

Supporting Information

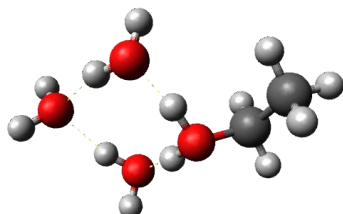
Single-Ion Solvation Free Energy: A New Cluster-Continuum Approach Based on the Cluster Expansion Method

Virginia C. Rufino and Josefredo R. Pliego Jr.*

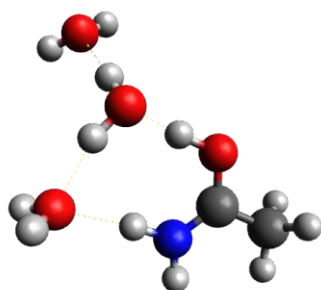
Departamento de Ciências Naturais, Universidade Federal de São João del-Rei
36301-160, São João del-Rei, MG, Brazil.

Coordinates of the optimized structures, obtained with the X3LYP functional and the def2-SVP basis set (ma-def2-SVP basis set for O, N, and the ions F⁻, Cl⁻, Br⁻, I⁻, PH₂⁻). Solvent effect obtained with the continuum SMD method in water.

CLUSTERS - Cations

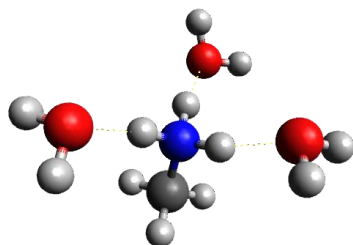


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C	-9.11224761698594	2.30979139517344	0.01462146055328
H	-11.24083213201882	2.23907629663645	0.11777444025749
H	-10.62361874052087	3.33306238889805	-1.15369517585672
H	-10.56937390615064	3.82120453937888	0.56784375711131
O	-8.05186096017892	3.25647066351774	-0.34686203443313
H	-8.99041390182912	1.46359203802680	-0.67301401476265
H	-8.92538262901344	1.96492836063248	1.04196873211918
H	-7.09518859053708	2.85925308311116	-0.17031866486565
H	-8.08524201392637	4.13593862067384	0.21295824505484
O	-7.89823339424070	5.39911821656948	0.96802371508140
H	-6.92581820491746	5.41388756290051	1.14291777243337
H	-8.32122884278116	5.45011811560443	1.83932836951159
O	-5.75566952513579	2.46132407246860	0.24901704370522
H	-5.17105864428694	2.18049178491198	-0.47269796819437
H	-5.35875784694664	3.28740949447630	0.61963004815790
O	-5.18248062185888	4.95049397916536	1.28683144823654
H	-4.52725142645054	5.48896896775649	0.81535271005665
H	-4.87495584368081	4.94210976604484	2.20798400353884

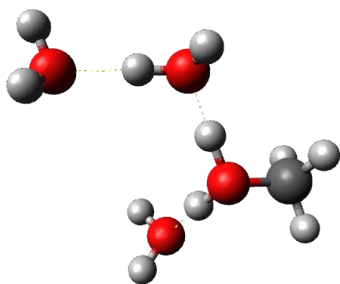
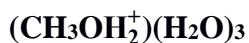


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H	-9.86168771226592	1.22447432932158	0.03426610811897

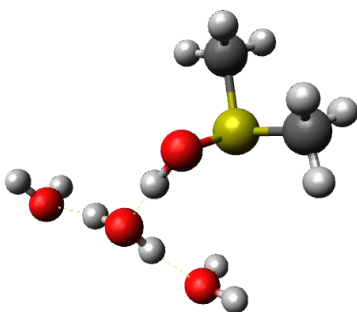
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O	-10.29900241794470	3.57379583809300	-1.13384461646640
N	-9.12709465863161	4.17054180104093	0.73063227572694
H	-8.82674846759667	3.92149490599104	1.66946310260035
H	-8.78720630940416	5.06620089275601	0.35218101289056
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H	-7.05136272495670	6.72373288841774	-0.43573231624646
H	-8.24864947135372	7.51521165683132	0.12426675626809
O	-9.55479694252001	5.66458119656779	-2.24880792322504
H	-10.28973876732599	6.28862472226865	-2.48554451755237
H	-8.95629612454266	6.17347034763486	-1.65288515190874
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H	-5.24292308601871	4.20783137920904	-0.52154694437351
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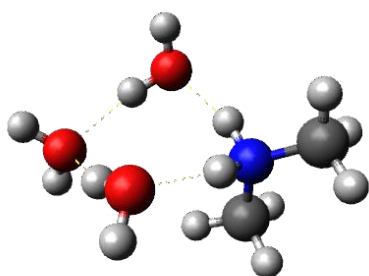


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H	-10.43466318998621	1.89404140413423	0.04741896492864
H	-10.52671384875948	3.52226988227801	-0.72297697833036
H	-10.46237351165375	3.36849660310225	1.07248521028221
H	-8.27104975841880	2.48703875616629	-0.75748223863165
H	-8.34106225660324	3.94966035234088	0.16574021549733
O	-7.78168650206171	1.83361695782051	-1.89129776779279
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O	-8.00323385310223	5.40740140737901	0.28761073566291
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H	-7.59883738030830	5.78115200963841	-0.51264525238904
O	-5.23002493095639	2.50995025300064	-2.23711707837543
H	-4.89560538892408	2.21317407302553	-3.09750294870583
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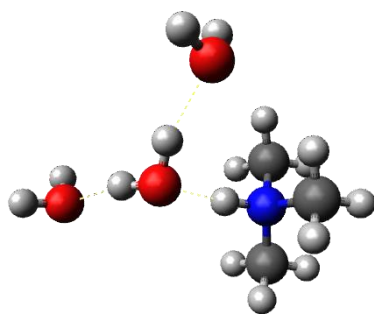


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C	0.11694237224113	8.00396785387464	2.80487491925589
C	1.88696222828755	6.62539834144446	4.41874396032025
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H	0.74137032547024	8.90074624199156	2.93837927220861
H	-0.58320128404169	7.87864484791568	3.64241752175852
H	2.55217056089097	5.75852991286861	4.52662697422792
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H	2.45897929699858	7.55907668527234	4.52924281766453

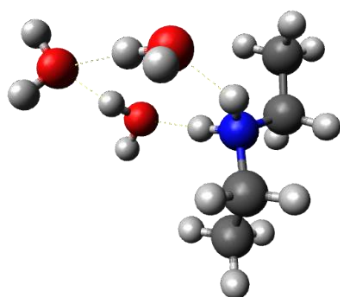
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O	3.37891512758140	3.88939050740027	0.51201984301785
H	3.74312761760620	4.69434209195995	0.11190322574459
H	3.87151619428557	3.78453007380641	1.34062626837293
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H	-0.41123267127452	4.80698351714821	-2.10630216648658
H	-1.57954307703379	4.05117218819647	-1.46582744373543



C	-8.89592817688339	3.24894006525601	-0.24921195191554
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H	-9.64733211393746	3.71319494680703	0.40163687079514
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H	-6.23538816746704	3.45919074357429	1.89182881299308
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H	-7.04401807963806	2.32330950503685	-0.03770922871056
H	-8.03105661901697	2.07983228881706	1.26058121468507
O	-5.64556131162585	1.30544205091554	-0.65857391220610
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H	-5.91297210368123	0.52174045876003	-1.16141534499820
O	-7.73265582145816	0.77983253045272	2.53791416617496
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H	-7.96966099164930	0.96410102430461	3.45855374931084
O	-4.99875771888852	0.50117880076876	2.01853696918654
H	-4.32996238365133	1.01686018269749	2.49485889787229
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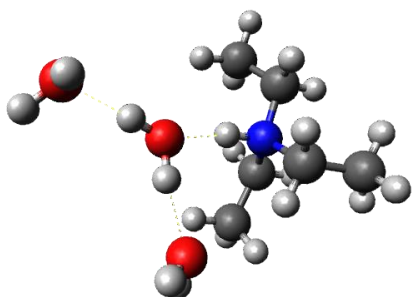
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H	-2.98113551810087	3.90515346385579	-4.44792287243892
H	-4.41313002656590	2.88469694682625	-4.07750198370321
C	-5.03933038026275	5.53378375642904	-3.93104794642688
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H	-5.84241112786805	4.93758472296501	-4.38411420600779
H	-4.35794861173259	5.89125089434738	-4.71307968471529
C	-5.11402247718635	4.26537111790664	-1.81887888954658
H	-4.48810747967961	3.70770568592396	-1.11109442525171
H	-5.93119737320873	3.62610415338997	-2.17788678414020
H	-5.52504378435177	5.15553798264130	-1.32629574709736
H	-3.48788576305669	5.28411169380696	-2.59449164722154
O	-2.07849599835933	6.10889144053203	-2.21633726288542
H	-1.67595861729844	6.26189230399936	-3.09828282332315
H	-2.17159194590300	6.97789241366042	-1.76126216121730
O	-2.52327816356348	8.31107095515418	-0.65147652024681
H	-2.98540417377694	9.06919399048541	-1.04090874749986
H	-1.71526347990679	8.69227727965119	-0.27424418182325
O	-1.21041752701804	6.02840669499279	-4.90761204668096
H	-0.31073369718690	6.36837076758972	-5.03480295017834
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N	2.16754366354546	5.35745413234231	3.34689386553791
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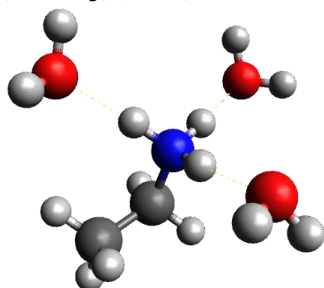
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H	1.65529836239372	5.18293992902234	5.38050563491767
H	3.22923781489681	4.48187716296161	4.93543819581691
H	0.48337248320184	3.29483526678545	4.14279892213090
H	1.56765892227890	2.68565330458113	5.41938961567553
H	2.08072744085684	2.61010027622717	3.71847955014665
C	3.08512493768360	6.54124816328722	3.29436920947470
H	1.18892415159785	5.66995357492563	3.13503391951173
C	2.59536415611798	7.72801059307729	4.10166812953852
H	3.17790608352386	6.81023475107981	2.23295286376959
H	4.06971720969239	6.19561024858466	3.64105351125203
H	1.60447380534976	8.06822513789062	3.76037515311624
H	3.29803246256585	8.56219965163748	3.95597897681333
H	2.54664314596647	7.51323718526050	5.18004434074572
H	2.40509787241446	4.74610624792029	2.54392197945589
O	-0.46370919164098	6.07764498340403	2.61732917601810
H	-0.54098274904003	5.96793518613143	1.64264011560046
H	-0.76606041910283	6.98162093058032	2.79037074441635
O	2.16990291053026	4.35369144865884	0.62440389496128
H	2.83925901327470	4.73213740483116	0.03556134241466
H	1.32280131875330	4.72716613555879	0.30177823380825
O	-0.36483360468136	5.60662260823218	-0.13669340643861
H	-0.22141176473825	6.37359413792661	-0.71263297025161
H	-1.04875963636916	5.08376597378086	-0.58404992154127

