10850455882859	7.73319220382421
H	12.90246462178148	9.52063698545047	9.54420321004496
O	16.89776765420753	9.67985335622469	3.72461328790087
H	19.78283098808003	-0.27199852726538	3.12322917780495
Cl	13.74842844044863	2.48283779457118	8.09560394054671
O	13.67611493144066	0.64609051187811	5.92812490027207
O	13.96827158113136	1.05791904408292	10.45735842560966
N	14.11825348394236	9.32478423350880	7.99803736181604
H	13.06404173291735	9.51279135469528	6.32365570305092
H	15.49073409379707	10.72736934271622	8.01735746251452
Cl	19.34431649375933	8.40966065842532	3.96593297324209
O	19.67353566541759	7.42395103345596	6.55203530733754
O	19.54779531673664	6.31102730586447	2.14986886392954
N	19.01666481590669	1.30245840889110	4.06104533063917

H	20.10110996828286	1.63484949151934	5.67671162077942
H	19.08043795524688	2.99963073164148	3.01913388066106
C	19.76315196413972	11.20226441920692	11.33258077560433
O	19.97133094228101	12.95696425708588	13.52919014062727
O	18.94008323950295	12.62934680784254	9.10023939186612
N	19.62647482173093	4.24447037052942	11.51261818850798
H	20.71113552949699	3.84243776470655	13.13049694542893
H	18.11999098469114	2.99728125026808	11.47925524006711
C	14.17313845141118	4.79983247419165	15.64444884065291
O	13.84955341882610	6.27466855570040	13.27663676479698
O	14.29457461814038	6.55202502722742	17.76130963914896
N	14.59289383668976	11.73517449969522	15.23118960435777
H	14.50088598940096	9.78352842174208	14.98372146263257
H	13.37377112725807	12.36649210971653	16.78971604345589
O	0.54978710167842	18.07048989986475	7.90017113299317
H	4.11031937054081	21.38132534637110	7.37478841180664
O	10.84122495246350	23.78844600274687	3.32950470285067
H	7.63687238891203	13.82268786091874	3.62282442038980
O	5.89695869987000	23.56773170398970	11.30982098218505
H	9.33409649204795	20.24707918695579	11.97052975396196
O	4.97524184765970	17.77466762368747	16.08750335285603
H	1.77131920247084	27.68906954789066	15.69036785512306
O	10.41317931977731	23.72722151624448	11.58115852482588
H	7.14008088006650	18.35010132299522	10.52216844633628
O	0.48335718504074	17.21257059847673	15.97438508967628
H	4.54160272012984	26.51248574138333	14.54387849651518
O	5.07647043405143	17.71925862193611	7.82209104912573
H	1.68726502724898	23.08234668407984	8.69600780623790
O	6.33298666987872	24.19501693325755	3.32200985817661
H	10.38620418610060	14.90159285975056	4.87691658735354
C	2.64551271564320	16.27496275960189	8.03659287324699
O	2.50563099645862	14.51649232850902	5.87186843572214
O	2.61646247748808	14.86014652088264	10.41121434286830
N	2.90363848374553	22.92003928450352	7.14775552084300
H	1.81418329135651	22.76254507783879	5.49003349295404
H	3.98325436730995	24.54689772706289	6.97066064962146
C	8.46728895075842	22.43203813341540	3.75935327409984
O	8.36172766266827	21.49991226152780	6.39448206940812
O	8.24131878507569	20.26642420558296	2.02940987080013
N	8.54226485144020	15.41133263594427	4.39813618481698
H	7.56625539854030	15.94362230233819	6.03356861149244
H	8.53907878264209	17.01609418022202	3.21965081871965
C	8.08349469459050	25.26424492050329	11.22271505233913
O	7.89659476772011	27.09489169483335	13.33373090903332
O	8.22985290771709	26.61337539027673	8.81484919380432
N	8.32615379324268	18.55383503412200	12.09123337591771
H	7.21442517002662	18.48547580537646	13.74097923077076
H	9.59150034886574	17.06279116092276	12.15450523894707
C	2.54446409542926	19.06645737398032	15.59167091781345
O	2.49612365015323	19.99282681505830	12.97574023949256
O	2.21456466205026	21.18775844872419	17.35107536872032
N	2.66728000978382	26.05850319811240	14.99187670422636
H	1.74035650289572	25.47830497389968	13.34292964983442
H	2.60442482569584	24.50410682160087	16.22507458516579
O	11.63255450606793	17.92517395762350	8.06988864192411
H	14.92210321200778	22.85007484112920	9.09046896166905
O	21.07178209572286	24.00142108122695	2.59441112160607
H	17.39755211506927	14.77574387449415	4.89528213636368
O	17.22279752225490	23.16310079466483	11.46204094244793
H	20.95330219953606	19.60701097712502	12.25643399721400
O	15.81765643941067	17.44152904288296	16.14060864618019
H	13.09980721112339	27.51387112832940	15.68449980008096
O	21.72415537248983	23.25580252482029	10.99957721195200
H	18.36736063200097	18.25917157579908	10.85569395990323
O	11.30510665974431	17.93705472246312	16.49156962524282
H	15.84982715585983	26.50835887810307	14.40871429718795
O	16.17373546011366	17.92686914400283	8.25535695574591
H	12.22747968911589	21.71279596230110	7.66185523913722
O	16.70043558119151	22.98470895338111	3.22054938727153
H	20.14993549869627	13.48202609899693	3.81956234083541

C	13.88737293862315	16.34070612551027	8.39430545825009
O	13.97407692561200	14.50080759978185	6.26386671865349
O	13.76738258434465	14.97871366950408	10.80288206356750
N	13.73557452145670	22.96456935594098	7.51036623816756
H	14.79704935547463	22.58553616269977	5.87502591674343
H	13.04969351488180	24.79416194088304	7.31153376796172
C	19.29544776987588	21.97909125265755	3.31495905567822
O	19.87806841511097	21.12061461245375	5.91845861855093
O	19.55107887461581	19.82093856827895	1.59089324675809
N	19.28309957561007	15.16444173374066	4.45141842831604
H	20.20714011632188	15.76745391848231	6.09363437651650
H	19.37852355640407	16.65439641226515	3.14123945830360
C	19.42568125233408	24.81753066075158	10.98341280270416
O	19.57989753439321	26.66879145393462	13.08806537327930
O	19.13660222194890	26.15525132889944	8.58180846286739
N	19.55877378081528	18.22440274104109	12.43664452036905
H	18.42899351855460	18.46602662504528	14.04590345597702
H	20.39508921913687	16.44684142358006	12.58328017363668
C	13.70117432124309	19.23678846564569	15.85556773186726
O	13.56406836974091	20.13505301729067	13.23831620112542
O	14.07471752749939	21.38047819726707	17.58302209185007
N	14.03910798382401	25.93282526897509	14.92002815477253
H	13.04119858178896	25.33236483055290	13.32451790646915
H	14.12519787785238	24.37391933318682	16.15461369184117
O	22.88023663886774	3.39077793483846	7.23840229666973
H	26.44447229472415	8.61380666432886	8.35034738423395
O	33.00520614558558	9.74776320620797	3.01878674553080
H	28.75766957914507	0.73310424954528	4.13683877219604
O	28.52276316695836	9.62696231626912	11.12317104529400
H	31.93052452968559	4.46559761601888	10.09959411691279
O	27.34147287470453	2.79449325636001	15.49237576313254
H	23.65044110474759	12.49352158798597	14.96444073815735
O	33.04312343981235	9.69350049531649	11.07354012116502
H	29.80689235682407	6.33996718779334	11.65793080483125
O	22.82130079400615	3.04593600802130	15.49498263465279
H	26.65100071803773	12.44907706445018	16.35520268137745
O	27.37056890092365	3.43604083072884	7.81374301200349
H	24.17920174539761	6.79942616871286	6.89468552979493
O	28.49383555880067	10.04890043159810	2.99102347700722
H	31.59058429543391	-0.29198904232177	3.03163274468055
C	25.18515180737258	1.76580903132120	7.55770069718958
O	25.45563464578433	0.20448696540883	5.26489772450345
O	24.85843621858404	0.15113639130281	9.77871893269369
N	25.11232934031709	8.53722831368762	6.89694499028491
H	26.04178631231411	8.90172215443409	5.18547539651532
H	23.78816303704664	9.95331914811173	7.18445248474030
C	30.65810428320131	8.29105050341673	3.39170391953697
O	30.54742486843313	7.27464524441686	5.96641472376875
O	30.50726184257669	6.22682857226323	1.54708009772820
N	30.62121385481251	1.28238133115010	3.74128320833577
H	31.48570187444663	1.85339384989252	5.42190184203601
H	30.63404790144451	2.86229676011588	2.54133391393157
C	30.78221797264139	11.31019795798054	10.85459252736210
O	30.76985116835269	13.12562088510861	12.96084155557517
O	30.69911959632710	12.61173658047483	8.43023813753394
N	30.73108841632679	4.59555244135241	11.66527045952675
H	31.81461738601385	4.32789337722553	13.31131392894065
H	29.39268949901650	3.16755599030040	11.58265443580587
C	25.17272190323884	4.53166185742328	15.20018493963459
O	25.23044965941681	5.69566564751242	12.67747980276402
O	25.28464091409433	6.50308649686091	17.14589673142440
N	25.30848249824140	11.46014392575955	15.16304927392765
H	26.09321075661106	11.20564035823744	13.37652335273241
H	24.95765813503925	9.65286423101575	15.89983561325351
O	33.96497414321380	3.74802081707484	7.34690946180859
H	37.44216318772735	7.34599388005240	7.11387632379123
O	44.37113569668485	10.07716856502241	3.33287525238228
H	41.20127101663918	0.09314762993191	3.21629102550914
O	39.28836622909234	10.09302898158743	11.30554090746948
H	42.79649481836680	6.47311382291295	11.55664456667490

O	38.66027973138105	3.77899265347577	15.74961085606901
H	34.08343359445364	12.89916866729893	14.52340129950282
O	43.81699932418934	9.94844825808209	11.33459271220755
H	40.69255740330532	4.44291475523987	10.15954135264511
O	34.14805538145067	3.43714609752427	15.58697341960441
H	36.92405645636318	13.91588638873411	15.63864223761466
O	38.49517721710627	3.91382063462057	7.49912209938274
H	35.31123972960024	9.29565809261414	8.58274412296366
O	39.86609290696234	10.49537748914716	3.14975193372405
H	43.93975033590014	1.21414419005060	4.48352910438675
C]	36.26562696074439	2.17429590979657	7.66253497173465
O	36.41958306720037	0.37278051846143	5.56878486612258
O	36.24046366246126	0.89729734635050	10.09795845123722
N	36.44073126249601	9.04077426873198	6.98037277609839
H	35.27217841974385	9.06747674516448	5.37345820826493
H	37.72240690566034	10.51166599481990	6.80339947095847
C]	41.98323163125905	8.70732287400310	3.62026729590979
O	41.75748203440963	7.69558051988583	6.20685433152822
O	41.82675565438389	6.61277718802323	1.79696947750721
N	42.09165170270027	1.69865686891745	3.98075567694118
H	41.11038879983453	2.22340051307440	5.61056723231060
H	42.08412614808694	3.30346344158931	2.80472258953900
C]	41.58677694137769	11.65198008749926	11.09020914586974
O	41.65956021551334	13.50477606584036	13.15302414190811
O	41.66952203717235	12.92674919930622	8.63055679040969
N	41.95652846318679	4.68605163334823	11.65878638400352
H	40.96046392895799	4.45430784790704	13.36163258298802
H	43.36687323383881	3.32732371512776	11.58242861542366
C]	36.32473845942876	5.19536887055984	15.19856131529389
O	36.33293758046317	6.06581627569968	12.57200006769452
O	36.06180193994098	7.33553242803403	16.93564883198859
N	35.94846429656566	12.35928737579717	14.89493399589913
H	36.82510734833028	11.82645217003740	13.20341093758983
H	35.97806775204387	10.75106271564331	16.05090155745611
O	22.61003487076092	17.18502921403584	8.31886134957496
H	25.91829393269859	20.83784872241516	7.29664132580972
O	32.64456508413193	23.73694778543173	2.93072316673543
H	29.64717075832170	13.51415224625542	3.21584102502700
O	28.39981837895125	23.38911114915306	11.02639060396967
H	31.55261236355570	18.08183215889916	9.95559719972733
O	27.91933119089640	18.42982666289831	16.09738645797329
H	23.20738470092862	26.35563928181164	14.26717557354040
O	32.92729391286175	23.59430524629841	11.06467150417960
H	29.44388556235234	20.05693146149369	11.40225809588095
O	23.64524044050160	16.81954250362438	16.07080663799440
H	26.11201948230232	27.15007701915194	15.33907875913390
O	27.04575935226574	17.51278913729064	7.38726924783889
H	23.02292897984336	22.12921181601270	6.65132238910845
O	28.13102244613894	23.62887418015772	2.72084016207600
H	32.31128673351404	14.70490389454995	4.53790027232972
C]	24.99754003956816	15.75451997525816	8.23460116585958
O	24.79027685861184	13.70129256329645	6.39155584173165
O	25.65184166846212	14.80041820614245	10.75050182036297
N	24.95716865250917	22.52010441262940	6.89505421725164
H	25.74494276010875	23.30450532886024	5.25738603481070
H	25.18915923051311	23.77152022095355	8.38598970520898
C]	30.38395041746571	22.08172159442509	3.24486847308505
O	30.31239363794613	21.11103430193294	5.84059976303122
O	30.54649625701530	19.97099192730391	1.45241895590716
N	30.48861610009453	15.15866836720551	3.93905483353819
H	29.42544542207259	15.79476993418553	5.49026991092036
H	30.55693308401255	16.67262275271057	2.65508776516647
C]	30.59681976009992	25.13095983837859	10.74197650425350
O	30.48680597868256	27.03385214637818	12.74751199848911
O	30.56276303650678	26.30293643023223	8.24953562607198
N	30.34132721574865	18.29961859347704	11.50353042376329
H	31.40806070025871	18.17411181494515	13.17136197808464
H	28.98540739842457	16.88047016139570	11.50892880627429
C]	25.22182808443798	19.05174290623476	15.64064866566623
O	24.95913978425618	19.93700861957074	13.01257619274636