((Et)₃NH⁺)(H₂O)₃



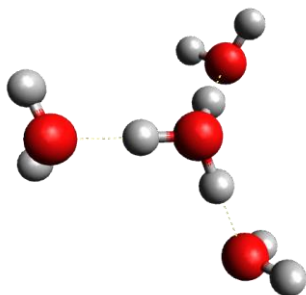
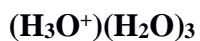
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H	3.00719183350408	4.51075741620484	4.88327776835397
H	1.30072293881688	4.49738311368784	4.42694229317567
H	2.70206696795870	6.74085142589809	6.04168401943462
H	1.56745971366358	5.51535369366730	6.64033700353255
H	0.99064077617606	6.77448990988894	5.53280357978409
C	3.72778503358471	6.66205281579308	3.32925966386547
C	1.30604749950356	6.54949275102367	2.73262244227724
C	5.00475189089885	5.90471013499735	3.64405464578448

H	3.54540998558126	7.47549818249971	4.04390395923949
H	3.80819780502484	7.11444665120546	2.33488029227205
H	5.03676512141659	5.51332520038706	4.67126918992533
H	5.84711191627348	6.60306630597953	3.52747486706796
H	5.16690402437989	5.07696627816266	2.93740450710060
C	1.46829034921288	6.89925494414847	1.26313381712387
H	1.15621698886387	7.44964120394639	3.34295001698322
H	0.43913441426032	5.89105845328877	2.87848287612962
H	2.22820613917424	7.67307224549811	1.08621044326187
H	0.51069079226075	7.29488535697884	0.89349338925366
H	1.72215240954014	6.01343918263053	0.65911134612585
H	2.67055215780438	5.00379048259470	2.66203737446693
O	2.96267294793217	3.33067053253549	1.96985938800255
H	3.52727717985308	2.89787912794255	2.64852809769166
H	2.71328242533893	2.62346737074816	1.33554986197280
O	4.49483800085896	2.45255790399890	4.08801954162193
H	5.41351402160798	2.76154043414732	4.11025101369609
H	4.55164515154752	1.51276284413894	4.31786079340489
O	2.28198969048271	1.19866862880948	0.26262924636463
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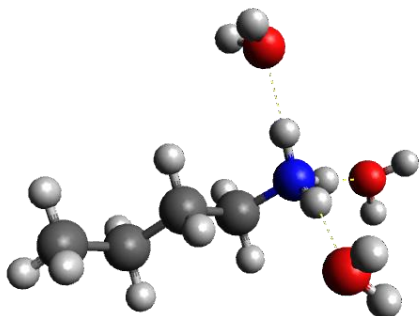
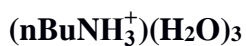


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C	1.86560748867101	4.79395603466327	4.42923576923509
C	1.05211902115066	3.58663831695879	4.00302221920051
H	1.31932665237270	5.41641191272379	5.15152358189446
H	2.81084847643861	4.48740036257906	4.89840465567065
H	0.12339923915124	3.88417599964348	3.49036395355670
H	0.77446744002019	2.99779411029962	4.88952899959997
H	1.62879804315950	2.93296401673286	3.33023688140086
H	1.36643715947427	6.17869178719905	2.92602318646497
H	2.58803969097193	5.10825410529408	2.47647660535625
H	2.91925338219427	6.38245006659355	3.53226786629795
O	-0.06516662748368	7.28743508143718	2.48638072232557
H	-0.75168845707331	6.84031425989759	1.96805638726744
H	-0.54806673612101	7.67801889307865	3.23111606552254
O	4.19107687439758	7.55048532490635	3.98738213499016

H	4.86766941009384	7.70274371863946	3.30974257426876
H	3.87473349373662	8.43780759502019	4.21759921289671
O	3.13559103505772	4.00311308862057	1.10240302387684
H	3.71192039671054	4.44305623531637	0.45870611347710
H	2.41211515082214	3.64330241232693	0.56621130607542

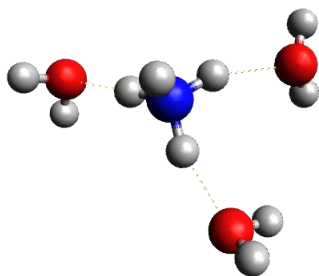


O	2.05594504392954	1.82398319337451	-1.15045797603284
H	2.85301813656348	2.40807299956268	-0.87687606316187
H	1.71238001899620	1.32175150799568	-0.32951329661765
H	1.32166371981111	2.42927619019673	-1.52670416768296
O	0.24152700987671	3.36678540740795	-2.12261962707298
H	0.11923618784739	3.16911212047029	-3.06566586815435
H	0.53598966062817	4.29191124610948	-2.10561222960314
O	4.02619779894559	3.34245391540451	-0.52980435124013
H	4.22055030348521	3.39222051130247	0.42006791507999
H	4.85857713049311	3.05276389053475	-0.93708393430138
O	1.18973340802455	0.51251069552733	0.90479869854952
H	1.90047225341046	0.09902750343769	1.42136791854108
H	0.72563932798842	1.08173081867599	1.53965298169660

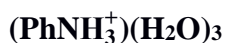


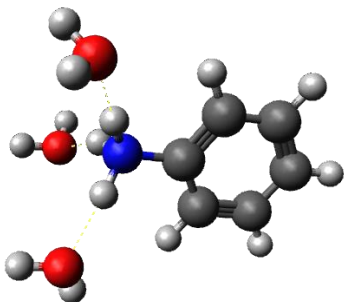
C	1.95694410517648	1.28778788857584	-1.38533055029580
N	3.19975651791617	1.55503805912197	-2.16455827985366
H	2.99948846970059	2.16099664670571	-2.98946096240267
H	3.91186563192470	2.03934643658285	-1.57993487370336
C	2.24781469411059	0.47898136883891	-0.13012102647744
H	1.26528367627038	0.75404570699425	-2.05266306175290
H	1.50338278489227	2.25824676609901	-1.13680649574191

C	0.97907206782815	0.11185601768081	0.64452628835069
H	2.92575324675304	1.05591631692743	0.52317459098523
H	2.78958137351371	-0.44192782327384	-0.40976020759017
C	1.27962148712483	-0.65713960399441	1.92908303856388
H	0.41384672478787	1.03003863614114	0.88499398362937
H	0.32115445947859	-0.49189507964460	-0.00529448994415
H	1.90011490140210	-0.05991828411761	2.61761419230869
H	1.82788331619841	-1.58992434982570	1.71456665145299
H	0.35524313053820	-0.92946142943770	2.46266316604066
H	3.59059069801721	0.65817993418583	-2.51910436343293
O	3.78867806912511	-1.09540196028073	-3.09580992676280
H	4.70036586738232	-1.42104062678030	-3.04340282519719
H	3.53989099064157	-1.24262647683128	-4.02161087253344
O	5.03171595262732	3.07332170998928	-0.51172320551468
H	5.69516146780364	2.57883371851334	-0.00700283276711
H	4.58011999879067	3.61446625724848	0.15370001546511
O	2.63418999524524	3.30953225998795	-4.32475688126703
H	3.37856159464644	3.44765861456662	-4.93141843178158
H	1.88991877810431	3.09063929602676	-4.90701263977785



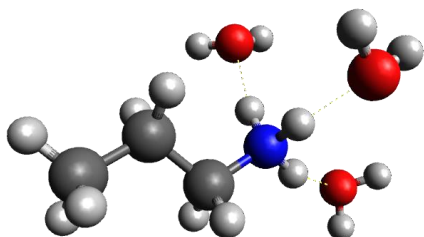
N	1.30643912573307	2.56879086221091	-0.38725662419893
H	2.08526077484695	3.07699376489348	0.04283685784949
H	1.16037885351531	2.92151491469992	-1.35544461309519
H	0.45039804729495	2.68698518450981	0.19587560899671
H	1.56131480568858	1.56526644113543	-0.48692488404439
O	1.91663849920470	-0.09108795017367	-1.25288536425681
H	2.85817163166023	-0.32149528094461	-1.27854393526648
H	1.63402919632842	-0.15199178912128	-2.17865490949593
O	-1.00654112814916	2.91941093828840	1.27642457764313
H	-0.69442546823280	3.07451953858508	2.18172601258820
H	-1.51054215944755	2.09280867877684	1.33546882332213
O	1.21730827318329	2.96700299446115	-3.19240875268802
H	0.86344917442711	3.78784795417588	-3.56972213290393
H	0.70875037394691	2.26972374850267	-3.63542066445001





H	3.76706096439613	1.41225001985673	-2.27911906460639
C	3.38555911881689	2.37352338360657	-1.92783881937244
C	2.26853996625184	2.43166490982054	-1.08804398033406
H	1.76950703617332	1.51267207039088	-0.77280055244562
C	1.78750652265713	3.66880641423332	-0.65023315213350
H	0.90981985088440	3.72072585376879	-0.00237185385285
C	2.42182388146399	4.85117730148817	-1.04350088310974
H	2.04693430306241	5.81828417623631	-0.70318779984347
C	3.53918318325161	4.77703027278150	-1.87523445654721
C	4.02669982295556	3.54890945099660	-2.32620478360416
H	4.90373128800901	3.50563578466871	-2.97570251072808
N	4.24303539503089	5.99631083096458	-2.26070340064507
H	3.65970775318187	6.85890823735464	-2.15740816166765
H	5.11906399775421	6.12242347320389	-1.69885862118069
H	4.59253613091095	5.94196053544974	-3.24182086477543
O	2.71556649636519	8.35450813192023	-2.00975445342542
H	3.08438394157548	9.05814171807815	-1.45430451268973
H	2.50782741883853	8.79304677632691	-2.84999069104493
O	5.65537722786888	5.70497544202030	-4.73804634267777
H	6.22565096068453	4.92400859802339	-4.81076413425654
H	6.23852478366712	6.44680606942580	-4.96126210055695
O	6.84422370229101	6.13303077758279	-1.25361787433898
H	7.29194740158011	6.93801122865783	-1.55734191082370
H	7.01647885232879	6.10931854314348	-0.29973907533966