O	24.46050892938415	21.09042422693838	17.37735741321535
N	24.98978339979564	25.63664358767583	14.71322329854194
H	25.81993193044737	24.87233837054723	13.09548239714181
H	24.81976478001422	24.15144934657870	16.02890379420700
O	33.87706572605110	17.82940978455303	7.51668538028433
H	37.25431789890676	21.13868132962313	6.91000596656835
O	44.28808663655325	23.38231777837550	2.96095516779953
H	40.99777779394879	13.75408816263408	3.30420634017220
O	39.42108387559459	23.62041356071186	10.83831176389730
H	42.66403431823674	20.29028441298099	11.81185125215525
O	38.13324803706758	17.35725286830511	15.79395607827638
H	35.25564895887236	27.63485614940242	15.39432707747285
O	43.92812794197524	23.73165528616525	11.29194587379612
H	40.54504573536710	18.34584485284868	10.32128308727236
O	33.61644784949609	17.63459297669362	15.66204049579226
H	38.06203557509662	26.54683125103315	14.27212362486718
O	38.40079649741409	17.68548485081512	7.54424238142192
H	35.08451198405236	23.01686568585693	8.40615637675529
O	39.87330840287198	24.42031558665149	3.01877893151328
H	43.72631341024483	15.00835402944378	4.45315652470649
C]	36.05899882603183	16.11662531178676	7.80569366877203
O	36.00900880858568	14.26668006467371	5.72732746638529
O	36.03907293582946	14.86089324238148	10.25216483302119
N	36.19408382126799	22.79617494631536	6.78337982199441
H	34.98918361395165	22.80723811358809	5.20223697055701
H	37.41940235306898	24.31560182939004	6.58978569717349
C]	41.73045213646982	22.36497212929488	3.42546338732091
O	41.55058097411174	21.44861778125536	6.04221986650979
O	41.19399939586362	20.28288725391951	1.66821907667835
N	41.84842775168125	15.42191633056621	3.98850468599960
H	40.89407636675196	15.98223777288937	5.62534666884034
H	41.74821372334124	16.96272551954726	2.74163921535224
C]	41.60420152772006	25.31170620471474	10.87782466916468
O	41.38684576739524	27.07010678964031	13.03879777167456
O	41.85615021386707	26.72253332229098	8.52043250536744
N	41.71915670295906	18.55941033468254	11.89592173949302
H	40.60888107882215	18.37544320228690	13.52985866525906
H	43.04742715689146	17.12058499137469	11.93385091064848
C]	35.96969851786369	19.09387471868809	15.30944302713347
O	36.13848487180545	20.05089249962085	12.71938292245143
O	36.06377670941078	21.19548915389536	17.11707446793928
N	36.20157075176904	26.02934761150527	14.71135606204756
H	35.30060412609136	25.41394671487996	13.06320914982229
H	36.18417004967517	24.48468728918286	15.95780960074557
O	28.80224239240803	13.82799989050473	17.95912936921961
H	28.62645091064832	15.63249622842602	17.39235083288284
H	28.49270228437434	13.86848365012774	19.78726447454188
O	11.63915653073698	13.48096863849300	18.84040544740707
H	11.44042422357467	15.27513495862736	18.25603309219453
H	9.94208860023720	12.74383872617063	18.70170121468126

(101) surface of NH_4ClO_4 without additive:

O	20.22557387499651	0.43037616766546	9.47848827506613
O	11.21111134969533	0.75343393453632	19.27665529771903
H	16.89551792769682	4.45958556951523	12.45070866154541
H	7.00663493311568	4.81153081809924	20.83716702450256
O	11.30283176397134	10.77858465669210	10.91992358337590
O	2.54287589589450	10.64806409459990	21.46426897679245
H	17.39027905810187	7.40314023931130	4.15112549665376
H	9.74930204798608	6.66064028848009	14.58125903293340
O	6.06939093455005	5.83428318716253	4.35047982228792
O	19.09974448960152	6.25921771837571	14.26018186155797
H	8.82435847896872	9.38331951690313	3.17718856686638
H	0.52737613469427	9.64018455044172	11.08084640707661
O	15.13299574426798	5.32031874680269	2.42932987619882
O	6.14525845526075	5.18872761139698	12.93527506532600
H	8.98141473026563	1.58348661260981	9.51233431120386
H	21.86462110964360	1.93519090977453	19.62811797261168
O	6.13952403409130	10.34865649206827	4.59391661127067
O	19.11456339495109	10.76250574810279	14.76329028831262

H	10.67099892957068	6.72457461201011	2.93960652358463
H	0.71202625190601	6.66199655814808	12.32337912500294
O	15.07009828133740	0.76472988205259	2.74365911526136
O	6.03953053112090	0.64386442017204	13.20440786638652
H	7.29708349337707	4.34435711531212	9.34333805593278
H	20.23423577295139	4.62609919519989	18.64526296792673
O	20.52180355722908	4.92874965846885	8.95993904354280
O	11.59596251834660	5.25646002176630	19.25378699622565
H	16.76155880671950	1.27857115384304	12.13287703998760
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H	38.96422989158701	19.49120184598849	7.19757979230046
H	29.73044034571263	19.91352001547683	16.87129774447951
C]	26.93829605861024	19.22253452604653	5.79338151271725
C]	39.76966989788593	18.96134186472416	15.89466923808806

O	27.70697567424421	19.24562795250290	8.48779475822431
O	40.50588255793421	18.64688645431743	18.55415236071235
O	24.20998767810127	18.96165559894515	5.59070444573272
O	37.04677814141425	18.85912272736141	15.55668343040444
N	32.37367569382109	19.15604269442209	2.31907176642158
N	23.55377915869993	19.33834448488310	11.87853107940377
H	34.02849772721165	18.12053559431173	2.68617708395087
H	24.01104264446907	19.47698669679749	13.78013098858867
H	32.10101091337473	19.29755033585433	0.39525280894806
H	25.20207885339268	19.37626150698930	10.77174334167302
C]	36.06529557111456	13.52435763849413	3.97786506304326
C]	26.33236507848497	13.99368246566222	14.25352083019067
O	33.28572321618201	13.24438392462988	3.75449917617654
O	23.69495451824926	13.76641768829551	13.45609862003528
O	36.83442915376582	13.45899207986074	6.62294211366670
O	26.36881329773243	15.10903718229432	16.83401730685414
N	30.21997826743902	13.79102040121339	8.28630028751797
N	42.88253950825654	13.72054182194197	18.23546274869175
H	29.09962020042455	12.83759444162368	6.95755990783116
H	41.60839615468943	12.44888422356831	17.39364777459914
H	31.19520067019485	15.23659002021407	7.38362609208567
H	44.18924011608249	14.19306951568369	16.81460992348539
O	5.36865437516683	11.57526500383451	25.64537395796712
H	4.39851187748843	12.44676802699531	26.96031502080701
H	4.09132685953527	10.97306225115316	24.38763253332450
O	26.01052892317788	11.05870129432263	24.88008376644930
H	25.25954059282403	9.55016353474457	24.02671526383124
H	24.56151646695213	12.00718726226749	25.53682683834880

Ethylene Glycol adsorbed (001) surface of NH₄ClO₄:

O	6.70615368457587	0.58063728696005	3.36340322046234
O	7.17338583092286	0.58994041245285	16.63241899002806
H	6.18975252174635	4.62217802482888	7.72302231009076
H	5.41504816631835	4.63686319992977	23.06575791415392
O	1.27037671177052	10.65035648167787	10.23269666472190
O	0.93678508802481	10.92718247684600	23.54532176123711
H	1.39907181543352	7.66380480155023	1.88228258638382
H	1.98488361282999	6.99633326500008	14.46419817555756
O	9.78630314629566	6.33088596905995	8.92986606104240
O	10.49897162918415	6.37976278664039	22.37828090158564
H	10.44511050021204	10.13650733161920	4.13099121501322
H	10.69133549127509	10.16260137293123	17.70781282102785
O	15.89895951543497	5.13434808330563	1.72631081489498
O	15.80949529809192	4.68117302000791	15.06439611212373
H	13.93106831425175	1.16751075705999	11.38920332923755
H	16.00837639662014	1.30002155980977	23.48570628771302
O	9.82976660150611	10.86147266302497	8.65294999207853
O	9.49813094445525	10.82418222685866	22.11051142832019
H	10.85860462946452	6.93765135775571	3.79961769321152
H	9.93531894174306	7.04417868895877	17.37590175529154
O	15.81987575455885	0.57536211081295	1.66072103647741
O	15.41301232845910	0.15476113545440	15.05803080210800
H	15.37138291292419	4.00308461847314	10.89329254048066
H	14.57912516931086	3.68475545659307	25.19002961757929
O	8.17241299840193	4.83434704629952	3.99625011969620
O	7.03250936935472	5.08954105360729	17.19550423239806
H	6.88780723850476	1.51173990994549	7.97319896603529
H	7.13514087141411	1.97270580572023	22.21359381714327
O	1.33539442851608	6.10101948857394	10.28634705899546
O	1.40394309663647	6.39611082246552	23.42239592151386
H	3.43862687746719	10.16185887874973	1.34045665898506
H	2.08793491376859	10.18818863316024	14.42930587932265
C]	7.69528767091797	2.85682297942223	2.06017011078739
C]	7.17988589541884	3.01713871159774	15.27899423290887
O	5.80288773085615	3.82175403196709	0.27131630967809
O	4.91503789263330	3.18624804808015	13.65882878454448
O	10.04412871061605	2.19870714999430	0.76384320365748
O	9.48147438249433	3.31593074907223	13.79166683116733
N	5.51158841211383	2.88410649750528	8.34648141087333
N	5.47619325030843	3.03105977405027	21.91933661970161

H	3.85029780840290	2.44638327875627	7.39541828924126
H	5.49513449493392	3.66751774148774	20.04568679547528
H	5.17042441201060	2.96153209740604	10.29867115547373
H	3.90457475460128	1.87838388863589	22.27108571093440
C]	1.43280530704215	8.34328361632462	8.66524558203820
C]	1.12126955562388	8.68637013497029	21.89160770261953
O	3.90072922240815	8.38655460859843	7.31429412870703
O	3.37606592373687	8.99488131925427	20.25132826071428
O	-0.62263231536727	8.30945332349524	6.80835544401717
O	-1.16036397537171	8.48517000233601	20.31867394997048
N	3.23816777636638	8.35876075296778	2.11720999720723
N	3.04013157249893	8.56825861065595	15.02171229555148
H	4.48045642104586	7.03333938431197	1.32650131501090
H	4.82256349842040	8.50968931030164	14.20521684529050
H	3.58846412930222	8.48109195824047	4.07777687315328
H	3.19345039716514	8.60076661298280	17.00522460972161
C]	9.85198997726756	8.69449769585580	10.40705162581427
C]	9.31866937645532	8.51580376484346	23.67834322089820
O	12.23477149405618	8.76511486197206	11.87841611791496
O	10.72784203125022	8.99788818910340	26.08715176364129
O	7.68513942210755	8.83978143527416	12.11671468487206
O	6.68611754397191	7.97902929458503	24.29388828661931
N	11.78939993006970	8.68190174904637	3.99785215013647
N	11.36396561731906	8.39694494266381	17.15359013907104
H	12.86668504243909	8.65902048403177	5.63998584989707
H	12.93448326252072	7.92345535942721	18.24451435163731
H	13.03403473209432	9.05077420238748	2.52314565092757
H	11.87520685461839	8.48943006863137	15.23713673498957
C]	16.00648181578873	2.83024241678096	3.28761422354131
C]	15.65819587066768	2.41943307623632	16.69684189279906
O	13.84526089459482	2.84084081347216	5.05270714314744
O	13.38271790520575	2.60577162594622	18.29596315072455
O	18.41402313464856	2.76762577660119	4.67938864611439
O	17.92747509791289	2.19298094535404	18.25825238844545
N	13.90433509197520	2.81579393554640	10.31099010622776
N	14.46930299478422	2.55424910108393	23.53168355677043
H	12.18233701760159	3.74244282554429	10.53716918302333
H	12.78309169960952	1.52514041521155	23.40673394319951
H	14.11786056263782	2.40981604833690	8.38209320899198
H	14.56033816791114	3.70223698227331	21.94111351932013
O	23.84848483728393	0.51835419100024	3.58086252077127
O	23.90474871144999	0.61812562658452	16.86308936567682
H	23.63073707595119	4.31018595935349	7.88233915949277
H	24.19588053242749	3.68760115548045	21.88828448127872
O	17.98675948575071	10.60893207119191	10.44244671769981
O	16.91157375328152	10.11151131000292	23.32852630848781
H	18.61152886404684	7.30719342988003	1.87740332297772
H	18.63225897633459	6.72383838982962	14.95944915509956
O	26.67248254259100	6.19176006284661	8.31476187220570
O	26.83760104961799	5.84769239650711	21.62350534653825
H	27.19305060821792	9.98335700060347	4.34289481878043
H	26.82455354897154	9.67302327940688	17.07654278297201
O	32.61871388774476	5.24519311178168	1.61436926905545
O	32.64630993629327	5.17695747868362	14.83884859691694
H	32.23499114448259	1.50412797784073	10.66439286466718
H	32.63016501012178	2.03771964474779	23.62285704084217
O	26.67075235281466	10.70730129597637	8.76060387406237
O	26.71121720383806	10.40852407962388	21.63407622125817
H	27.58889034342369	6.99282820476289	3.18954500411755
H	27.92958776069803	6.76016036781303	17.86765539601729
O	32.52229570691860	0.69010794219183	1.75175314824801
O	32.43919721533103	0.63522855508425	15.02422608483200
H	31.11197749447755	4.45950751059819	11.25307048275481
H	30.79254659203098	4.68565045016107	24.30633166639004
O	24.57187883496059	5.00211792945185	3.02140921485049
O	24.05423487106826	5.14986281416033	16.83706582815678
H	23.59678541168198	1.11984054094871	7.93571077758891
H	22.65998939159154	1.06429915821311	23.11244113575875
O	18.32606663718407	6.06695192551175	10.46661411330754
O	18.64799266975539	5.92105623608234	23.32955255638533

H	20.32225643795619	10.06671444892086	1.37345283237205
H	18.95933839409397	9.83773746819106	14.25962368559353
C]	24.47308261144038	2.50548418363597	1.69272936498119
C]	24.04845555378554	2.91418963728360	15.20388213777554
O	22.50742018537431	2.60216623447988	-0.22940079716676
O	21.77086104404102	2.93158111562426	13.59837791034368
O	26.96151564318272	1.94541575485397	0.61855753671847
O	26.34009369928823	2.77949301100175	13.67386307709833
N	22.52521422073303	2.73108219610428	8.31433280610957
N	22.57982410454929	2.53329112939948	21.79289537349064
H	20.89329518609723	2.71048206484859	7.21822718371681
H	22.54229833889891	1.71594736029400	19.99480324748709
H	22.05693422124972	2.77837297032747	10.24094106170454
H	20.97036635085571	3.64577977211713	22.09375136416967
C]	18.26581917121364	8.34049682586974	8.86082432369176
C]	17.90957568764599	8.11666175402125	21.71323002294338
O	20.69634426706117	8.51040600594208	7.47063630163417
O	20.17552879471052	8.98820873788089	20.35688298011642
O	16.18841499060261	8.16625931314577	7.03321145741222
O	15.99127601547122	7.23683046405293	19.90773578301645
N	20.26101621003517	8.32722333098627	2.29903184069619
N	19.82841348579102	8.29555788005979	15.12274295013915
H	21.84793763042375	7.20526213371092	1.92636267623640
H	21.54755717609599	7.91841265549828	14.26390959200392
H	20.28816847152103	8.67482918257220	4.26130415478580
H	20.13149499180965	8.70209928548949	17.03759047062878
C]	26.70373711225585	8.28967751534171	10.15480477301008
C]	26.73371392848348	8.13671941671604	23.27609727633418
O	29.09288472896573	8.14438803493538	11.61301590578624
O	29.04981730743874	8.19673386811691	24.82839176527894
O	24.53475741778863	8.13687024520671	11.85358833105668
O	24.47102581084922	8.04459687816927	24.82626364453411
N	28.53472355162880	8.61394795726150	3.82322192208811
N	28.35285365240449	8.42435692432884	16.90456173363239
H	29.61722623940328	8.12163269560058	5.38398485394489
H	29.94998094313248	9.23344819708551	17.70907139185518
H	29.75399538501819	9.39129718471240	2.48112015446603
H	28.69724675981833	8.05075851161352	14.99006024656268
C]	32.69115525373263	3.01593447606569	3.27752352256058
C]	32.55204352424467	2.97184147182477	16.54985814631003
O	30.48620146096435	3.11672397514364	4.99700012213753
O	30.21715471047265	3.13804303002687	18.08185676124358
O	35.05851452286312	3.00853837147138	4.73354127290018
O	34.76961279414189	2.94327628857142	18.19975362211875
N	30.81464803321421	2.80945100933662	10.22376131016865
N	30.99284726227292	3.06619454482374	23.20719521242089
H	29.06295014622727	2.03595533407653	10.65970477351479
H	29.41870901708906	1.86428663189893	23.30967576504714
H	30.85320615057748	3.18054116022035	8.27268717483478
H	31.05678534068875	3.62556159608527	21.30795731538332
O	7.41043743941968	11.93356085469582	3.94946508909639
O	7.13854281874529	11.95881357481920	16.87864894162218
H	5.85703351116420	15.78556778809795	7.64432555756613
H	5.79368424117330	15.76427345272216	21.90255915306321
O	1.36652917631652	21.79792017226453	10.37735549816689
O	1.41796954911498	21.96634619700822	23.58351961176330
H	2.88873726003622	17.80125360795299	1.17547969811401
H	2.76705756052184	18.02967822929536	14.07919403546620
O	9.75252828858215	17.40152789096639	8.85008717952901
O	9.15322244825589	17.64940644530114	21.88419510638533
H	11.38466097754337	21.14907893346491	2.26873727268982
H	11.47041638059898	21.17441938034419	18.42972324763612
O	15.53236057836676	16.26606922279806	2.16865369781340
O	15.46410393529366	16.22319548308107	15.62424585046019
H	14.20004289043356	12.52137801244860	11.54313613726013
H	13.18075542492731	14.23487409182285	25.21919435424032
O	9.88694298095424	21.90299759409065	8.29716336302969
O	9.89960339577042	22.14468714796741	22.22443684832998
H	9.84934814014481	18.50817289201374	3.44657242749124
H	9.94140058685989	18.41555536805441	17.72488851668440

O	15.96002422181405	11.73268164858017	1.95069465943071
O	15.58975839214276	11.69501472794716	15.17651182835102
H	15.28576001368500	15.46420572350165	10.79656238098906
H	15.77153401671015	13.97786302024932	23.18133269468451
O	7.05089885552570	16.49095311343291	3.72179918712403
O	6.97535370508438	16.48848212644912	17.14371009153065
H	6.81189830066658	12.76127883661312	8.16298691220964
H	6.47492818676008	12.64554613922917	21.38602008369027
O	1.21390787223976	17.25013261285363	10.51618411644570
O	0.92465383053869	17.44166402790980	23.90844372128808
H	1.24198804405505	20.55968024880031	1.84217998074077
H	1.52261014940895	20.90877500804122	14.80486089179107
C]	7.18431246359334	14.11803335163578	2.20048954345484
C]	7.10214821669716	14.31180278634932	15.39536594118199
O	4.79571869915453	13.85629322153720	0.78439341779758
O	4.77866930281647	14.33759402928543	13.81309313745678
O	9.35631620363044	14.22866602591798	0.52690642247892
O	9.34235243525721	14.49785357801353	13.79570578627797
N	5.40473211171776	14.09541888004524	8.54464422450144
N	5.02447472932634	13.97670372051479	21.56957101524524
H	3.67770364309120	13.44522016593236	7.87495423829767
H	4.00546783712705	14.04209728677908	19.89160867885205
H	5.25960796722957	14.37050387998303	10.50582248543043
H	3.75488019409622	13.38827314821321	22.95930718488907
C]	1.28418123859237	19.46818798834033	8.83807977847258
C]	1.07747472181960	19.57933777105883	22.14155510077003
O	3.62832928896794	19.35183989219514	7.29680608536138
O	3.30867241685080	19.24704977299071	20.49900233156450
O	-0.92350784392471	19.50240711688637	7.17411874041345
O	-1.23903580996765	19.74010651593993	20.63425872496019
N	2.86761411306037	19.47948741484239	2.19194096292704
N	2.97438455186022	19.62551978816243	15.21066175890581
H	4.47458232076989	20.59699921227220	1.89737139186720
H	4.72030344470760	20.47018856239831	14.88395878214943
H	2.91596535056230	19.03230370554725	4.13031665459619
H	2.90211294374962	19.13123499157307	17.12671826191953
C]	9.66424722309678	19.82725460746542	10.19467951547697
C]	9.37272106918932	19.76254017286566	23.70217380494950
O	11.85043512270616	20.00932081143960	11.93097209809021
O	11.52368180931498	19.30816715170607	25.38579858473376
O	7.29867284186532	20.10018903860174	11.58685114714316
O	7.02676039729412	20.08599762626059	25.09302724114967
N	11.46913879723711	19.65833198348306	3.56096920755757
N	11.45365926631094	19.59857704628122	17.25080225998273
H	11.49506335468217	20.46280971100352	5.36549587747289
H	13.15307225433526	18.60583938056465	17.37485553298887
H	13.08266644652718	18.54527256977635	3.25009570877008
H	11.28254428034413	20.16802551807849	15.36403552924883
C]	15.74992999868618	13.91416358211774	3.65372221732115
C]	15.37713149381149	13.79763605458725	16.99554674397932
O	13.44664533690460	13.63140394518289	5.22497317452507
O	12.91499975909393	13.59875593304745	18.31119569066673
O	17.99050327319953	14.07139228415163	5.28543914574788
O	17.44175604056455	13.67194647528839	18.83845204318084
N	13.83870780249405	14.14274792311219	10.48712626080458
N	13.93815482690473	14.64475566187780	23.36526651309830
H	12.10876265497713	14.91089762174619	11.00427193415337
H	13.95899627807630	16.58603436404824	23.06065264139300
H	13.76682654566046	13.71519819235572	8.54951153916925
H	12.86656770367482	13.80746941077456	21.94535993423396
O	24.16566848498155	11.79071033986409	4.11991965924622
O	23.88115011584697	11.53642363353263	16.91501591776408
H	22.82654612003938	15.67669981566032	7.90247143235443
H	23.01537633222659	15.42665735672682	22.00228836271722
O	18.42353056788136	21.83543617747947	10.49277628680528
O	18.68596104516903	21.63230720327913	23.82315129735364
H	20.04060212828802	17.69497697726631	1.28648066112072
H	19.84073437918351	17.74020378316715	14.29770372492390
O	26.58255368127807	17.10565970578263	8.65731832267332
O	26.36787500713740	17.41986234831260	22.16063280062929

H	28.22384681385074	21.14435023776727	2.36388427065650
H	26.81096683765204	21.03960874310576	17.20069084842003
O	32.45953501669577	16.31275616338390	2.02263811470998
O	32.29153667476868	16.51506324844932	15.09327429449462
H	31.97919630253284	12.57975331162919	10.78381593450131
H	30.50723862918097	12.28403600217925	24.17322505944922
O	26.87702395289922	21.62633019040812	8.61870899940123
O	27.13825293286799	21.91097367641970	21.88046239273159
H	26.82271339792171	18.42530039277345	3.54998114933940
H	27.31984852889662	17.97386085772838	17.94876550643779
O	32.59939470545318	11.76308213006666	1.79009535117343
O	32.69981402797023	11.98600625943660	14.97595876439810
H	31.25145727269478	15.67926070447477	11.19572943068243
H	32.01387220811890	15.14322294205644	23.69070270438789
O	24.08268019088323	16.35014651692933	3.78998277716460
O	24.01333344417711	16.06908104025254	17.23235424710395
H	23.56959171606110	12.58807161958003	8.31838657856277
H	23.72052976359956	12.31863394522431	21.68522613937176
O	18.13193496086963	17.29561105279555	10.67710868247390
O	18.55709116451619	17.09311005726326	24.15446496208034
H	18.28939215535848	20.40854478724275	1.89348577669324
H	18.34556152243131	20.53439728172058	14.90192472022455
C]	24.09028409165197	13.94886322833311	2.32151928489661
C]	23.91824707807315	13.92639711158174	15.47053640050669
O	21.70086059382510	13.80112663763260	0.88635102273380
O	21.53174936572684	14.09433069448425	13.98762785874679
O	26.27596945828265	13.86579790143903	0.66352895936160
O	26.08730186836685	13.96655218736037	13.75357079908476
N	22.22418695094721	13.98135144144798	8.69874632552865
N	22.29238949683054	13.60226689489932	22.14291118335514
H	20.50227123461757	13.46930521861392	7.90725145490336
H	20.83886063296058	13.38505738992795	20.85161358955483
H	22.00295690246682	14.18887957712483	10.66077033716434
H	21.60993740397862	13.21786427919998	24.07609852990291
C]	18.27498300688348	19.52466436598860	8.97710816347952
C]	18.41861168825677	19.23828450512707	22.41017707484390
O	20.61593115566571	19.28147010256701	7.44221166676137
O	20.49664872113953	19.05142815345139	20.55746289518785
O	16.06695725642915	19.57890969328946	7.31031274977195
O	15.95399841999394	19.24557213188289	21.09592412742654
N	19.90952828273231	19.35342430471876	2.32957667836137
N	19.90831058857080	19.40188296559199	15.34684280663282
H	21.50613464021833	20.50793416744771	2.14066387569387
H	21.56196037382341	20.38582050366709	14.95193797752260
H	19.86282821610881	18.87644518912454	4.25876183819970
H	19.90530780997873	18.99772799135061	17.28902115071959
C]	26.69700245715872	19.34786919588186	10.28099616908144
C]	26.54850885351089	19.80730311147405	23.65416757096676
O	29.00918166296816	19.25064804018956	11.85122404367909
O	28.57701247780189	19.55438077795621	25.50106860157327
O	24.45398977865432	19.54802209898945	11.87537079402891
O	24.11233882069511	20.33213192369772	24.85658741447828
N	28.38418769828098	19.65346535478583	3.65391579141677
N	28.14188038726478	19.57318031201959	17.14434407196887
H	28.39727353958078	20.43750791091323	5.46643645448535
H	29.73486126549575	20.08549218688312	18.16553299879935
H	30.03768691582514	18.61741421386244	3.31895153486455
H	28.63563694493096	19.20759906049983	15.26005075840654
C]	32.55960227000765	13.95139360185010	3.50636772735339
C]	32.41339521796353	14.21138437656998	16.62779030997531
O	30.26280712616054	13.80853118174378	5.10387837170255
O	30.02178655989847	13.93369879034103	18.06815797593678
O	34.83374929380084	13.95876369247457	5.09344335506294
O	34.52588080159253	14.36664217362400	18.41911698212534
N	30.67789163191228	13.99802887165450	10.34825652964419
N	30.45261636009969	14.01214313970605	23.23788252787699
H	28.89755843204577	13.49781442817945	11.00161303280372
H	28.79068301140076	15.02755969588704	23.57345930324783
H	30.58352004337674	14.20487106887332	8.37308217279715
H	30.48531208215061	13.66202392402798	21.27734918323130