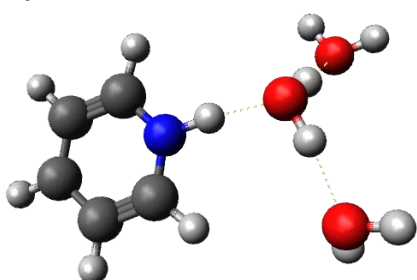
(PrNH₃⁺)(H₂O)₃



N	3.93085333107218	5.43582461333938	-2.40326598357095
C	3.17536171109135	4.36031279303545	-1.70118626504253
H	4.91742079124006	5.49266495512648	-2.07344949626252
H	3.52584198558025	6.38315175089352	-2.27158894179134
C	4.03359112492296	3.11441442681886	-1.52258101315967

H	2.27467764329310	4.14775557504986	-2.29448783268130
H	2.84794368661254	4.75808187740964	-0.73054391798056
C	3.23638176139627	1.93077642063527	-0.98521856089785
H	4.49140554797765	2.83982871917627	-2.48949213639267
H	4.86650305270158	3.34967146157893	-0.83774751847112
H	2.43671119615936	1.63702694695702	-1.68356908536500
H	2.76363986791770	2.16493700041806	-0.01669201759097
H	3.88943778297022	1.05747314562123	-0.83580271353618
H	3.98076591445637	5.26986749687550	-3.43043037580753
O	3.48291006224874	8.24657225976195	-2.13924731127711
H	3.57572883073007	8.70901765816216	-2.98630335378008
H	2.64833671090206	8.58249126035783	-1.77661947606869
O	4.16414627473742	5.20084938105217	-5.25295822290437
H	4.64881963155584	4.41511379136335	-5.55121459458980
H	4.68588182782033	5.94231074274965	-5.59778811326842
O	6.73542108523565	5.49319599084989	-1.92214098095841
H	7.02563662744982	5.18781702111181	-1.04846320089677
H	7.13984355192841	6.37006471165558	-2.01071888770622

(PyridineH⁺)(H₂O)₃

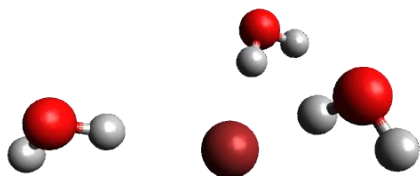


H	0.23284295005133	5.41043491893579	-2.33891879250460
C	0.21823143076194	4.62508702543269	-1.58319649087191
C	0.24270581424267	4.87620982687128	-0.21970013307972
H	0.27865632484564	5.90421862995235	0.14115278640978
C	0.22479651194468	3.79535304315958	0.66612994020450
H	0.24510577640944	3.97323790155687	1.74361231117793
C	0.18176617798484	2.48882106470708	0.17009167705254
H	0.16655090480420	1.62563023320452	0.83487516876999
C	0.15772576058821	2.29679353583823	-1.20212669115290
H	0.12326789428517	1.31290687407917	-1.67170245872180
N	0.17567926165300	3.35674521244736	-2.03071134599956
H	0.15783499014474	3.16368102100090	-3.07355764163019
O	0.14542136097527	2.67160086034960	-4.65643526410718
H	-0.67649416484179	2.95913128368075	-5.11770572429073
H	0.13187828617822	1.68585989782766	-4.66755977490683
O	-2.20358055936674	3.56179638791986	-5.83468333743148
H	-2.29863816539646	3.43460972038035	-6.79113208933147
H	-2.36444471759739	4.50901892696581	-5.70301745732863
O	0.19184478461440	-0.09860884683405	-4.47338427127081

H	-0.66866763009476	-0.43753590672081	-4.18087775546225
H	0.35010700781336	-0.55327161075501	-5.31503265552460

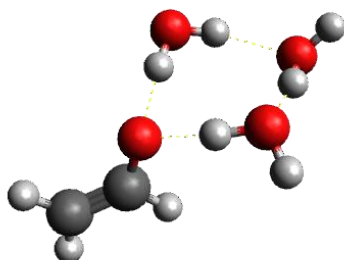
CLUSTERS – Anions

(Br⁻)(H₂O)₃



Br	-11.06724107169761	3.96643790294414	-2.51003994945425
O	-7.95715944646623	4.19915702212709	-1.35603588062784
H	-7.99585941923735	3.83842863241144	-0.45829714941989
H	-8.87778439044221	4.12230508101356	-1.69460630434683
O	-12.21968784566007	6.73978518136423	-1.13249492172048
H	-11.88233687477442	5.90957402083792	-1.54035515270033
H	-13.07564425596230	6.49092009260559	-0.75342042524549
O	-10.93217962018242	4.61826733963033	-5.79027091419001
H	-10.97801966390429	4.43852826510513	-4.82383996863135
H	-10.91040741167298	3.73854646196047	-6.19447933366357

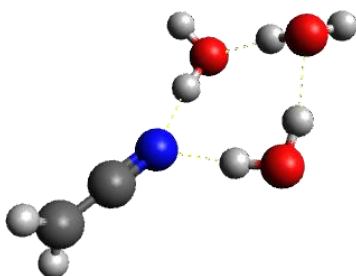
(CH₂CHO⁻)(H₂O)₃



C	-6.98694584501726	4.54629013805451	-1.56483512778507
O	-7.40904097135662	4.13035074451327	-0.37973066285780
C	-7.53173061740266	4.27291085885776	-2.77261248809037
H	-6.07924284204249	5.18510288135701	-1.54863299576841
H	-8.42948743386130	3.65318818314517	-2.87674678530541
H	-7.08037545324471	4.68661424570741	-3.67790806871052
O	-5.67294877444602	4.41137797045586	1.49736213130382
H	-4.81061011969547	4.09964373968580	1.18928299995343
H	-6.32677614729608	4.26590494264337	0.72208415261684
O	-8.63919218554973	6.04781328955582	1.21238067905057
H	-8.22092189381274	5.37417898783895	0.61908395284146
H	-7.90111698605459	6.38258608334207	1.76196367831121
O	-6.22397089208595	6.83018335324586	2.49961565545493
H	-5.88078733110991	5.95467514780930	2.18168921395695

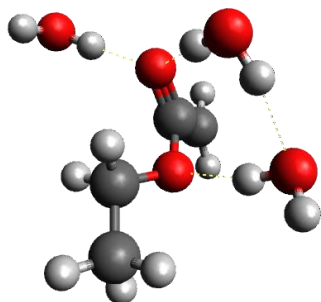
H -6.09829250702451 6.81710943378783 3.45937366502838

(CH₂CN⁻)(H₂O)₃



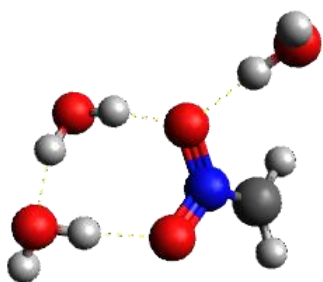
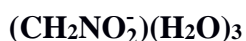
C	-5.68481649652223	5.16243712249381	-1.71584026246548
C	-4.40775793759992	4.84343183098409	-2.02235476466706
N	-3.27024644093058	4.56074833781514	-2.28714662025990
O	0.70676160433886	4.54035875829223	-2.11743902364961
H	1.46186381473026	3.95543935289354	-2.27563520430485
H	0.11095112294610	4.40944412223039	-2.89879406846138
O	-1.38330172508716	3.75316205694620	-0.39037563425220
H	-2.10172087975009	4.03647706882459	-1.01879519206744
H	-0.56270523259279	3.99790385883199	-0.86840360093813
O	-1.18651477074154	4.21452059928273	-4.02039789530367
H	-1.23513670563513	4.85249496591912	-4.74716025388718
H	-2.01027511407277	4.37364013742831	-3.46980706509412
H	-6.46746930174716	4.40120190269722	-1.75294443275577
H	-5.93370193733584	6.16614988536060	-1.36292598189320

(CH₂COOEt⁻)(H₂O)₃

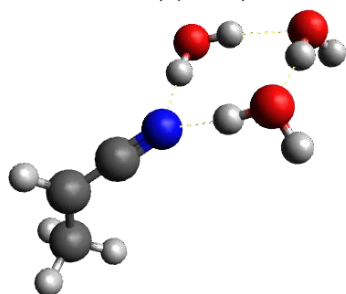


C	-6.91067442936428	5.05029832915541	-1.97566974252406
O	-6.45346628797208	5.93062180091554	-1.14404080458223
C	-8.08933861292117	5.05374498431379	-2.65158682091717
O	-6.04965442111358	3.96604129301313	-2.26153360896532
H	-8.76839765434452	5.90321830327027	-2.55518561803898
H	-8.37172581902232	4.21625140391965	-3.29102891246674
C	-5.33779324592482	3.38593950261488	-1.15144052565623
C	-4.64085270981475	2.12772358464504	-1.62849067579254
H	-6.05969716877147	3.15535752596136	-0.34996225695051
H	-4.60880773460291	4.10846366742651	-0.75198267162058

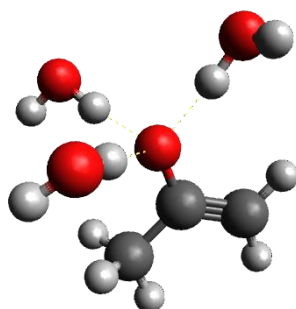
H	-5.36207269350795	1.40007134565746	-2.03264696835552
H	-4.11048052809767	1.65468064859242	-0.78682732326054
H	-3.89617120869865	2.35138109322637	-2.40933071226220
O	-7.54912592982665	5.97040773245293	1.30858227985936
H	-7.12957306851340	5.93905122499062	0.40454435728164
H	-6.83134792948667	5.73762860827140	1.91438994737879
O	-4.07582394144432	6.85468702757384	-2.10433938789203
H	-4.91843847508659	6.53216477299084	-1.68987974853563
H	-3.97103811139715	6.27343220533687	-2.88171252234315
O	-4.33339994788520	4.89560893307951	-4.23435583815982
H	-3.66714600583971	4.23773531215436	-4.48130987838304
H	-4.94060407636414	4.42887070043784	-3.61544256781343