C	15.39926858089861	7.05256100571291	29.65152506525891
C	18.21571183012101	6.80508714756618	29.83569579296781
H	14.51541575153561	6.11213203628005	31.30594947381660
H	14.88231881734692	9.08398061914423	29.69367525718853
H	18.74725400967701	4.77589402646286	29.78094349750105
O	14.52580074334524	5.96220224266695	27.36588141826307
H	13.11554351803541	7.03839301652708	26.72564291387281
H	18.85970795097588	7.57139547438727	31.66612779236486
O	19.50768273900884	8.12649152350837	27.92116904214954
H	19.12848585958041	7.29314655324156	26.27545981993373
O	54.61170367920916	12.80497562386713	26.83348397511906
H	53.99461293090137	11.05804765128408	27.35607937672739
H	53.25172543881590	14.01091735751671	27.19889852633843
O	45.82014547516867	13.48578316555124	27.87733237547803
H	44.86998087106588	11.91323455231455	27.43313026094509
H	44.58269354860132	14.75879019089459	28.41788833322147

Ethylene Glycol adsorbed (011) surface of NH_4ClO_4 :

O	6.87152179796780	1.10486711080416	3.62428032208828
O	6.99539506133245	7.76504339971097	11.63426486316859
H	7.07576616600588	16.46917154052167	9.37425183805742
H	5.79170345481552	6.75130465009813	16.06229576506169
O	1.20081695891504	12.75157740409633	7.43296457920708
O	1.40991273957559	1.07040111410633	15.53937386602212
H	2.70303540063181	8.10566548305334	6.51376809252421
H	1.19352809249888	12.72356902486625	16.48997146118220
O	9.80915011656054	11.22198911593794	3.02382801704733
O	9.57673363775173	-0.19901998583950	11.09768220011186
H	9.73266560593921	17.28097871443711	2.70014551427845
H	11.23698068745329	4.33961656914195	12.11610025365061
O	15.35628649184452	4.85448253358533	6.85241152678905
O	15.32664909877483	11.45669494503485	14.55878171766500
H	14.25952667272345	5.67661428665590	2.42446078518845
H	15.65968102910602	13.72207842628434	9.02824020289424
O	10.09107334181519	13.78106113257438	6.75562014017101
O	9.95293743288312	2.47559663240131	14.75144567204405
H	11.07863878555369	14.34880194391017	2.29794159155427
H	9.87519185321652	4.53634025617038	9.18069636569466
O	15.54712704570611	2.53261578852556	2.95304398244506
O	15.51034910704435	8.55571561775199	11.07236574141601
H	15.71728087161232	8.53638335477617	2.95703712870471
H	14.24648096353737	13.31665952006261	11.90125013221752
O	7.12239073429124	3.75770678029357	7.30623645934225
O	7.15412514321374	9.83009584092997	15.64175008119983
H	5.72575052205933	16.77683511082900	6.45684462835148
H	7.15136550245410	3.82403994484337	15.61738093465154
O	1.53302881424840	9.92940194468405	3.88223787999905
O	1.57392106462949	-1.26016981153036	11.64724145562166
H	1.38486035876736	7.64111754904771	9.43663899556575
H	2.20495956399187	15.78665422566228	16.30338418194028
C]	7.31492452433479	3.76395717039446	4.50824391585837
C]	7.40495537038724	10.23806010808658	12.86251158985095
O	5.42774549315494	5.42766536120833	3.43289161725934
O	5.44379074950141	12.03186020685681	12.02923005013125
O	9.88552343569668	4.47752200140664	3.74382144878262
O	9.90712967981803	11.19767215228687	12.26759549638565
N	5.55358793051033	15.93894664369398	8.24314507309467
N	5.42447975728285	4.82057733957125	15.80619520510916
H	3.86790662981438	16.49524826060404	9.10893382145624
H	4.38675259936194	4.58588376723800	14.12752167973746
H	5.52312518254802	13.98199092665840	8.06221888042047
H	4.31080175306748	4.07565192336888	17.22428954606826
C]	1.07268846506419	12.62775484208361	4.63754410604713
C]	0.96118109891969	1.21922394017048	12.78314345731836
O	2.99159125844956	14.23497924563308	3.52687501825428
O	2.64441241693774	3.16547622953683	11.69831161784414
O	-1.47262526067950	13.29989387177139	3.76932715221152
O	-1.67218073632131	1.83315691832888	12.25606914401160
N	2.89546331310003	7.15734666894314	8.24413987594947
N	2.78363934979945	13.89629579074836	16.35735633232224

H	4.59983954395944	7.65797140975444	9.10037930718841
H	3.61752807175120	13.48391717627610	14.61331247675868
H	2.90144362165341	5.21594195038605	7.94527750475834
H	4.22310719998980	13.63380547717268	17.77841984498400
C]	9.47330202565103	11.22208650486352	5.79997347459468
C]	9.44903459361142	-0.18155388410388	13.89854964253120
O	11.22954954922636	9.37262203431229	6.92764833250827
O	11.33225338055317	-1.86737651741672	14.94944010918469
O	6.87089765922323	10.61714333182694	6.47375164516438
O	6.88775448679998	-0.84830613041963	14.72864543470624
N	11.45265679494753	16.29027214525694	2.42196491996023
N	11.37579594536840	5.15497433057637	10.31821431944401
H	12.59129603092122	16.61695742472816	4.02226308797801
H	13.09407680751168	4.67690232967228	9.47478154325689
H	12.43389252544131	16.96304957734208	0.87762811308124
H	11.30963195666022	7.10760419995018	10.45965535180979
C]	15.87290294928173	2.34656218683860	5.72661385477789
C]	15.56711542726170	8.71369504372466	13.87204984867425
O	14.01541648739496	0.51104259495825	6.72368333402161
O	13.45609743895645	7.32044537621649	14.93045645343577
O	18.43102547302666	1.57147798134167	6.36571278250518
O	17.99371732128265	7.79779014247754	14.83007769955917
N	13.95078908413189	7.60668460365981	2.74758781052179
N	14.11475521727059	14.25206500597096	10.15808181133412
H	12.95840038657991	7.79442358026806	4.45244082873117
H	12.44087054702772	13.76821357818004	9.23137380125441
H	12.84098931570996	8.44396595659293	1.37926729667097
H	14.13442486061042	16.19868016243756	10.41510441779591
O	23.70973670055105	1.07531247262094	3.79846068193532
O	23.75345461305342	7.79925300970652	11.93409878791402
H	23.96697470933493	16.51124694465017	9.45295884801546
H	22.46943043715820	6.82367031932661	16.16987372351901
O	18.29730886438241	12.64292068036275	7.30038136215219
O	18.25425678743155	0.93284459331445	15.68349363997215
H	19.90185752534300	7.82391273566159	6.55757771154570
H	18.10997954071381	12.78255928628134	15.53229891282385
O	26.73308053386036	11.25772459285202	3.21562843272766
O	26.43310849848109	-0.14783199352394	11.30378529331785
H	26.53355031629794	17.29509586999017	2.88754292288960
H	28.02010074580483	4.42238531485906	12.35225774201084
O	32.07027222949338	4.84915032928323	6.96236860697403
O	32.17254231765190	11.39253606345967	14.94928887251318
H	31.07826549283441	5.73867341794455	2.49854803082159
H	32.30686791888582	13.82966867363064	9.41917385381101
O	27.01175743450969	13.77030519130587	6.98211322708759
O	26.78632147361551	2.53102805197370	14.95615705187885
H	27.98834039661180	14.41184498945169	2.47021527065353
H	26.73542317442518	4.61417946987675	9.38225362444123
O	32.27285892032598	2.57339991066751	3.03605796737005
O	32.50441644869110	8.69697771006128	11.30743843438392
H	32.49199137091789	8.63743914083157	2.99581947152135
H	31.04329080265072	13.30095533471526	12.35421342713650
O	24.06613440655748	3.76156295353451	7.44085065954998
O	23.40173150555485	10.12970806111668	15.80072739406033
H	22.54268866183003	16.80365763778276	6.55823787980856
H	24.00950213784225	3.95253329567608	15.80072931024262
O	18.54426776649090	9.76679402007234	3.79476593476916
O	18.48951365688706	-1.55119349104064	11.88780549617727
H	18.30745509874478	7.65959932944263	9.37269799563334
H	18.59079477010615	15.17425660273728	17.63029675048886
C]	24.19425616164497	3.73732108382019	4.64048020565288
C]	23.83264437055761	10.38723874312389	13.02819058019798
O	22.28937157019385	5.40289036762881	3.59081525662707
O	21.80066817042152	11.92174013401410	11.93177881083461
O	26.74728671441117	4.42893944252975	3.80522294782087
O	26.29907074033053	11.50115266830761	12.54185136008884
N	22.42916127294422	15.94308828652226	8.33648297388093
N	22.23128897825167	4.86446929962918	15.95748195436084
H	20.75830699397155	16.45046640394742	9.24985041135865
H	21.24181804429285	4.50949409819143	14.26954068672830

H	22.42371451533415	13.98651705694353	8.14937417180249
H	21.15631566422701	4.07913609835293	17.38370363510749
C]	18.12438875910867	12.47488820998185	4.50541072884766
C]	17.94208206669810	0.99162881600040	12.92483779802257
O	20.03149928352886	14.05507474472670	3.34330426914144
O	19.74960335158863	2.82466556475527	11.81884425360065
O	15.55991655716252	13.16804744192510	3.68555993379146
O	15.35921287825798	1.70146717134479	12.22929332919792
N	19.90109980374839	7.03866467599591	8.36926181742519
N	19.51284165353555	13.96997844223869	16.31832683033598
H	21.53755437572596	7.56860455110135	9.34566215450486
H	20.28015877852312	15.03089774968820	14.85111784976361
H	19.86872508947432	5.07977055915954	8.24842846010178
H	20.95530498230594	12.84928832199816	17.04248729903922
C]	26.39530735816033	11.23031944443666	5.99330563235207
C]	26.25654651868844	-0.12847916843814	14.10640753730659
O	28.14985541134720	9.36387682022228	7.10500469269263
O	28.12272350032198	-1.82761284738228	15.17266139420832
O	23.79287570408729	10.60878934395714	6.65029436675809
O	23.68643737142582	-0.76532337132913	14.91155328679169
N	28.29334828566279	16.35214124001729	2.70914050102930
N	28.17426702382097	5.28047303619825	10.57320918741272
H	29.29523655896634	16.60685182892611	4.40469061106439
H	29.92798153582165	4.87933030240765	9.76777870722319
H	29.39898408225255	17.13260898044705	1.30448512693208
H	27.99298728795522	7.22392156725885	10.73684078611497
C]	32.69319196275563	2.38583551073814	5.79695977716507
C]	32.62694775139398	8.73102853392945	14.11210639005091
O	31.01235424365709	0.41464573591195	6.82893324437924
O	30.69527176244756	7.08758271417232	15.15396543981330
O	35.32838538480766	1.78191276524261	6.33563807279510
O	35.16604166091576	7.99540996031116	14.95357143221860
N	30.74957846805295	7.66149511402958	2.84615831759473
N	30.81694789037956	14.27987358445784	10.64255085642475
H	29.82569932129057	7.81202242770504	4.59492284129935
H	29.10873956327977	13.78546858805886	9.79035185806229
H	29.55669999347598	8.48752486564941	1.54118997257468
H	30.79195399092571	16.21775602359330	10.96301734012617
O	6.96159380603470	18.58478403129298	3.71746650810232
O	6.80639020821567	25.33113639140863	11.54075400519874
H	6.90383469174142	34.23606157871226	9.18050845132880
H	5.83142533544644	24.66132157178678	16.03500523798445
O	1.11602861564499	30.43680633686125	7.21017555391673
O	1.49198279118334	19.07694104917793	15.56555926047449
H	2.68126919308370	25.80025074088092	6.30632089003784
H	1.21852219226369	30.43429600011037	15.59384471512846
O	9.75031217274030	29.22357881137991	2.69322595892862
O	9.97254608531226	17.57734030144293	11.47085637309157
H	9.68162444156410	35.28664411449368	2.69448119249961
H	11.52416176384594	22.53011901055963	11.79397551448752
O	15.30656170312919	22.59190155397372	6.49086175840284
O	15.02169315262584	28.99057329926877	14.42627117569742
H	14.22081997753332	23.42580891807369	2.17216169090553
H	15.40926730890884	31.42826289865618	9.05995644021033
O	9.94423673885089	31.58698428401785	6.56110941881097
O	10.38059257256284	20.65487714498532	14.80465744576618
H	11.08638278116870	32.40201882858558	2.14304051243168
H	9.73723130519966	22.45687498528990	9.07114288187710
O	15.43523141832169	20.22071855631014	2.63349411606975
O	15.44145626310482	26.47466666756164	10.67155820346601
H	15.64134242381097	26.32666140882876	2.64502191786374
H	13.80810686830885	31.01490574620188	11.83769593654618
O	7.08672971069676	21.33769254902312	7.32230290140832
O	7.06574644502813	27.77169375979484	15.36109098634676
H	5.61113955476482	34.63966181818047	6.24188619915527
H	7.33387292346339	21.81780629318060	15.65281752870224
O	1.44831477878903	27.60389607654662	3.67284289333194
O	1.72003134568848	16.53933806931808	11.81615810051055
H	1.37834299004926	25.27210375288519	9.22147110534640
H	2.61867281832689	33.33896027254997	16.10834580936190

C]	7.35062377897850	21.27447415390474	4.52513346971215
C]	7.38203389766988	27.86637743282047	12.58050524310296
O	5.46297792497454	22.87998186788130	3.36483144901145
O	5.58231139155473	29.71841657962796	11.52908823072091
O	9.92413992292050	22.01645880287784	3.80759534968243
O	9.96575531479785	28.53986456289020	11.91571121792533
N	5.39773967341074	33.74101235200055	7.99213693198596
N	5.56217413737500	22.71195930533447	15.78524971317605
H	3.69835630306399	34.28213035019837	8.83072077676101
H	4.59780710571749	22.44980342603975	14.06392075869795
H	5.36551167369356	31.79328429991414	7.74953314750719
H	4.43264566600267	21.90607932166077	17.15888890277964
C]	0.95618268828141	30.30155878738382	4.41681370304392
C]	1.12312383804567	19.09040774021178	12.79201496369503
O	2.84174528930791	31.92831187582200	3.27722205077241
O	2.88721836809681	20.93718568161741	11.66012907409958
O	-1.60641596926456	30.93696962922954	3.57420256843759
O	-1.47999765488011	19.72337402856276	12.15584806888286
N	2.88837207046256	24.82488270071210	8.01873306974995
N	2.95903147762689	31.41446051289403	15.78553203070022
H	4.58050108079220	25.32196908242217	8.89963980852518
H	3.93770132664980	31.25191164033400	14.06870863872810
H	2.91787948627965	22.88733307447260	7.69494868239704
H	4.10359809470465	30.60688225880796	17.14262031482025
C]	9.38912029580545	29.07538085160488	5.45925707124196
C]	10.09128827170575	17.91886841397593	14.22279654602239
O	11.18474182221908	27.20057584346752	6.49584497942253
O	12.23618296073456	16.51692849128264	15.27446592187979
O	6.80362027789727	28.36603703569768	6.08449555704110
O	7.70471634225561	17.05168479073135	15.38342675734894
N	11.42553747138803	34.32592997634811	2.46162495930371
N	11.35422531502560	23.19591553355684	9.94912430193413
H	12.44121970038548	34.50448761275341	4.16038455184359
H	12.96307001132861	22.69627084817765	8.91071735661373
H	12.52780709127242	35.14091907111280	1.07423752648118
H	11.23806003098575	25.15626662923558	9.96974082467423
C]	15.86962283826301	20.07609753817464	5.39462713574588
C]	15.74185388559442	26.45094039639244	13.44881413589400
O	14.12423857350283	18.18260021714450	6.47936055072461
O	14.10759490892271	24.52921217143238	14.57327170673390
O	18.47572647964076	19.40547989864419	5.95651728318910
O	18.39474665449822	25.97121623439344	14.09887318412843
N	13.89396471719715	25.37184020774917	2.37342895795013
N	13.85530975136997	32.01699627311313	10.13758558666941
H	12.78510677126839	25.67158066664045	3.99515072616956
H	12.19744962040606	31.69649970119234	9.11597556082814
H	12.91020581871210	26.12132729053645	0.86620562383447
H	14.00446261810185	33.94145548491560	10.50748226590108
O	23.74204820348624	18.60720206207338	3.77135969060896
O	23.63621271613536	25.44730226693277	11.56921099029308
H	23.85311085849202	34.17938171346513	9.33921010983945
H	21.81949827647415	24.26255682588816	17.24229981711828
O	18.07425424942355	30.34451041594250	7.15218623318690
O	17.95003390195124	19.68494072572031	15.17009724561631
H	19.88612818585120	25.86212940710409	6.08023519594846
H	17.83954981872397	30.52926302811980	15.33666619492300
O	26.68600468385855	29.15163912610425	2.80064018017610
O	26.53685429833707	17.71585474708428	11.34474636185523
H	26.50004016386112	35.21618254086765	2.89156382733631
H	28.04518664468534	22.26613425810059	12.14281504731798
O	32.11334864044754	22.53364839535149	6.77422854922384
O	32.22746159687797	29.12435955376936	14.72743714004246
H	31.14306795087707	23.26033444522626	2.35685622046066
H	32.26838701006282	31.55856660900636	9.19334458421844
O	26.98644864621219	31.40741381299106	6.72796073477471
O	26.82772987056229	20.51020899708027	14.90824883043130
H	27.92085271900375	32.34474552130505	2.28032666821713
H	26.73028287936998	22.50813248740151	9.19421157355705
O	32.34931164197444	20.08299398784314	2.96958992739753
O	32.55054789672360	26.33310520672936	11.15565251208660

H	32.48530097131688	26.20552221822928	2.77473800275754
H	30.96796887988738	30.98317211395680	12.10414207807000
O	24.07267265863899	21.52246775476598	7.23641473942324
O	24.45360936544700	27.71811270335226	15.41718455839444
H	22.36497099734893	34.67853460517918	6.50275417151430
H	24.04085499594231	22.01224691703976	16.11002208714163
O	18.40275585994679	27.70697750727855	3.46608513663529
O	18.50735066083839	16.63541072317092	11.86461921802775
H	18.25449248919168	25.45963166976200	8.83027165122206
H	19.77134284596822	32.67093794130562	16.75807328436072
C]	24.27999070401389	21.30667325781974	4.45202674249403
C]	24.51521067656680	27.90464960816487	12.67021986427538
O	22.46071589332320	22.95554380287005	3.23591042670048
O	22.79149856957521	29.92386840896059	11.81857330844830
O	26.87469808743321	21.86786440501795	3.64129286876690
O	27.06988398337127	28.37840559932140	11.73130218819317
N	22.32456546860805	33.65424551650024	8.19232385772271
N	22.25927977735960	22.85655403737957	15.88974574375228
H	20.65034781917332	33.99581616298885	9.18091920975823
H	22.30248418513339	23.73740852144799	14.11186723576117
H	22.42223631864685	31.73142616367560	7.80428868952344
H	20.85238130024174	21.47434440689637	15.83172882735184
C]	17.92081198784685	30.35993418483017	4.35355911211133
C]	17.88070674792559	19.31883081953763	12.37935234039372
O	19.80690737636731	32.04153413629958	3.30408170328562
O	19.76290289445700	20.95264346179588	11.20432972167591
O	15.35436179633758	31.05029962866270	3.55345476642359
O	15.33394639147979	19.82198139096431	11.44577768918540
N	19.88272753865159	24.94935622802145	7.83275595661762
N	19.66625257022501	30.84729312194334	16.04669733445747
H	21.48106776332100	25.45318982016903	8.88292628265994
H	20.93679422485062	30.72139279849728	14.52508588640832
H	19.91196253721968	23.00409124874582	7.57926535221838
H	20.04247504718886	29.38993064627264	17.35999052588075
C]	26.30049702624117	28.96114068448089	5.56258947461084
C]	26.29835173166531	17.84223258542486	14.13991302400961
O	27.94727110156951	26.94304492335481	6.55988894486232
O	28.10555863982796	16.15878311175376	15.32139684689536
O	23.65993268695765	28.41102125745586	6.14678555239099
O	23.68711990081792	17.24055837969204	14.88750013646657
N	28.24729944889758	34.26702898370544	2.63161812447423
N	28.23792961607257	23.07423667308086	10.34671266686377
H	29.27852527998547	34.41322350875507	4.32051534786161
H	29.93781284921501	22.51574997341136	9.52180142335033
H	29.33139108831782	35.12224116738173	1.25368355148373
H	28.24226956865014	25.03672773619752	10.49455774674112
C]	32.73831805003346	20.01230920543640	5.74035790658429
C]	32.69937992386425	26.43514688180143	13.95051447102113
O	31.03670593291543	18.10356683636687	6.85324267747170
O	30.80667289007904	24.80762331233785	15.06937697854467
O	35.36329520825237	19.41530068626304	6.34212846567277
O	35.26307433721406	25.77253939636208	14.78628913019699
N	30.77035263174640	25.20210599174956	2.50457788421451
N	30.75389341955388	31.96797259924633	10.39924658448651
H	29.62667805988594	25.50125178028547	4.10520997439748
H	29.06915071936805	31.43066282248903	9.52702821306000
H	29.78423548544846	25.88564619835288	0.96808313650834
H	30.68580153225298	33.90021788330571	10.74276972813282
C	15.94589144578484	18.65839581238444	20.90436317595104
C	17.65107461615579	20.90204449522375	20.47044435572659
H	16.54325702304034	17.72564404241725	22.67721598376889
H	13.98467666778820	19.33590103120896	21.17918449106425
H	19.46154175541832	20.21035503556874	19.65803556104310
O	16.04767709887177	16.77835435614719	19.01665822643170
H	14.86135573206358	17.17989819564619	17.61860113156634
H	18.07589985127908	21.77423570183722	22.32216830377534
O	16.58613589336376	22.86451695776616	18.99500736398681
H	16.27982859461415	22.27910481287869	17.22996823543483
O	40.79120492805621	-21.85402924006643	19.14573834667485
H	41.52961030535747	-20.42785033516035	18.17147528606309

H	41.41188386943288	-23.34303915379419	18.18400218794910
O	53.81233365841687	-9.03743994713991	19.07557336367441
H	52.25463525573275	-10.20349966476674	18.98449653531452
H	54.25084072233444	-8.91702594838954	20.87287254169865

Ethylene Glycol adsorbed (210) surface of NH_4ClO_4 :