N	-6.95754055190823	3.90962193578504	-1.25496241499866
O	-6.73115459312039	3.77942671614916	0.03144222304878
C	-7.97544570008165	3.32876935574928	-1.82512087164116
H	-8.63673172737055	2.72532009569337	-1.20777120232933
H	-8.12404955136908	3.48395864017049	-2.89154564463111
O	-6.11699332226472	4.64785088295877	-1.91802357781746
O	-4.53613607598767	2.10293996288060	0.32566847292221
H	-5.36944719120729	2.62873264237510	0.32849997622155
H	-3.96642971982247	2.63998882204868	-0.26344343254067
O	-3.51201406306654	4.03320499381671	-1.46535822537922
H	-3.14556248519518	3.73220481090063	-2.30886128845261
H	-4.45594759822400	4.27479313532248	-1.66015337387012
O	-8.95298133835758	4.48667025487033	1.39006975099018
H	-8.77432220905400	5.36198657668819	1.76177777111054
H	-8.11366387297055	4.23523117459116	0.92647183736701

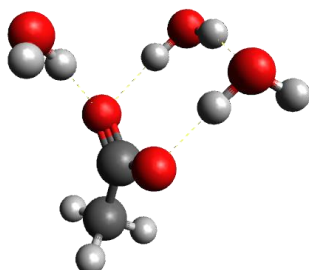


C	-6.12651784993033	6.82139331185862	-1.65374561234594
C	-5.75979542986643	5.36831072756222	-1.84422089438738
H	-6.58022167279432	7.03454330120027	-0.66412307444213
H	-6.85781724990778	7.17652482056708	-2.40316593591534
H	-5.23996425824065	7.47065157102308	-1.74366431886013
C	-4.49089115632604	4.91538433578363	-1.91783257133694
H	-6.55792036769468	4.61908717734780	-1.88789597348449
N	-3.35535500046189	4.50926352590503	-1.97399802801021
O	0.49876057017335	3.50129215239484	-1.52305810115990
H	1.04479022952487	4.29839137860013	-1.45617870469262
H	-0.05786933275737	3.64394142183232	-2.32832732197264
O	-1.84230249452273	3.68372074811974	0.17403315158824
H	-2.43618572313012	4.00746926265790	-0.56389035467485
H	-0.97408186219070	3.59102910012948	-0.26859108354071
O	-1.27149928005752	3.86562623946555	-3.61664909402721
H	-1.06414564040188	4.63013035530873	-4.17377728881133
H	-2.08335348141576	4.14043057024363	-3.08729479392646

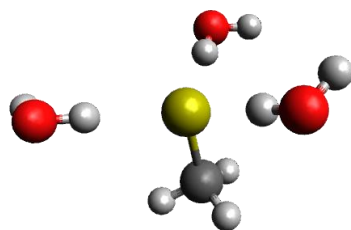


C	-5.72837589421008	5.07380711386053	-2.27019557503413
O	-5.24419216991717	6.06579067969753	-1.51649252376401
C	-6.60817904632232	5.53090852149175	-3.41225605669569
H	-6.04380784529949	6.20252816696392	-4.08268066813344
H	-7.46218489099905	6.11419831683318	-3.02645899669568
H	-7.00286272816403	4.69365873116464	-4.00619415732882
C	-5.47128202743905	3.76186377349412	-2.04599440373548
H	-5.90009219722094	2.99062969238888	-2.68972413208070
H	-4.83684937635813	3.44115535684719	-1.21379660603197

O	-3.90795958337597	8.15358914173365	-2.44169195855030
H	-4.26141904302599	8.39188433286938	-3.31002104942667
H	-4.43237852242012	7.34721499674373	-2.15968389791003
O	-7.12476590076172	7.68627690301160	-0.53926340176542
H	-6.42346970764543	7.09233588047131	-0.93796805202988
H	-7.54414318387676	8.12122854693023	-1.29462650142334
O	-3.73318471836043	5.62668043464634	0.59974490176427
H	-4.32671351398089	5.74200663578977	-0.20598944210541
H	-4.33705965062226	5.40066277506216	1.32113252094672

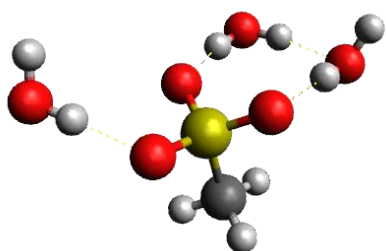
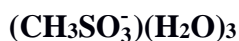


C	-5.70718058755912	5.52745278821517	-2.28237907463901
O	-5.09298189147630	6.60044377591931	-2.01961147860528
C	-7.12474109287779	5.63468770130951	-2.81110795267506
H	-7.20099704902525	6.43418861916133	-3.56236498244821
H	-7.78564546235164	5.91294068387380	-1.97318552430418
H	-7.47745843924138	4.68589320440548	-3.23650945274484
O	-5.21070778743167	4.36726375697600	-2.10943554177243
O	-3.92008816750971	4.05908755929136	0.35384608915483
H	-3.59699671565711	4.97929592491913	0.43672708168996
H	-4.38442732962882	4.07707601738385	-0.51394037748754
O	-3.31180425777022	6.84615771173273	0.03086655054559
H	-3.80291162788690	7.36709224162612	0.68322700253251
H	-3.92731058642923	6.77041738525013	-0.74623586798588
O	-2.73060664520636	4.28673126061757	-3.37013650911978
H	-3.58767178732018	4.31167893388551	-2.88281466888090
H	-2.66672057262834	5.15514243543301	-3.79235529325978

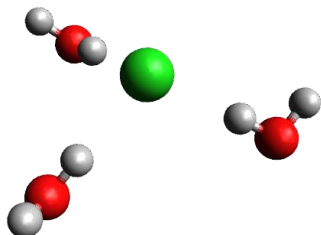


S	-4.38893971535454	3.72254220123202	-2.48031590348572
C	-5.49441470470687	4.94006436881493	-1.65252359513326
H	-6.14701381931586	5.44873646534933	-2.38123191722623

H	-4.91622087808411	5.71541562609070	-1.12401207288785
H	-6.14284573781208	4.44287890473702	-0.91309306981314
O	-5.66223548914588	0.98867799704738	-1.57581936417314
H	-5.24230460050048	1.85349551340017	-1.85436817972541
H	-5.31337443153954	0.82324931124759	-0.68792893189552
O	-4.32030076344394	4.76355448257787	-5.46044691634692
H	-3.42811126066410	5.11081542875425	-5.60492684847174
H	-4.31696869879452	4.43740379695694	-4.51478497784834
O	-1.66157567338481	4.16559344571887	-0.99861569811059
H	-1.29184091262910	4.99234076909540	-1.34150570852094
H	-2.52823331462418	4.04696168897753	-1.48711681636123

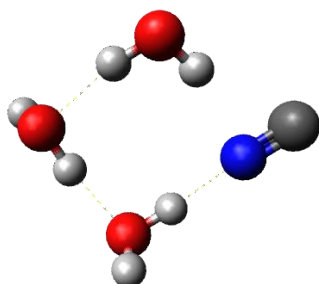


S	-6.62204232796195	4.49316671750358	-2.71511408991631
C	-6.81661146188424	6.25891107617516	-2.55686973843039
H	-5.84271694680644	6.73445890769893	-2.73183262429783
H	-7.18147324065479	6.47464838560111	-1.54415971012029
H	-7.54646317227566	6.58579974871888	-3.30777420772357
O	-6.11149372434629	4.24349668661041	-4.10924843150604
O	-5.64737014532983	4.04732431552116	-1.66147784482614
O	-7.98363306615022	3.89356825526942	-2.48946358386847
O	-3.39071476201001	5.16935266503812	-4.38031073112149
H	-4.30137485720712	4.80225087164964	-4.37208792670592
H	-2.88885663234629	4.55614055783100	-4.93735357261126
O	-8.08776768264818	2.62564290266084	0.03140693469277
H	-8.03710120311102	3.04045221655473	-0.85622319664226
H	-7.59291688405077	1.79890575917669	-0.05919720814392
O	-2.91900490967637	4.62206646018541	-1.57685443791682
H	-3.86598983990669	4.38844441247317	-1.48226160098955
H	-2.86182914363423	4.85006006133155	-2.52642802987250



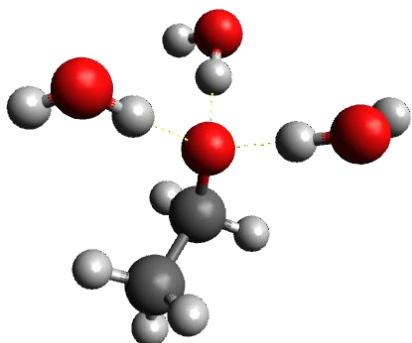
Cl	-11.25155303707423	3.77568666208321	-2.61404852701254
O	-8.38947527218013	4.35803942606183	-1.33159582159081
H	-8.38624901317943	3.97947670367596	-0.44070922807727
H	-9.28061486038066	4.14663491967775	-1.68729893983781
O	-11.64166875256275	6.55892032276759	-1.18902752545013
H	-11.55206755191122	5.68053436798098	-1.62220982141844
H	-12.53213471752042	6.55187270651578	-0.80867846854658
O	-11.04671099362832	4.69733003141787	-5.66671138982821
H	-11.10464235331450	4.38087566426770	-4.73692584326210
H	-10.71121344824845	3.93257919555134	-6.15663443497612

(CN⁻)(H₂O)₃



C	-7.49546834324075	1.95107631301092	0.58372959926723
N	-6.38372256894878	2.24527101794409	0.33623913107797
O	-2.68538029980421	1.44670501616281	1.63719455932301
H	-3.00591998687933	1.97271203273700	0.86411364667227
H	-2.31380451464725	0.63837818584571	1.25299359727306
O	-5.18410163854587	1.03881504476874	2.92136617778390
H	-5.74299238281104	1.36320444089229	2.19216334169326
H	-4.27608403847240	1.09714727366159	2.54867498076689
O	-3.81933586187918	2.98284682397459	-0.34731432297666
H	-3.69722131993662	3.89410103161458	-0.04167543374205
H	-4.76000904483463	2.75779281938767	-0.11047527713886