O	3.56990679765683	21.10373980035347	0.91280411011985
O	4.38354557161138	11.58528190345116	7.43696503303766
O	4.48840844527162	2.63490490244672	13.70426748165626
O	4.68018813065636	21.60395801761159	19.82501649521148
H	9.06013846618960	7.95725723266539	9.39524944485761
H	9.17314750508904	27.71585584312544	15.80147913467176
H	8.84527042637339	18.23546715553307	22.18327233376770
H	10.28067187129140	7.49441526214719	27.84140854767134
O	11.46310289294113	-0.10013182714330	8.92080880781573
O	11.37549649558718	18.89103338914987	15.40267437571218
O	11.32751173834185	10.08618212400163	21.91914097635589
O	11.87434710293084	0.14935389579706	27.65766699755242
H	2.34720318194020	13.73136473321462	1.63476721095413
H	2.11159930396610	3.32612721424473	6.88178899558915
H	2.30389566692958	22.00468887992408	13.13140924095139
H	2.29946510954322	13.38306800531630	19.72079717912145
O	9.59414947466215	17.62507353236157	6.39562787271866
O	9.54449941705615	8.58094492794813	12.78974122632418
O	9.47485757827725	27.83530754420009	19.20986390104009
O	8.85918875817167	17.82496238970690	25.57563953772591
H	4.25073119758769	24.35849685120265	1.70647418023694
H	5.38133745157871	15.14221408530845	9.24304184907276
H	5.61594631315896	6.31168829048902	15.96067839964510
H	4.94273185356152	24.97242150322774	21.11059172240529
O	1.96191497821773	3.70787505575627	3.59288170049064
O	2.67841111837993	21.78972596829750	9.79709608840170
O	2.77222790222243	12.84229600841307	16.36329545807417
O	2.69637256457606	3.83535071159191	22.80808379437492
H	11.73603124104905	24.55417249990161	7.57597763316228
H	12.40575476044291	15.21281429869164	13.17410905405528
H	12.38464196916622	6.40519165191533	20.37183324410840
H	11.85083176299171	24.88560474494266	26.94134968784260
O	9.33894460142916	13.86676436029168	8.92193192685387
O	9.46910546360210	4.88130548761719	15.41238732044052
O	9.41817051506331	23.85399977243313	21.38431530506113
O	10.78289549992843	14.12572906474830	27.48015966714793
H	4.58212870568311	27.72860752226482	1.55124846128389
H	4.81780879820156	17.28231539142464	6.86712690349287
H	4.56020182606095	7.86847293500267	13.32838819407451
H	5.22157825130590	27.96796202660661	20.09725701135579
O	3.34794647774352	7.15483203306532	0.93284507330488
O	2.59103692490304	25.60617170666715	7.36149137849456
O	2.59670322522513	16.56287966511199	13.78036457007608
O	2.26810214329812	7.47013215104992	20.10297891497938
H	11.67250278722698	21.89959151014898	9.30245203219927
H	11.48648536623641	13.53082642802274	15.78972574493187
H	11.37652556673554	3.90623376406367	22.19853190813182
H	11.32269389481426	21.63432028505639	27.42896654611567
O	4.99327127297372	17.68557806911514	3.59125367875725
O	4.27586868599142	7.82634369257687	9.96081893630934
O	4.26677990835353	-1.03429882623358	16.35658954949086
O	4.17050129514005	18.46325648496728	23.05996571838766
H	9.05814453300716	10.57443449528080	7.61100115386904
H	8.23539361873064	28.93643592257280	12.94972258657969
H	8.38785052986261	20.15141422261716	19.59623588159251
H	8.45102938057211	10.00096833913015	28.06067549763048
O	11.17588388029653	3.65376063545328	6.38899298949175
O	11.17378584588133	22.51973231421703	12.69442524148850
O	11.20681086593762	13.64971607163549	19.12787093703016
O	9.83502275000086	3.46366142492998	25.27288033394654
H	2.67827352553104	10.36107033164021	1.77936400091098
H	1.58177383099053	1.20788989199608	9.28767915679864
H	1.52262755567629	20.23512082807176	15.71208805350920
H	2.04040946390657	10.82524792845822	21.57069423821832

C]	2.76272110204788	18.94082831316061	2.46514718203356
C]	2.67876830874290	9.77459697325273	8.75041968077133
C]	2.75982385143181	0.90958323823570	15.04023703698013
C]	2.80684157912720	20.07554038833148	21.24716262630106
O	1.44566775436808	17.09900690228287	0.85516397487312
O	1.04930431747156	8.55425344594223	6.84298190302945
O	1.08568647378342	-0.35456639131596	13.18460568521520
O	1.35380585818682	18.48968137008065	19.46292255184168
O	1.09891272362404	19.82028420714447	4.51497849536645
O	1.16547024023885	11.08507901754109	10.64118236022873
O	1.23522131463640	2.33220325783538	16.86869748700070
O	1.09688524780289	21.78574769418245	22.58398324813122
N	9.42166642146714	8.62507961765764	7.56725810800921
N	9.46465980352455	27.68381942573253	13.84494004933442
N	9.42037968238220	18.63985670336807	20.32477699245623
N	9.14797785165695	8.70595965959160	26.69441661829024
H	8.27355100455131	7.66851609098054	6.27661954296691
H	9.19237815938086	25.85917194414450	13.16913137182286
H	9.14315063319805	17.04971206594523	19.20975692364415
H	7.72083631081416	7.67230952342440	25.81461696611671
H	11.33849170097330	8.31890886295892	7.19005065098695
H	11.33772880152911	28.17170747293262	13.44262518078944
H	11.35519104633370	19.04937225803905	20.31092865233417
H	10.15928802918888	9.63450362741887	25.28465734337326
C]	9.71002326844722	1.66891946965151	7.60885747311929
C]	9.64749489170557	20.57883781415479	14.02907282000436
C]	9.61740148693493	11.75844943812535	20.45782157858564
C]	9.43645207141637	1.33642044964647	27.02789218261627
O	7.97709813999420	2.79468538670486	9.50862672712814
O	7.96154654058281	21.88137150217581	15.83360131539512
O	7.93743825371854	13.10321899069959	22.22361826810551
O	8.25733201434380	2.31375156754955	29.34826939641143
O	8.21993763190227	0.22486397481121	5.76804613597317
O	8.15363954066935	19.14572519418102	12.19057576619284
O	8.16586099478341	10.28232378483219	18.63765435607077
O	7.77633405221463	-0.57166590855768	25.86189080650410
N	2.18002546681098	12.05906720992906	2.69691848188713
N	2.51438673632315	2.86414802086560	8.77740956376045
N	2.52633587145397	21.80957479924795	15.08802011509450
N	2.55158000088238	12.73656055749406	21.57684159289197
H	0.32347960287484	11.96493038018031	3.31914154304696
H	1.90517201501528	4.31370388484613	9.94539889585132
H	1.87626816449443	23.42485423788397	15.99435987276268
H	1.42850875202504	13.79300801893111	22.81287480946071
H	3.25767415114846	12.18931929485124	4.36534194189452
H	4.46906542975414	2.65767594162617	9.02064605500203
H	4.44492888770485	21.59428551113260	15.51816475351512
H	4.47950714547286	12.89662714439781	22.01291779249085
C]	11.07994734530620	15.66294791204187	7.62761001725285
C]	11.13506516671787	6.65873406693575	14.07288551738971
C]	11.08834489892209	25.78776229492156	20.24050844670274
C]	11.25337225122998	16.65995492638853	26.42700186740543
O	12.78239561899138	16.81299458370402	9.53920931396239
O	12.79638580006666	7.96332970127216	15.89629479183913
O	12.72313873611732	26.86474750964464	22.22655694907714
O	12.38658410873502	18.28093154725098	28.37138171408193
O	12.60778903897575	14.24051239585240	5.80070104749870
O	12.65640538048658	5.30929943629387	12.18975585371145
O	12.60259076712303	24.67006260391287	18.22706770463215
O	12.95706394958760	16.43024307463242	24.23402778553668
N	4.75399900384372	26.05812212728039	2.61443546842928
N	4.44885678928031	16.80938278417639	8.76861962930169
N	4.40553956863631	7.71318302016342	15.29563346986068
N	4.56303584077170	26.85857979317200	21.57862929648292
H	6.61302046191593	25.96413721261482	3.22905041473112
H	5.09681949062497	18.24719156632283	9.93034985965424
H	4.83847268881670	9.44148929324981	16.12030815745779
H	5.51665882131748	27.36345562785902	23.23937319864644
H	3.68413690954811	26.19642098918596	4.28808474682712
H	2.49707425798314	16.61284365724995	9.05005470617292

H	2.54089471647368	7.27484947278837	15.78512696979505
H	2.60180153812474	27.10736388536859	21.74090135062181
C]	4.17891135307371	4.98863172321630	2.47015651339912
C]	4.28493445621374	23.76144376850780	8.63779304496081
C]	4.31787802151513	14.78642321760391	15.04839580291314
C]	4.06719236027993	5.83681754611191	21.50997254358710
O	5.50518250322204	3.17041511380218	0.84162264532651
O	5.92208720451572	22.57800411876694	6.71529373048353
O	5.91327940836563	13.50090074022515	13.15102161614099
O	5.89142984121870	4.70852909034608	19.70075638412205
O	5.84378457894090	5.87128514718722	4.51718473927902
O	5.78965935885310	25.02003217973800	10.57149789489763
O	5.90764541291165	16.10599194193417	16.88822839231761
O	5.42195497357574	7.47220526375699	23.30539069389570
N	11.33430460834199	22.61404890416343	7.48920650987338
N	11.31614667409256	13.70806979014373	13.82513860893573
N	11.34472723593712	4.73179020353988	20.40008123494195
N	11.64825498944181	23.07716385317929	26.12230690566238
H	12.47527721010468	21.66094382762864	6.18993886952926
H	11.90017498009761	12.04548495269404	12.96513202567415
H	12.12283159416811	3.48692909169398	19.09902286744507
H	13.28567364110685	22.58099350675968	25.11457446345495
H	9.41301389277439	22.35529969462548	7.09287919887120
H	9.41861864849604	13.99772935573287	13.34731484623487
H	9.46136209537616	5.07324256640116	19.90074909136658
H	10.19433062668087	23.21443569050990	24.79593139727853
O	17.42802652453150	21.11259920303431	0.91406975041262
O	18.22202935085276	11.58060502782332	7.43090185621425
O	18.22117115818926	2.73718272336455	13.71730458880902
O	18.71262832167299	21.64145879352369	19.99412013794907
H	22.90354346831596	7.92466113319633	9.43721869173131
H	22.95544288582580	27.63733830466760	15.76600385225811
H	23.13069238846368	18.34252871798084	22.31407822938697
H	22.25352115257795	6.82582765334761	27.51180127539990
O	25.25416709611638	-0.12771268985267	8.91068604574156
O	25.20086601204785	18.78840367855085	15.37811354479440
O	24.92424834784665	9.92547283179414	22.09559144718936
O	24.61407148714651	0.22300000565330	28.28169311065880
H	16.20105737932129	13.73237865442863	1.62968642337460
H	15.93507347992545	3.35881507692470	6.84822926240799
H	16.14926741285889	21.83384420605136	13.28615476726799
H	15.98072455012834	13.46280158064584	19.68224927383816
O	23.38699484675541	17.58675617177579	6.50301544504834
O	23.34718669067825	8.53666899821832	12.83603568591166
O	23.20311479293960	27.68637860812429	19.13543210920148
O	23.37002928622715	18.22052648946008	25.77753064115889
H	18.04123365132639	24.32694191712914	1.76959924556146
H	19.15226286800633	15.13048810604601	9.25260895418741
H	19.23981253011283	6.30905832651552	16.03480138377871
H	18.73253742165875	24.94236689831391	21.37061161213558
O	15.76112981772419	3.75221981120129	3.57940683450157
O	16.44347990504961	21.75779431921069	9.90383822288365
O	16.44743514529292	12.98107112665555	16.37408750067058
O	16.28527870459837	3.75658754464262	22.66204739026906
H	25.52083781647235	24.52644106948379	7.55374502041954
H	26.37918446430573	14.91695154080131	13.24239233848730
H	25.87427232609012	6.40622968414497	20.05727289532023
H	25.36897352723263	25.02393808301164	27.33084573149952
O	23.10628177943448	13.83662142957877	9.04009548855652
O	23.24125684930195	4.81064381845069	15.42133218409563
O	23.60192821440375	23.90849593442092	21.61230042146025
O	24.04685092875130	13.92090418985216	27.15345380289003
H	18.34320561031991	27.69848819612093	1.61597235018345
H	18.63391814831343	17.30114658218006	6.89676586125579
H	18.48624755818755	7.99952015431727	13.38347990136086
H	18.55765435581377	27.69480944737615	19.80530518530032
O	17.21333107718175	7.16145358616415	0.90610179012645
O	16.34520558420087	25.55904569766480	7.43849232669942
O	16.37265161873067	16.71421960448490	13.79585069614642
O	16.16968836973204	7.57628781280843	20.21796364931443