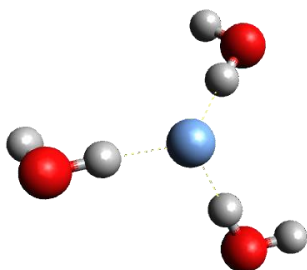
(EtO⁻)(H₂O)₃



C	-6.63779659567878	1.15644594487154	0.70619041362520
C	-5.53358772145329	2.20576574015674	0.78414413485268

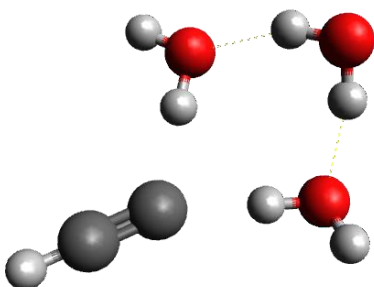
H	-6.69670759881489	0.71121160689935	-0.30183613905608
H	-7.61829071139958	1.60767411392152	0.93780365669426
H	-6.46382119284458	0.33757863072434	1.42392943730606
O	-4.25207916507236	1.69413236460220	0.51641076936318
H	-5.56390603016875	2.66966473717992	1.79488299787103
H	-5.78025846860524	3.02690286005199	0.07637374136770
O	-2.39458382908258	3.10245182440163	1.62954540902393
H	-2.66223565604879	3.22493608024757	2.55090373870803
H	-3.14328717167666	2.54848060021828	1.20470390699385
O	-3.49031190170242	-0.61684369843070	1.42265754273137
H	-3.83434132105097	0.28715196283556	1.10131785245510
H	-3.96162593025927	-0.78398501331618	2.25008894073706
O	-3.43145976995552	1.97523814764442	-1.90304633714519
H	-3.15476056160366	2.89978867315885	-1.97311189843156
H	-3.77653637458266	1.87368542483296	-0.94261816709663

(F⁻)(H₂O)₃



F	-10.38909158934325	5.40540317918599	-2.85640554162203
O	-8.99396864717975	4.61699599691236	-0.82196721072093
H	-8.57507001922614	3.77897831970048	-1.06484758657963
H	-9.50778597975671	4.89104151534633	-1.63244915703403
O	-12.77120513506022	5.45538271925061	-1.89742603648145
H	-11.83902943656642	5.44663692701410	-2.25923467484867
H	-12.69046024119872	5.85856995580655	-1.02185977663527
O	-10.51496831287641	4.38118660421137	-5.22940471938768
H	-10.44332377490413	4.74873907350685	-4.30407075627196
H	-10.17141686388788	3.47899570906523	-5.16617454041828

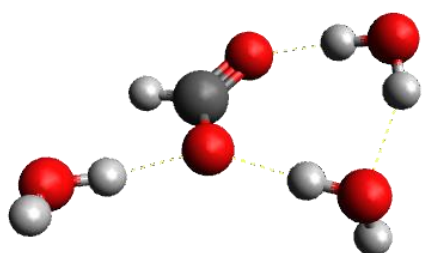
(HCC⁻)(H₂O)₃



C	-8.97693446253494	2.15205377657071	0.45104732955626
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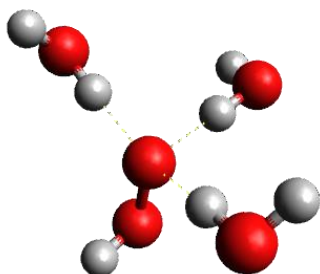
C	-7.93532349940818	2.55588283758007	-0.07609608251855
H	-9.88750260903354	1.80382306087221	0.91372635348847
O	-3.79244956417411	3.38698124302751	-0.17790035662619
H	-4.42013006726169	3.83509778355156	0.42344800545778
H	-4.38509775741453	3.07251384118754	-0.89821150718491
O	-5.79425800690514	2.66724175415427	-1.98591010746828
H	-5.73587288310512	1.76866325906591	-2.34276391918102
H	-6.55530125983320	2.62952995945667	-1.31970262084513
O	-6.09044152483520	4.38197667418603	1.06293463006570
H	-6.56232933036734	4.84672555570275	1.76818110944442
H	-6.75824903512701	3.76342025464475	0.64503716581141

(HCOO⁻)(H₂O)₃



C	-3.92389024713348	2.38145390616143	2.00805400143315
O	-3.88179619929248	1.11579345199405	1.97957565274285
O	-2.95554309531335	3.16936595183957	1.89954831632429
H	-4.93127769839281	2.84220727153438	2.14854485293553
O	-1.57998732518967	-0.08048525838165	1.00657254583659
H	-1.72226506480796	-0.22609559188060	0.06025135223353
H	-2.42057406543205	0.32887015696915	1.33368612345426
O	-0.35635848434812	2.36552944677444	1.86624015388470
H	-1.28385970571723	2.70852079833155	1.89386975691300
H	-0.49265003479012	1.47196762682786	1.49374437378979
O	-6.37701184694103	0.52537062522174	2.98438885315945
H	-5.46602474930407	0.62238234050418	2.61348517011502
H	-6.40103148333766	-0.37550072589609	3.33698884717778

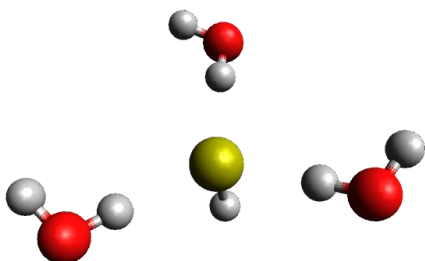
(HO₂)(H₂O)₃



O	-10.64061565451514	-1.93035487727876	3.66917083718877
O	-9.27968344511187	-1.49171395695747	3.35666318959590

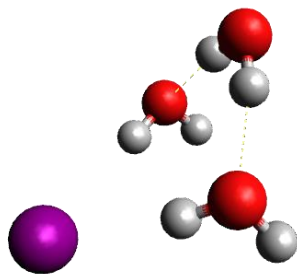
H	-10.95923663708543	-1.22662753324471	4.25620803838652
O	-9.44939994276350	-0.35131439414589	0.97623422986429
H	-9.38355294819119	-0.74479144649243	1.89901853703129
H	-9.05363173227480	0.52764205514357	1.05412750005630
O	-8.26502476293300	-3.52090523499993	2.00325284299764
H	-8.73527082269609	-3.54536733293071	1.15830968115236
H	-8.67264246771516	-2.75407168538162	2.50877927169132
O	-8.02360951260690	-1.94044389663413	5.60391565563234
H	-7.15876391560723	-2.31092047486471	5.37692599106180
H	-8.47625815849957	-1.77198122221317	4.71734422534151

(HS⁻)(H₂O)₃



S	-10.52467057092258	-1.78631264744038	3.46507286992164
H	-11.32025686487137	-0.93306966856223	4.15050414238964
O	-11.83537843029713	-4.53635109568685	4.39523709421266
H	-12.24532157721253	-4.91397057092605	3.60360078994599
H	-11.43113537762730	-3.68010145862352	4.08423426035437
O	-7.78249746485333	-1.25053939329912	4.92988388650002
H	-7.63381750323234	-2.02139275744235	5.49617829363574
H	-8.65088027872225	-1.43478517729933	4.47428741332381
O	-10.75521671360166	-0.46617834035501	0.56328929200573
H	-11.07036075541714	-1.16744989034720	-0.02463025036255
H	-10.68003446324242	-0.90099900001795	1.45581220807294

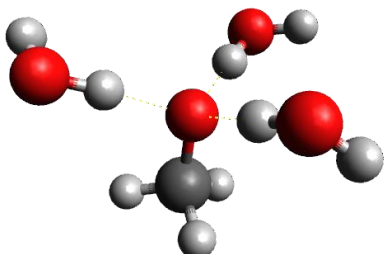
(I⁻)(H₂O)₃



I	-10.86622402091261	4.41355290815616	-2.99599184442490
O	-9.19231186374727	4.18566934248060	0.23266083812362
H	-9.68643132251170	3.52134991333336	0.73613812911982
H	-9.62812856451281	4.19195658403527	-0.64369348664453
O	-12.39817266505007	6.22659346782036	-0.26585572552305
H	-12.08009983407406	5.70789820354436	-1.03221254486525

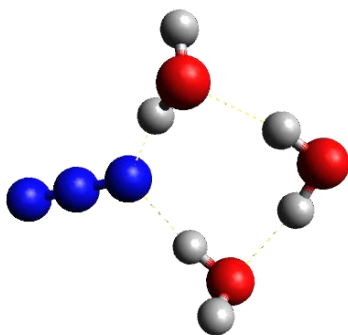
H	-13.10673597300196	5.68642592644825	0.11500665785456
O	-10.04678448757693	6.72678388888316	1.20236513524150
H	-9.62522963651442	5.88263332476646	0.93703442245912
H	-10.92595163209812	6.66060644053204	0.77185841865914

(MeO⁻)(H₂O)₃



C	-4.54168461148800	0.58630639887765	2.89768217887102
O	-4.74750209733956	1.97453476295318	2.83379193447842
H	-4.16668501738316	0.16742171265564	1.93948865348174
H	-5.47241437255029	0.03450643470738	3.14728573065796
H	-3.79704512753063	0.30890411526946	3.67246885264622
O	-6.96565402290023	2.51911603591389	4.02545449298355
H	-6.08490489851677	2.32131722410279	3.54116680372877
H	-7.60472645669426	2.68593528164941	3.31860849884541
O	-2.57495994251903	3.01212870348256	3.76751890941539
H	-2.77260053395137	3.30898394765060	4.66610397897411
H	-3.45546512924019	2.63480549568587	3.40956612218154
O	-5.06054123049893	2.84877148187707	0.38501341304410
H	-4.94884876213083	2.49057705518475	1.33178836359318
H	-5.67564779725673	2.23943134998971	-0.04610793290139

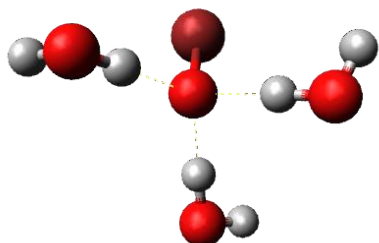
(N₃⁻)(H₂O)₃



N	-5.00761739500467	-0.46450777504920	0.62954161429841
N	-4.68888452614202	-1.25165459533367	1.46131329547019
N	-5.31992907155231	0.31417189485806	-0.18288562918989
O	-2.10472293370827	-1.66788599254555	2.37997311713471
H	-2.99834470099369	-1.47088787460503	1.98960761821589
H	-1.62532289861790	-2.12741336515225	1.67507076260597
O	-5.31350085921388	-3.88383032910915	2.13110531441281
H	-5.20221714620933	-2.94630965784737	1.82702236845457