H	25.44037007687406	21.88581956409525	9.30540638655938
H	25.22422228995958	13.54131855407557	15.95349382910350
H	25.33900522044174	4.17000527037813	22.33313434479443
H	24.31976185736379	21.94229471531127	27.28165021160809
O	18.82054701286846	17.70389488208852	3.61864074816277
O	18.09173441072153	7.83771568078268	9.97882758786407
O	18.00833175448605	-0.96398329820140	16.32327664666696
O	18.27869926669185	17.90303941032829	22.54037553122837
H	22.82657650305602	10.55621747118517	7.67861860463927
H	22.20825159918243	28.97160834613931	12.89705265402937
H	22.54953167382317	20.34725630327541	19.84492948236387
H	22.16847839736941	9.89903909520361	28.78537999013921
O	24.96322776831114	3.64219809671365	6.40195109475414
O	25.01454123844140	22.43694246403855	12.68645147407395
O	24.98127206765949	13.56131235725543	19.37157407346159
O	25.35435339272551	3.88648568197185	25.66951022411640
H	16.54035639737342	10.36209018470453	1.76157931780686
H	15.37926823548691	1.22219978827554	9.23053574929195
H	15.03824498407519	20.81580079071689	16.15605998995148
H	15.64447935972983	11.06010640585205	21.70445750231087
C]	16.60145390750829	18.95521854169764	2.46733257848752
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C]	16.48803742664876	0.99976963709413	15.00807412132042
C]	16.94080687346183	20.07088043709081	21.50357425218131
O	15.29978478430727	17.11044710204289	0.84953006823626
O	14.86781013888665	8.56455679024491	6.85641897260629
O	14.84380267647006	-0.27153496988801	13.14532167680415
O	14.85923677460072	19.22028297406038	19.84406916375848
O	14.91776639448586	19.84806892405957	4.49443411103145
O	15.00957680318912	11.12385623919994	10.63553792403790
O	14.94980032121973	2.36931613722471	16.86027612850481
O	15.95569338716504	21.69991551911328	23.54045894033802
N	23.23337259821394	8.61657511688143	7.61223863157336
N	23.31978630437273	27.63252715643967	13.81980731548162
N	23.40247352730481	18.65088155644362	20.37453720597750
N	22.26255975042831	8.77851821127593	27.08881769176897
H	22.09556428048658	7.64988976354459	6.32150022663070
H	22.97440475681195	25.84253870896286	13.09062623563758
H	22.58487413683613	17.18208848082163	19.36396159900542
H	20.69666704551140	9.10410454319587	25.95685690665800
H	25.15516152873604	8.35964838378486	7.21498070604366
H	25.23708539491021	28.02424202013652	13.50921513077373
H	25.33651011488343	18.70105331074095	19.96726599020806
H	23.81289218587037	9.24603786811448	25.97817535115970
C]	23.50203537714402	1.65581372386643	7.62181945798940
C]	23.48004355330413	20.51114146164965	14.04004419949976
C]	23.32231048525720	11.66468723524252	20.61117618710575
C]	23.41156867898892	2.17529856446343	26.72142732228181
O	21.78268334075432	2.77757333082795	9.54076642372295
O	21.83650932271023	21.82239504709979	15.86765895739515
O	21.58939184990314	13.00904002005825	22.33256007403257
O	21.69125976276830	3.67836140762243	28.31325980638772
O	21.98768105189159	0.22940550258481	5.78675599875247
O	21.94292046032304	19.10505553086074	12.21223357905041
O	21.90248297064420	10.26867639818627	18.69363254144126
O	22.01598172828950	0.99470344953865	24.62801210448498
N	16.03432026706620	12.05560309627755	2.68456956196648
N	16.31779311687622	2.88317459229482	8.74604569989543
N	16.41590956811476	21.88462633999733	15.24578599256640
N	16.21773472260042	12.94409144272242	21.58354132585031
H	14.17549512130275	11.95376814590520	3.29828651419318
H	15.69035667928276	4.32380726021998	9.91617230467476
H	16.36755598357298	23.76054478799562	15.85693894737918
H	15.12383080688780	14.12097894144613	22.74082348672450
H	17.10571011044756	12.18338324746316	4.35718103679154
H	18.26986208152107	2.67832325367402	9.01182618161228
H	18.20570408811717	21.18649437879383	15.69616726775340
H	18.15211542930639	13.09563907811428	21.99286909465679
C]	24.85761298018467	15.60412715150129	7.72227849688043
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C]	25.02908764717349	25.83748033731463	20.17674941605781
C]	25.26536761246333	16.36971345176454	26.66856112466588
O	26.59865832415775	16.72781883901943	9.61168465911571
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O	26.75430824694161	27.16519719408899	21.91472772886084
O	26.37784347118373	17.29628593635574	29.04535165972797
O	26.33847642442731	14.15666474312956	5.87478616530022
O	26.45404003667650	5.26527114950355	12.22425234680949
O	26.42499407875106	24.65069770536687	18.10944534726362
O	27.22266310792536	16.08349736212790	24.72080213209363
N	18.52230270873184	26.03292554714074	2.68340767897634
N	18.24539282862103	16.81477973238525	8.79005204885516
N	18.21444935322978	7.83790910747965	15.33490435601351
N	18.21063997149743	26.84396450392266	21.55114342463668
H	20.38027888936444	25.95968893715632	3.30571269566849
H	18.91049335792750	18.22708459878371	9.97336588063063
H	18.79226120294597	9.48817824261453	16.22480050684752
H	19.27935171202199	27.75268120824375	22.94046673447563
H	17.44439618071323	26.15972000206174	4.35194449798480
H	16.28942032852939	16.64780135123688	9.05528038472363
H	16.28780820128243	7.57764816995403	15.71194465353193
H	16.27224093226200	26.97089301601497	21.92455935027956
C]	18.00521693025258	4.99664262941839	2.46672731999668
C]	18.04222291350419	23.72662090459017	8.73129687125975
C]	18.03753015094882	14.91744332123835	15.10046681889348
C]	17.84304550591958	5.69465034490862	21.46750833397756
O	19.32308274867229	3.14946088377546	0.86673340355420
O	19.68407045014796	22.53862563538800	6.81529472054884
O	19.68330623356466	13.61833001860631	13.26002901068241
O	19.50882554332402	4.51908707176700	19.54013683500824
O	19.65908428723288	5.87666587965621	4.52382823020843
O	19.54136117533654	25.00883974008051	10.65482210104275
O	19.57900762456643	16.23364314576791	16.99327449571265
O	19.42604619246389	6.99869302837332	23.33055563057139
N	25.10666672118148	22.58889441011430	7.48460865314346
N	25.06943087353375	13.64539895261869	13.98080072990173
N	25.03667231053027	4.66585028721724	20.42910142645168
N	25.64157282677903	23.20571442491907	26.57786041038636
H	26.23826922177806	21.61825082509770	6.18916553690713
H	25.33903056733826	11.85498294704720	13.21441641530342
H	25.85029711562930	3.31795571722682	19.26254637003351
H	27.51574888492912	22.40256447755554	26.94729453190579
H	23.18228126538967	22.33947080058195	7.09981737369254
H	23.24224630990099	14.21103664050682	13.48562237253472
H	23.09621831885584	4.74053336538732	20.05410754169990
H	25.32266130988874	23.32158561088209	24.63123517412062
C	10.46113358251217	-20.23302995760830	32.80314042956893
C	10.70093638847231	-17.44991050737062	32.33202382456036
H	11.72068597516407	-20.74643667553795	34.39547078280945
H	8.48555466742711	-20.64595942346654	33.36357638173635
H	12.46681024495849	-17.08454201444610	31.25941301401183
O	11.16321636011012	-21.63554692896083	30.62721568167727
H	10.22845587930220	-23.27606076115627	30.57855742793071
H	10.84446599906377	-16.46949315301089	34.17640648141079
O	8.56684727247895	-16.52198749031994	30.98400390147716
H	9.08432934164443	-14.89269240276966	30.19630863325152
O	2.33451244268889	20.78097264501474	27.73277920795904
H	3.15426335438102	20.05218115488809	26.21036485118418
H	1.45401629037801	19.30967468639146	28.50338542583361
O	21.78905370956689	11.90421517108915	31.06203346918582
H	22.75207753523312	11.68501764210894	32.62966414199180
H	22.65744069151060	13.27608383282253	30.10129299770670

Ethylene Glycol adsorbed (100) surface of NH₄ClO₄:

O	0.87971318208550	4.29236900728606	7.53970125993944
H	4.06803556741526	9.43592442208775	8.73014766833190
O	10.98560813911754	10.03937157831968	3.59604426487521
H	7.72727672232555	-0.05106072304049	3.50957731757257
O	6.02662949747722	9.55659279120264	11.37432723888570
H	9.67137930460553	6.27251579292689	12.16820826668902

O	5.02893571886222	4.25807354136347	16.19376719009684
H	1.56274183793706	13.82300486625567	15.51550057038095
O	10.49715603701504	9.96882642966604	11.91767854565365
H	7.44299351259969	4.48935566671232	10.63992836442835
O	0.61592021226172	3.27205225331295	15.90870331750121
H	4.39219631640267	12.60982078557794	14.55448869832548
O	5.36532732524089	3.69021791593751	7.96605968467000
H	2.05137046124663	7.51465852429335	7.10099652500001
O	6.48896247404311	10.45107003689585	3.34845166767714
H	10.56512960289408	1.05949253021007	4.60176721767475
C	2.88210737891436	2.40606520276100	8.01567220853570
O	2.81448226719441	0.52472752479310	5.94977770724514
O	2.46962462541480	1.18056434451429	10.45787552648705
N	2.87223104846525	9.31145051305373	7.15362774273121
H	3.93514745249872	9.67556013279474	5.51907686006497
H	1.44681221219362	10.64427528442614	7.27981564658869
C	8.58834872750722	8.64640420376924	3.89825779322846
O	8.33620678662831	7.70575710702922	6.48704508988655
O	8.46597061167321	6.54132586467006	2.09921938686782
N	8.67064082382438	1.52974372380134	4.26773957930994
H	7.82960487231927	1.97773245642573	5.99641993124168
H	8.56333334942624	3.16506772933012	3.14982178178108
C	8.12627780871171	11.39552181561935	11.42798541316171
O	7.68658199367795	13.14505303522795	13.55581010027879
O	8.32407913851909	12.78509027962850	9.05674473160816
N	8.49815579775530	4.69579337561299	12.29213417215434
H	7.23957818442018	4.84462257005418	13.82710333262144
H	9.60482854943080	3.10272458921241	12.60386126779139
C	2.50792292244343	5.31075524539576	15.61344537401609
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O	41.54680710222300	21.43296523645383	6.01925268131747
O	41.17367667262364	20.29784431903582	1.63723279332119
N	41.84652459905214	15.42624635263299	3.90934064766797
H	40.88355592504287	15.97329833841741	5.54523381980833
H	41.74155162427868	16.97434252397326	2.67110335470252
C ¹	41.62128039622677	25.29342204431907	10.86336282189724
O	41.42384337727039	27.05032213756851	13.02699415490400
O	41.85165107454019	26.70824558682979	8.50490363747161
N	41.73099708057194	18.55573470965503	11.78592186268049
H	40.62780234715278	18.36098216193251	13.42312296718428
H	43.04490487329203	17.10280653113870	11.79663455000772
C ¹	36.02215146450143	19.09273574673749	15.30774351139159
O	36.10737660662691	20.05292766473760	12.71464488016837
O	36.16382932679383	21.19088878760914	17.11617920262865
N	36.24606258837781	26.03870087899107	14.72028109869617
H	35.32759785845260	25.43482574703498	13.07681248695224
H	36.24211353698756	24.48789187162782	15.95920521262175
C	18.87905418091750	-6.77062600746449	19.39290223304529
C	17.40086606163426	-4.80120639201192	20.79543524250345
H	20.67615943524679	-7.15760079175352	20.39404847892970
H	17.80449782173424	-8.56001897578315	19.29140470461091
H	18.42166463340828	-2.98037719276629	20.76187769195597
O	19.39446005901205	-5.96552879181546	16.86908621311324
H	21.24744960011041	-5.64713178687777	16.81994682564664
H	17.19250844768238	-5.38533797910860	22.79846399046782
O	14.99842829588458	-4.33847367600963	19.71562814700107
H	14.11759644128651	-6.00751106646107	19.49733738609440
O	27.75832830327923	13.93376841730010	18.57979618233401
H	28.04732738313152	15.68157690210192	17.92346882939502
H	26.78010052922710	14.17497300887168	20.13739907448032
O	11.87123678002500	12.20206560905816	19.29109010867480
H	10.95029482701979	13.61978995298034	18.46919397799585
H	10.63225741617670	10.87662597053017	19.67136525449179

Ethylene Glycol adsorbed (101) surface of NH₄ClO₄:

O	20.22517858208568	0.42845709409374	9.46969534728119
O	11.24229787410187	0.84379030481106	19.28560629542515
H	16.84648773427489	4.56837442100974	12.43700488925136
H	7.01206655401949	4.85348562368589	20.84715903453641
O	11.30601297617331	10.81203421884017	10.95857633066461
O	2.49617130526665	10.61990843011564	21.46840043777637
H	17.37629686489893	7.39722268289336	4.19976482668290
H	9.73060781135210	6.69059578859702	14.60728337169731
O	6.08526411999449	5.85838357119214	4.33573996607187
O	19.10047688319688	6.35244704872691	14.27696166011841
H	8.85369099307403	9.39964940568828	3.19567717295206
H	0.53339534892911	9.64021436087134	11.03982365787850
O	15.14072423279041	5.31290783242474	2.46838053555877
O	6.14768361638600	5.21918249998834	12.94388834062769
H	8.97999889643018	1.60667164920927	9.49951148576559
H	21.96206026414167	1.90649770135566	19.57989844335149
O	6.17020584099575	10.37051914178917	4.60288507571536
O	19.22838006500185	10.84542193403163	14.86755587434681