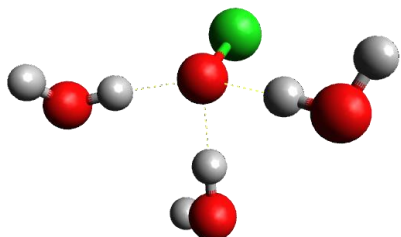
H	-6.22513454592122	-3.93055634382181	2.45553313600877
O	-3.28197186457618	-3.57197120767061	4.08796029497726
H	-2.76407905259420	-2.91472132216150	3.57489936922168
H	-4.03778500546635	-3.77328343156180	3.49552873838963

(OBr⁻)(H₂O)₃

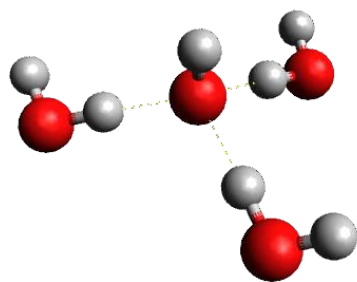
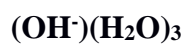


O	-5.01163256994430	1.42790584977747	-1.60070937690896
Br	-5.19846937244847	0.22165198255811	-0.20752232057982
O	-3.95122791860887	0.24243511736950	-3.69938221346176
H	-4.33883038956612	0.65451633531521	-2.86692683009362
H	-4.50824051379589	-0.52731152808681	-3.88029841103402
O	-7.37640639021226	1.66215458471507	-2.75360228166352
H	-6.48925936488350	1.55805635574780	-2.28928078103635
H	-8.03369791758694	1.40477572909373	-2.09217863910087
O	-3.99316690079002	3.68401387399417	-0.75857446050324
H	-3.11929419708027	3.47399891484801	-0.40135998148956
H	-4.37895446508339	2.79539278466772	-1.04102470412825

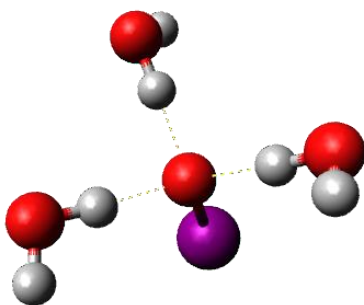
(OCl⁻)(H₂O)₃



O	-5.41015064568283	1.54110265066635	-1.34918902607993
Cl	-5.35633169873088	0.11830510023171	-0.37085680714596
O	-4.39485010748139	0.85180209000065	-3.72127140279970
H	-4.76909916330025	1.08636402937808	-2.82432466267060
H	-3.49087539605238	0.55535356641374	-3.54712005599820
O	-7.72949015117810	1.43030384071352	-2.63716038137348
H	-6.87215575684055	1.46875157753401	-2.12001392646034
H	-8.40607182583233	1.22095591264911	-1.97780625694169
O	-2.98135115002123	2.60241310609655	-1.13057181848357
H	-3.07660838757597	3.48380359979441	-0.74361092262460
H	-3.91218571730425	2.23845452652207	-1.16892473942244

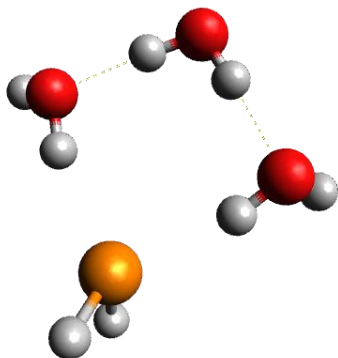


O	-5.12759615287669	1.38353645481436	-1.59537620534519
H	-5.28168241196719	0.72596703555249	-0.90146136807422
O	-4.23029163866502	0.22086617310764	-3.74925940513764
H	-4.54923913268738	0.65174695554059	-2.88370578615003
H	-3.36128671661178	-0.14790049361634	-3.53918486325734
O	-7.49486941860959	1.93754141193683	-2.66004226057477
H	-6.60053807487493	1.70211733085750	-2.24523326762148
H	-7.92142666527120	1.08778576923984	-2.83678854257933
O	-4.14548836909332	3.54650005420921	-0.53534785547771
H	-3.27718589101234	3.30954418323147	-0.18076493871530
H	-4.51004552832985	2.67979512512666	-0.93036550706734



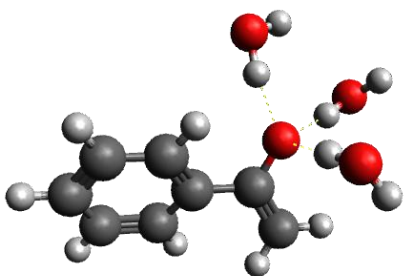
O	-5.07739535971080	1.14047478454800	-1.63481197184759
I	-5.28156260528699	-0.00824576459638	0.01779128601736
O	-4.26738990555921	-0.18452118883270	-3.76022744056566
H	-4.56627066668739	0.29765450356127	-2.92679669840580
H	-3.34617539987675	0.08894386141703	-3.87417150238710
O	-7.35096621502676	2.26825171613808	-2.40538964399667
H	-6.51146983589699	1.81372533724559	-2.08954758953061
H	-8.06287048321717	1.66065051189286	-2.15868954061554
O	-4.17006808119926	3.52155242611756	-0.96127560261759
H	-3.28156694703838	3.40362221860723	-0.59853449722666
H	-4.48343450050032	2.59550159390141	-1.19919679882417

(PH₂)(H₂O)₃



P	-4.67092801414171	-2.57903278107940	-0.38805772259646
H	-4.73387825742638	-3.81785764027117	0.32509784303379
H	-4.75414839388586	-3.19191173550058	-1.67890781608110
O	-2.47795744071870	-0.28307387887160	0.31256580351249
H	-1.69608017251460	-0.58945941787710	0.79536203521117
H	-2.97915954871806	-1.10965500422922	0.07724907748568
O	-4.48731827346663	1.43052272037080	1.19943859778606
H	-3.73272181395369	0.85741444328085	0.94007955448142
H	-5.28169658009564	0.92903814198118	0.91714282654062
O	-6.74544468818590	-0.11573681188030	0.36723670437944
H	-6.25872023984489	-0.94631641706819	0.11719829649745
H	-7.25655657704792	-0.36502161885528	1.15224479974945

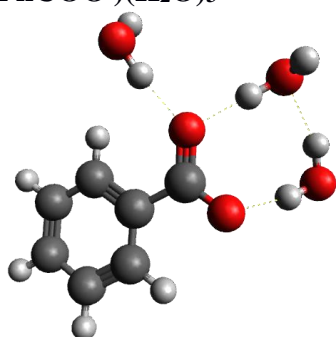
(PhCOCH₂)(H₂O)₃



H	-3.07555313442020	-1.50410641788436	3.34446357780956
C	-3.51362586120853	-2.14559705870627	2.57765654263278
C	-4.51927819020741	-3.06875851801379	2.92908346509062
C	-5.07858553871335	-3.85716085941060	1.90665790667262
H	-5.85812164796044	-4.57793591704074	2.16090143973443
C	-4.64330431873261	-3.73605169869385	0.58337516959284
H	-5.08865478460942	-4.36481953282780	-0.19166693975034
C	-3.64528421084759	-2.81441714826246	0.25090274314657
H	-3.30476187857328	-2.71254891257472	-0.78281319732150
C	-3.08094967910637	-2.02025542705095	1.25582502230211
H	-2.30217915023131	-1.29500773194514	1.00477610379354
C	-5.00054722849759	-3.23151792568447	4.34373425347899

O	-6.22674251478814	-3.73095583340662	4.49413071947820
C	-4.19573156881394	-2.92447762457693	5.39496556195810
H	-3.17778965959968	-2.55843284896089	5.25441066274907
H	-4.55669385916894	-3.05597155108027	6.41926903448364
O	-6.00582330425229	-6.21471368124119	5.37346162497767
H	-5.53653171794956	-6.15254269137046	6.21682127035191
H	-6.09382217439890	-5.26719267110816	5.05587334479876
O	-8.47279282796517	-3.35907707879373	3.10885493708897
H	-9.01915913005509	-3.06220331215384	3.85095024914872
H	-7.57407850653542	-3.50295511247701	3.52398174845472
O	-7.94682608920305	-2.82468087868694	6.33505556882364
H	-8.42447115801096	-3.61399914591794	6.62607509226726
H	-7.24601186615088	-3.16444042213081	5.70714409823702

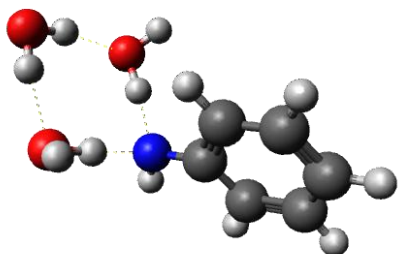
(PhCOO⁻)(H₂O)₃



H	-2.72981444106177	-3.81655083699756	3.36438557242670
C	-3.53621349428071	-3.29616922857039	2.84539355277768
C	-4.86666222886265	-3.63522329779181	3.14396667199948
C	-5.90411486570917	-2.95951947186679	2.48193770700097
H	-6.94033061972801	-3.20666674737859	2.71473195771209
C	-5.61768031757670	-1.97142522764327	1.53643708447444
H	-6.43385909388257	-1.45271114187555	1.02882559032632
C	-4.29006201454944	-1.64367011453557	1.24264502140254
H	-4.06404988448239	-0.86956199698716	0.50473426109319
C	-3.24913500523656	-2.30774760114617	1.90069349007837
H	-2.21172427405005	-2.04827229346788	1.67432139199565
C	-5.16231710034093	-4.70209162225837	4.17559560136582
O	-6.37828758346545	-5.01941151030924	4.38404743266495
O	-4.19119807171503	-5.22174742676018	4.78698523194445
O	-4.49081371577476	-5.37685735840928	7.51830953145447
H	-4.28870568497129	-5.33223174622654	6.55362428327334
H	-5.41279021680250	-5.70363959064841	7.50751289875860
O	-8.76221086552214	-5.09012794855639	3.05220506334839
H	-7.88195722174962	-5.00442524333288	3.49148625020814
H	-9.37954914496674	-4.67565439013161	3.67119720635588
O	-7.09681268000214	-6.22602946822188	6.69024541154211