H	10.68546295380262	6.73020422707893	2.95372895903249
H	0.71201202604774	6.68997692407808	12.35110209133745
O	15.08042523587828	0.75769712265924	2.79213154845859
O	6.07867602638643	0.67357307103445	13.18364974268843
H	7.31332634326663	4.38030796809211	9.31559276815327
H	20.31643476624183	4.60412785410146	18.66983130294696
O	20.51730949559629	4.92821228271987	8.97623158756027
O	11.63218573546327	5.34942805968620	19.28711332744339
H	16.79285754873252	1.37768185424662	12.26354575471828
H	8.67690737297336	2.07376886344177	20.74564357638056
O	11.50761626486883	6.26998291174333	10.83418559603625
O	2.47662663329492	6.07579048829289	21.08034390622326
H	19.12638097490800	10.07616298505952	5.04454543491086
H	9.19641443674959	9.84976155741890	14.34000704514088
C]	21.43737226297047	2.46174740599770	7.97084764595838
C]	12.46161911249108	3.03207252741353	18.00404369567761
O	20.63690416201120	2.23146370043946	5.32306944915777
O	11.56017572402988	3.07708964741382	15.33296684816345
O	24.17404982285757	2.32294093341935	8.22904397832394
O	15.19313703975553	2.75969647444236	18.04710250572264
N	15.72851788612965	3.00871278941327	11.94142550554447
N	7.21345502998747	3.08250877155876	21.69719179637809
H	15.20824401495560	3.10917173192826	10.05607698025230
H	5.51034376667832	2.07098830908309	21.54295845387150
H	14.10616726240925	2.97720521376617	13.08046062591326
H	7.69553556141159	3.32773486473050	23.56978792632466
C]	12.43124210707223	8.60224104155620	9.65580622278755
C]	3.37062115978786	8.41287020329107	19.93388540306355
O	15.21421717656478	8.74254419423309	9.91928682277260
O	6.20060140163542	8.43572763885924	20.00291909396035
O	11.75826273885338	8.65992205346875	6.96920091366867
O	2.47542817843508	8.71628807867022	17.35364818548607
N	18.30601038989414	8.37446019699229	5.64206087878643
N	9.61336381872777	8.39108251900556	15.59771783543329
H	19.66629070111876	7.19894228105713	6.47429589762674
H	11.32193494300794	8.74613916008040	16.50372265237390
H	16.99503631194543	8.77277977821792	7.07899901119476
H	8.20244407433579	8.25917647207947	16.96883036294200
C]	5.01549346198716	8.02750552424205	5.68314252696840
C]	18.13577955764833	8.46694200460078	15.83919864071365
O	5.73683512827495	7.89446735751229	8.39402711481996
O	18.98105465051141	8.05683130336345	18.47108279516258
O	2.28120771144894	8.14132630255740	5.44480214982077
O	15.37934654384780	8.55756870775660	15.69538951317213
N	10.42036633184507	8.55808231830984	2.24025450417223
N	1.74418801521073	8.29769922510805	11.87629973236935
H	12.05226117042756	9.65102061798765	2.53333548316136
H	2.57508366798323	9.05854814827184	13.47520099404855
H	10.03495939663016	8.44701634683472	0.33322447074662
H	3.18546026283262	7.84201849835216	10.59242979403073
C]	14.20309420664115	3.12130476008775	3.90978985635486
C]	5.09052949375423	3.01791268294731	14.29055363621490
O	11.36091858512060	3.17369520970309	3.75974078511848
O	2.29858595792727	3.05157440275771	14.02928457893448
O	14.98470549026901	3.33116492929669	6.54964548598055
O	5.75139121429452	3.17387003204636	16.98102560655471
N	8.06942235578222	2.87900394028079	8.28646872447667
N	21.06957060593056	2.86950509774296	18.10275291809675
H	6.64989150927359	1.94442544954734	7.27362503419431
H	19.67616216930255	1.73047235275990	17.28559510371115
H	9.36957969808325	3.55630725509693	6.97561510711980
H	22.43170459108516	3.18823073550241	16.69481814162810
O	42.02416846594861	0.34298953223176	9.35057173100773
O	32.98658451600879	0.31081708290375	19.53639168506687
H	38.69539785177763	4.02189774344682	11.65324987763060
H	28.79730584573390	4.68005072866981	20.60483430969397
O	33.45781845222273	10.30156005161060	10.85332938528728
O	24.32822914754287	10.62524897755858	19.08729413296193
H	40.74190435639977	6.21775214776501	4.93313049338141
H	30.67608100027424	6.77342788738249	14.25723262268648

O	28.17204155950398	6.05980182735413	4.43746808266748
O	41.01647681158986	5.70549110275480	14.46218248406853
H	32.62985201100425	9.91794480919850	3.01610120849142
H	22.63691807682055	9.88404198868044	11.62833473251301
O	36.56412584689484	4.81728434439981	2.75639151730455
O	28.05472561366772	4.76116482074326	12.83038983620570
H	30.11891156632553	1.11785900814911	9.36751558992117
H	43.93057989185803	1.66721791300541	19.72941602344603
O	27.94358520588052	10.56566843751163	4.68023701409176
O	40.71441710694319	10.20983100695537	14.93177492480181
H	30.78829943634451	7.23765085274530	3.08364662857095
H	22.58078943145599	6.72206359873727	11.17763575279043
O	37.10464477923432	0.29316375655231	2.72021119319147
O	28.05979896517494	0.21059262138580	12.69452203137089
H	29.67211001634464	4.28492817665382	9.13563445540576
H	42.05677220747013	4.25890163257953	18.94387429845080
O	42.09957648274448	4.88558070762635	9.37192846136072
O	33.56216408705558	4.78095593756813	19.17883752714318
H	38.83546742485684	1.01418395963925	12.78328895300190
H	30.35757070625537	1.82330132006509	20.69618552250776
O	33.25548275292433	5.75721991579007	10.90550544169428
O	24.06923597436218	6.66315273605505	21.37200361463487
H	39.34193473586372	9.12300076320671	4.27292290720846
H	32.13113794771149	9.65693803078642	14.64631174173761
C]	43.09778169494823	2.62004904917194	8.08948511884783
C]	34.38005728080382	2.32172084497483	18.15964132973959
O	42.22634349128325	2.62530445311459	5.43418400360184
O	33.66446487570473	2.16675219302547	15.44509216986863
O	45.84642211126754	2.55406781209785	8.24417046872571
O	37.09238801747734	1.98752731322269	18.43793088566617
N	37.64962383561511	2.38986620207644	11.99353620010425
N	28.91810088130122	2.93727068603386	21.54613739840212
H	36.89064882156864	1.71818913483717	10.31810472666712
H	27.17669838664942	1.96815738611546	21.41905486229227
H	36.16243572747597	2.74790835720547	13.25662694996766
H	29.37715309678260	3.25373905916509	23.41313851983438
C]	34.39776656761501	7.94818253726659	9.65328337038055
C]	25.21343782138548	8.02335083096515	19.22646602377080
O	37.17938063556534	7.85263657276150	9.95664214268541
O	28.01352568941731	8.02100859858117	19.64756362104473
O	33.76530099054674	7.96633993483379	6.95665940419972
O	24.63847544622948	6.68824487859068	16.87074128249667
N	40.21143953805352	7.98291890464002	5.63033517164455
N	31.46921963216183	8.03773877104384	15.55254152868368
H	41.77623778162897	8.92497912912768	6.37062923950088
H	32.94185343629314	7.14585531807637	16.51867678652499
H	38.94815186172034	7.72168026817076	7.14553105430140
H	30.10631902480257	8.52592231093864	16.89328468715683
C]	27.01092609863387	8.20786592346580	5.83803323527401
C]	39.77255709326929	7.73295533421335	15.92047685172160
O	27.88191746332852	8.08503735172565	8.50313720085846
O	40.50451669601642	7.52784455131340	18.59387146344587
O	24.27548552134286	8.03542896824989	5.72413774663631
O	37.04333747737422	7.60343616445094	15.59935187594439
N	32.39059966903623	8.10983682859685	2.22831986702024
N	23.68930111530797	8.22597965324171	11.82380311983004
H	34.00489037083832	6.99678024003070	2.57667713040525
H	24.17308808454077	7.93217209723424	13.71117246343822
H	32.10513977598523	8.27874562734288	0.30852118471463
H	25.32879547049459	8.32126128285644	10.71463746790662
C]	35.91384931197041	2.41691861799276	4.02937132681225
C]	27.08496072484306	2.43571184415034	14.04794984606695
O	33.10730301955778	2.08082524063223	3.88136561454509
O	24.29621507427167	2.43999762394908	13.89377858484302
O	36.69881569661881	2.52259501686009	6.67020101198961
O	27.90110292482006	2.34547636532499	16.69316739593805
N	29.75426904570698	2.60078929309780	8.11975399035835
N	42.89765815440516	2.58298534234611	18.32067772220096
H	28.03695809305626	2.27001333671189	7.22376220854445
H	41.53686432522389	1.36052577530990	17.56238699499189

H	31.16163700449362	2.68027912210312	6.73704472951578
H	44.13591919933828	3.01346204155170	16.82383080998695
O	20.21710909815317	11.49905387422251	9.45257429441820
O	11.94866395217789	11.48124483254863	19.51050137134893
H	16.92499974717354	15.33251522818601	12.72261928820008
H	8.96171999136286	14.84375023468036	21.34521328483483
O	11.42697329285670	21.98112011553767	11.03351083500590
O	2.87689509285270	22.04493952860148	21.39315951623365
H	17.44060931317793	18.46009305319843	4.18814135372437
H	8.81266366317980	18.21706455088334	14.43340275831848
O	6.36728112857728	17.47087210732923	4.26965427816568
O	18.95146339888452	17.38831086109954	14.29674703406559
H	10.59605528084468	21.74900491009580	3.08341218347871
H	0.51191819199936	20.83392240443020	11.17254040676084
O	14.75537065777210	16.59121764092416	2.58573954636370
O	6.20862530159434	16.32201961218697	12.90595470782885
H	8.84576733363741	12.70071554827432	9.31903148010621
H	20.82034957125935	13.60679341068858	20.18930793684133
O	5.86619200079884	21.93185713431331	4.74122248614414
O	18.75152832261763	21.89430559657804	14.65694267951268
H	8.96880378469994	18.92817899103678	3.04453433201398
H	0.79929829623721	17.83074124589645	12.30008559355746
O	14.64234517258618	12.02398931613251	2.60244382390928
O	6.04570338197943	11.77234725694654	13.03234447978991
H	7.37876699772650	15.58098631181644	9.24884544744647
H	20.04392607906312	16.27257027184134	18.47653015559528
O	20.51999736455771	16.00073407960901	8.95132382749238
O	11.66223729413859	16.00828560661819	19.49982885015048
H	16.90666302971488	12.39149901048611	11.41370259098845
H	7.10920434444378	12.43406423729538	20.43057987636228
O	11.47691754302583	17.43411272010884	10.78370601291207
O	2.95670618096844	17.47954974481301	21.25552399355139
H	19.18904145673388	21.13716388899338	4.96623188293958
H	10.00183624498593	21.20311150217053	14.56220541952333
C]	21.40582649973785	13.53667359970143	7.92497986952238
C]	12.78552788917644	13.81068914315386	18.17652728555483
O	20.51405592011182	13.30901229921219	5.29568654281890
O	11.82639282696790	13.74112464519608	15.55848414287005
O	24.13999248699317	13.36092415678910	8.08746646426823
O	15.53446577862344	13.98129911493158	18.18962853946091
N	15.78204131159459	13.93460160132807	11.89149753536590
N	7.21484100048097	13.96146516557436	21.66311724510870
H	14.93180303069846	14.65718601576635	10.28024651472765
H	5.75457993059893	15.21839128110843	21.21606235655377
H	14.35860990217835	13.40202643322145	13.15507553599283
H	6.89777707260254	13.24455110681044	23.51947678771808
C]	12.43014809926505	19.76730165909102	9.63145915390958
C]	3.78743491423233	19.79482726242904	19.96177870742124
O	15.21897202418226	19.81616481773104	9.79112990366138
O	6.58070040985975	19.86952101188255	19.96780859482923
O	11.64441446124346	19.93991783593263	6.98073405204924
O	2.78580442980785	19.87236861939331	17.39560727886130
N	18.39597447381232	19.44453540704138	5.60454785177986
N	9.63098122138558	19.57763430767907	15.61108460908801
H	19.77674700159253	18.27870541964012	6.42196749716872
H	11.31248940208519	18.89153575016348	16.36043670495872
H	17.09387031298060	19.85775093964043	7.04851595434578
H	8.39936040571459	19.98249633428847	17.10232613819128
C]	5.02198559341286	19.46511710023927	5.72146456273661
C]	17.73344829761894	19.49393229614868	15.68732827978389
O	5.76184023947390	19.23887861045433	8.41812369294116
O	18.42044250594927	19.31871958080928	18.37144307537893
O	2.30338647644575	19.17467380286513	5.46015337401223
O	15.00244246156792	19.40604853991191	15.33834960452911
N	10.47855390374267	19.97524328763101	2.22005435234816
N	1.77504312889810	19.50160848272115	11.93941448545841
H	12.17940815186745	18.98714827460215	2.49296464790241
H	2.55890212458862	20.20048598434466	13.59251422812783
H	10.15311623846671	20.21308343159664	0.31341610639141
H	3.23656180584714	19.17585481177339	10.63909714004638

C]	13.77960399877447	14.31583943410437	3.92559280823814
C]	5.12890629945472	14.10805459992042	14.22787348234007
O	10.98998417223601	14.40824018380045	3.83216233165875
O	2.34390066632854	14.21115023950310	14.02633055905589
O	14.69608531940204	14.31750847234331	6.52495341547312
O	5.86895514889017	14.17293825382550	16.89704168946045
N	7.89529044851302	14.00968693038056	8.18062619978570
N	21.03739640671616	14.56534664701022	18.44611150628182
H	6.28620403734136	13.17542737235350	7.41230370837428
H	20.34380181777851	13.39441236761589	17.01125589930639
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