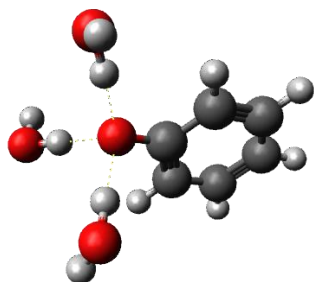
H	-7.09938577954045	-7.18559390491762	6.57330326757386
H	-6.82857569572882	-5.84899183196694	5.80763552022266

(PhNH⁻)(H₂O)₃



H	-2.92161114662154	-3.13374882584156	3.79309108874929
C	-3.59421767832188	-2.81215781311636	2.99089280116397
C	-4.93034029728655	-3.30716135999065	2.98496623857278
C	-5.75478663804296	-2.85827532172414	1.91253473180328
H	-6.78786411768473	-3.21519708551252	1.86281491294541
C	-5.28041526961515	-1.97982548643055	0.93790238909154
H	-5.95508296935850	-1.65941858386885	0.13767778718625
C	-3.96353725838587	-1.49859903270687	0.97206678078324
H	-3.59612262881925	-0.80753644001797	0.20923550196102
C	-3.13142646558119	-1.93040091263727	2.01414802241178
H	-2.10025477146340	-1.56748275778597	2.06992402474027
N	-5.42797915992591	-4.16226526642980	3.94414380650555
H	-4.70493433694338	-4.34935669420161	4.64258169684272
O	-6.52961822290881	-6.44416210748555	3.14687795281910
H	-6.32422934855385	-6.56203395083222	2.20843421051543
H	-6.08158965468701	-5.54478626152709	3.41997548856908
O	-7.78274985558993	-3.48346541443184	4.96338920619618
H	-8.02509913474608	-2.64734366895635	4.54009157239753
H	-6.85075391811911	-3.72894227699762	4.56615901563244
O	-9.10136672915641	-5.71958750380689	3.89855797794311
H	-8.26013298629166	-6.10060642734739	3.55326513815663
H	-8.78554741189687	-4.87944680835086	4.30480965501337

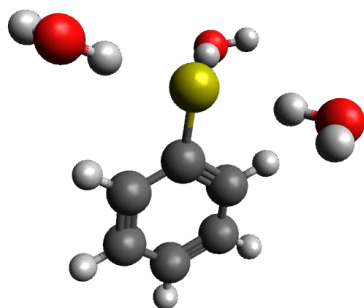
(PhO⁻)(H₂O)₃



H	-3.75414144514597	-1.97087874781013	4.19962771144924
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C	-4.04660940162496	-2.11093395288151	3.15554347553471
C	-5.03387344492663	-3.08068506442007	2.84183545841066
C	-5.38625673578493	-3.23159656930048	1.47690601465836
H	-6.14916162299262	-3.96879011263958	1.21033894265727
C	-4.76731566247380	-2.46918955802977	0.48443928793025
H	-5.06008621931942	-2.61889682854302	-0.55945952697933
C	-3.78510326524123	-1.52421636152574	0.80965342070098
H	-3.29912276889366	-0.93321838161126	0.03031695163157
C	-3.43488580223427	-1.35324056300293	2.15505487845906
H	-2.66824525950506	-0.62326148755119	2.43326891965438
O	-5.59324939494276	-3.83886435499969	3.78470536416627
O	-5.38327985565495	-3.04880873469832	6.31956565118982
H	-4.64454470195407	-3.54524057269523	6.69881457017508
H	-5.42893192465946	-3.34831606184726	5.36182649235661
O	-4.60816167626007	-6.32539455310239	3.45617553203960
H	-5.01206053668752	-5.41977639784894	3.57404865066382
H	-5.19566870307390	-6.78496738049392	2.83997222535098
O	-8.20825621153481	-4.48457869845413	3.63815907132831
H	-7.24378655475845	-4.21908595354454	3.64856241342160
H	-8.69323881233131	-3.64823966499987	3.61039449520070

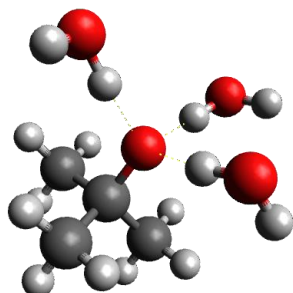
(PhS)(H₂O)₃



S	-4.12098185491584	3.85017883874747	-2.44830198666218
O	-5.29350956264534	0.97496133323472	-1.63386967223306
H	-4.91105172264271	1.85431153356245	-1.89092028237223
H	-4.97206589696972	0.82785678140123	-0.73219212988931
O	-4.93521463053904	4.84215230524361	-5.39907911580118
H	-5.31454523790504	4.06694523671153	-5.83759894847367
H	-4.64829350473783	4.51058171339675	-4.50951398554469
O	-1.38888420180573	4.54033588213392	-0.96750888536057
H	-1.05529834444927	5.37489882606257	-1.32834043880609
H	-2.25944841314730	4.39546698977079	-1.42333816712369
C	-5.45205880223058	4.78135599200507	-1.72506172667793
C	-6.79074694603716	4.48969106604165	-2.06899180226746
H	-6.99255418748342	3.68511423195916	-2.78066552343987
C	-7.85447317045937	5.20527494160882	-1.51628469148203
H	-8.87667059658084	4.94774221668303	-1.80908817513313
C	-7.61695902528553	6.23916638422624	-0.60149048971271

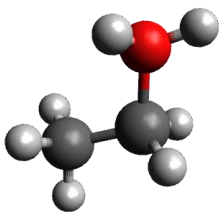
H	-8.44733286418114	6.80161438226681	-0.16861270853250
C	-6.29660389604720	6.54573219693748	-0.25457699679457
H	-6.08831956040748	7.35514191254916	0.45139088527076
C	-5.22908568002286	5.83038673197530	-0.80735490327852
H	-4.20639190150647	6.09013050348222	-0.52144025568544

(TerBuO⁻)(H₂O)₃

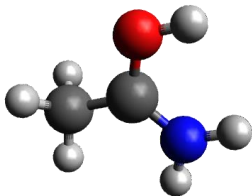


C	-4.86687185683743	-1.82918573727164	-0.20154071259414
C	-6.39804912126276	-1.94402505445497	-0.30627120572772
H	-6.69996448749894	-2.63352975411004	-1.11117568443747
H	-6.85237360755186	-0.96160430014599	-0.51780154323517
H	-6.82717157100091	-2.32449172618912	0.63464975315820
C	-4.27475387089046	-3.22152874461590	0.08679805002372
H	-4.67291409758882	-3.61813346518377	1.03539152976683
H	-3.17745401939535	-3.16800362176686	0.17469801340106
H	-4.51738007547781	-3.94634284629959	-0.70777165927880
C	-4.30941345631144	-1.29661067005311	-1.53410522045198
H	-4.55886960655324	-1.96305960241249	-2.37658278709083
H	-3.21224552640289	-1.20054886537912	-1.48777452261797
H	-4.72899168369627	-0.30205018690626	-1.75809943884491
O	-4.51945502963852	-0.94134071212457	0.84890055472782
O	-5.20475462896283	1.54504527422110	0.73865575740188
H	-4.96049995533728	0.54900040136252	0.72297447897753
H	-6.11586621484990	1.58546881116155	0.41779716754336
O	-5.75679569095008	-1.10224759878785	3.12420243659402
H	-6.17373868285192	-0.23327910416176	3.20390869980175
H	-5.29841923295446	-1.08654265726127	2.20985903085272
O	-2.08144702513632	-0.75262442204495	1.65275771144481
H	-1.58500735716816	-0.36078913046959	0.92118870171120
H	-3.03815320168226	-0.85970628710634	1.29066088887409

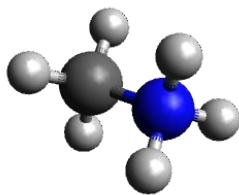
CATIONS



C	-10.45516705288023	2.92293997425734	-0.04172043391443
C	-9.05983939158388	2.37938013235377	0.03945517624366
H	-11.13519508629352	2.17452749607902	0.39169072636123
H	-10.75753338693025	3.11161256785572	-1.08201463030959
H	-10.55915900447394	3.84859354146941	0.54487671226037
O	-8.11959898572827	3.41623538464697	-0.50331005838429
H	-8.88286460712867	1.51608696818334	-0.61042990792570
H	-8.72627743622816	2.16472803328408	1.06199338657911
H	-7.19332652068518	3.10265898724842	-0.54266862631991
H	-8.12248852806789	4.24594691462193	0.01734765540957



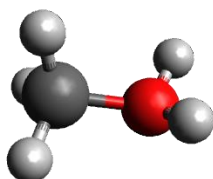
C	1.77724823073223	1.65456227180120	-0.85524904863996
O	3.00377028389951	1.57991884311012	-0.41927008177134
N	1.23434073124181	2.79566146555194	-1.16795445765022
H	0.27966499737492	2.82412747160261	-1.52135657949368
H	1.73950710638273	3.67922240174882	-1.09522211412693
H	3.44509681851541	2.44701509721652	-0.34164616422910
C	1.03843951906809	0.37729835545113	-0.96030998508748
H	0.08615378507181	0.50319521082494	-1.48742901657995
H	0.84807478716140	0.00564952427579	0.05970948612059
H	1.66860374055207	-0.36257064158306	-1.47391203854194



C	-9.00802654592665	3.01691422800551	-0.33884499966076
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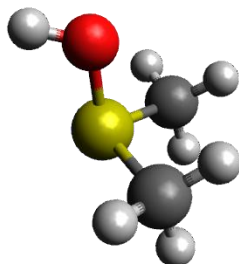
N	-8.04757806319765	2.42902033517660	0.62842083759358
H	-7.23224260438094	3.03762922548504	0.76939593312967
H	-8.48355716859207	2.27931322730428	1.54671544771675
H	-7.69690322871953	1.51949135459374	0.30286769255360
H	-9.36798596459710	3.97239754975615	0.05888844176704
H	-9.84638601336512	2.32445472418954	-0.46979113512121
H	-8.49298041122094	3.17275935548915	-1.29342221797868

CH₃OH₂⁺

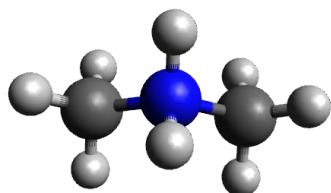
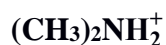


C	-10.39090787591007	3.08232621377786	0.02136318795034
O	-8.92508382727869	2.93002804910666	0.00937049859023
H	-10.79471723438174	2.06752689820732	-0.03756709776401
H	-10.69489855991203	3.69750447635962	-0.83197818810586
H	-10.63369145910420	3.55469853645356	0.97764495702938
H	-8.595367444462740	2.49893601389890	-0.80530583230056
H	-8.45324359878587	3.78226981219609	0.10367247460048

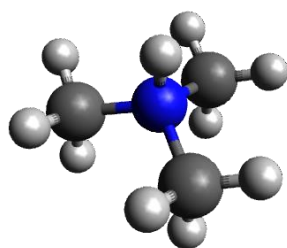
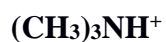
CH₃SOCH₃H⁺



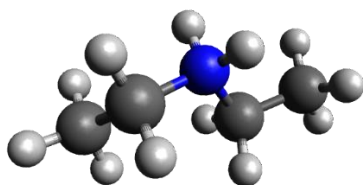
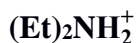
S	0.30768695120301	6.38453560689891	3.36018848277294
O	0.01121594897355	6.21482936618238	1.75653008246077
C	0.60173142949261	8.14353455185167	3.44806521282883
C	-1.33534194403003	6.24564651112279	4.05289571017155
H	1.54949006302032	8.34162494281138	2.93067849836553
H	0.69059786216213	8.38747566340435	4.51725841362248
H	-0.23900463393251	8.67767315781971	2.98609069594656
H	-1.64861927995900	5.19830067336529	3.94798134007118
H	-2.01348424350670	6.93363604233958	3.53146210652294
H	-1.24267405324889	6.50965297920053	5.11826499036476
H	0.49979189982551	5.43926050500342	1.41627446687247



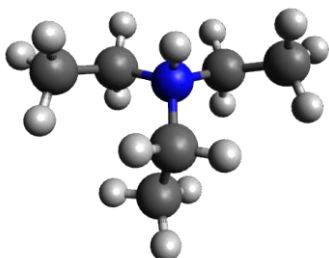
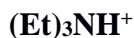
C	-8.90873170040300	2.98828243242455	-0.19298018145455
N	-7.66667177422674	2.82348967860982	0.60785227176757
H	-8.68841649582079	3.62406803061630	-1.05814813508148
H	-9.67431168845313	3.45822375906037	0.43590820184790
H	-9.25085843925573	2.00241358147017	-0.52982004859681
C	-7.10331185152922	4.09619852177887	1.13311070975834
H	-6.21182060758617	3.86934330600375	1.72897492910600
H	-7.86033312050504	4.58596939269415	1.75753340559537
H	-6.83555307333920	4.74169239003536	0.28839968491734
H	-6.95609197983575	2.34955340116652	0.03526277984232
H	-7.85900926904523	2.19242550614013	1.39633638229801



N	-3.97958143762654	6.14643801836740	-1.89349766965056
C	-5.40470489641498	6.50625598883218	-2.14082755932457
H	-5.98306008524150	5.58624120816614	-2.28363940260036
H	-5.46562834466731	7.13079634842502	-3.03976914148429
H	-5.78325029179740	7.05972960351966	-1.27222902899645
C	-3.11233066544931	7.35313160583547	-1.77459792891928
H	-2.07210181234608	7.02794436196019	-1.65252321984923
H	-3.43195341764342	7.93470142839424	-0.90033050267689
H	-3.21350960474166	7.95640363295664	-2.68472882495850
C	-3.83438474147191	5.24170984647950	-0.71858482911706
H	-4.43286772146109	4.33993417351429	-0.88932596966421
H	-4.18842682314933	5.76816356268426	0.17677477847760
H	-2.77807426422828	4.97153542807545	-0.60506570485877
H	-3.65261589376118	5.62403479278955	-2.71728499637743



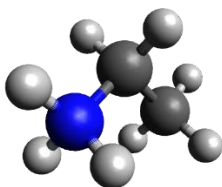
N	2.16086087972950	5.78576880915513	3.24110876494368
C	2.00043504645312	4.80333706427063	4.36472364734366
C	1.14024920741943	3.63266273096034	3.93760597884137
H	1.55817377101835	5.34756119596603	5.20817700345576
H	3.00979141525150	4.47608481767317	4.64986799193033
H	0.13542733976714	3.95973539683526	3.62661440764469
H	1.02758622332300	2.93951802336503	4.78390539818188
H	1.60643859214301	3.08301195386814	3.10468444589800
C	3.26989896728844	6.78757528818911	3.39205538097159
H	1.27164003663265	6.28525450079921	3.10528321239810
C	3.11743934945906	7.64460102461455	4.63191018955066
H	3.25260625485955	7.39900370331618	2.47996551481774
H	4.20643213024725	6.21312731079203	3.40034986281070
H	2.14081617919232	8.15467952626922	4.65039731766488
H	3.89787525216413	8.41985286079229	4.62378065310468
H	3.23266006444162	7.06182342554105	5.55757276238705
H	2.32305929060994	5.26610236759264	2.36903746805523



N	2.258273	5.793540	3.044243
C	1.957279	5.186795	4.392124
C	1.139815	3.913242	4.309258
H	1.462328	5.961385	4.993182
H	2.934588	4.983152	4.849200
H	0.110592	4.082365	3.960130
H	1.080163	3.479412	5.318482
H	1.620399	3.169006	3.654846
C	3.202703	6.964868	3.182547
C	1.031442	6.097554	2.211280
C	3.883518	7.343058	1.879167
H	3.947811	6.655944	3.925989
H	2.628491	7.798098	3.609666
H	4.386965	6.474720	1.423534

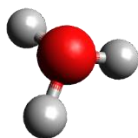
H	4.654755	8.095643	2.098828
H	3.195189	7.781332	1.142460
C	-0.002555	6.964895	2.903743
H	0.607170	5.128814	1.918106
H	1.398529	6.576738	1.295797
H	-0.488326	6.454452	3.748021
H	-0.784681	7.202561	2.167858
H	0.414363	7.918510	3.260592
H	2.775279	5.074985	2.519865

EtNH₃⁺



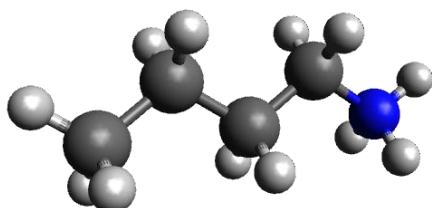
N	2.21752967853705	5.72305665174775	3.20879376612482
C	2.06998510343645	4.75917889189441	4.34571868500161
C	1.12269641834171	3.63566028973341	3.98967115051323
H	1.71223771972117	5.34284338611604	5.20361257948662
H	3.07607795998975	4.38414923360321	4.57399446634393
H	0.11254784097916	4.01609263224428	3.76927551549958
H	1.04994045023491	2.94270428363748	4.84085498828988
H	1.48503639718562	3.06648130356740	3.11873451627070
H	1.31939713661610	6.16345920926983	2.97028322456311
H	2.56320607635793	5.25769847177922	2.35985161777626
H	2.87684521860014	6.47684564640696	3.43755949013025

H₃O⁺



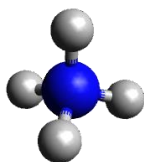
O	1.82322557966720	2.05185761775306	-1.00295481569697
H	2.78385740197037	2.23431501012614	-0.92893074565989
H	1.49432823397403	1.78983966717796	-0.11747820581479
H	1.37754878438839	2.88701770494283	-1.25758623282835

nBuNH₃⁺



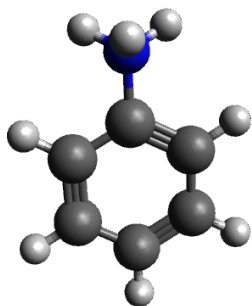
C	1.89018591804012	1.57159187069502	-1.07115389709004
N	3.12591851674589	1.78913466813295	-1.88724052290792
H	3.04990465756772	2.63176939752269	-2.47064621298630
H	3.95577475666168	1.90041757526741	-1.29066148320885
C	2.06353476191366	0.39681279388051	-0.12588563509004
H	1.06969047167947	1.41145548761001	-1.78257786362506
H	1.69857816056796	2.50566796767459	-0.52547346639571
C	0.78540867480724	0.08180793340506	0.65662902255469
H	2.88332551230239	0.62303517077255	0.57758991383275
H	2.37490055534258	-0.49327033003395	-0.70195020992671
C	0.99274785200105	-1.01941638299992	1.69192418916803
H	0.42353458658439	0.99742074997478	1.15773583655136
H	-0.00694061733244	-0.21417249609895	-0.05185065280805
H	1.73214914659449	-0.71617065053291	2.45124755306398
H	1.36247700817858	-1.94562241590600	1.22038261158187
H	0.05530826376299	-1.26256490667738	2.21696376102320
H	3.30554177458223	0.99471356731355	-2.51510294373721

NH_4^+



N	1.44545342403431	2.70286435324947	-0.67319882177380
H	2.22989556561697	3.24191579576873	-0.28816457230533
H	1.18730843746819	3.08413747610210	-1.59125906659090
H	0.64106563236058	2.76259266438762	-0.03816541119433
H	1.72954694051994	1.72151971049208	-0.78002212813564

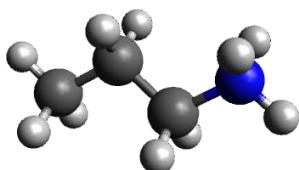
PhNH_3^+



H	4.25387329641357	1.56464264063212	-0.97829097664594
C	3.69836697201992	2.48145208694064	-1.18671444507386
C	2.31072315682809	2.52177322986716	-1.01531167259636
H	1.77665562986605	1.63230802396367	-0.67427872844472
C	1.60534309238205	3.70223213158144	-1.26783990236322
H	0.52355568980802	3.73884548131762	-1.12399980391323

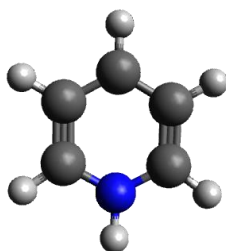
C	2.28036483149023	4.84709430697439	-1.69786345223802
H	1.74108500171111	5.77478763591116	-1.90278502835923
C	3.66069258028412	4.78235144673691	-1.86679798639988
C	4.38534183183740	3.61924274924179	-1.61707339851199
H	5.46854967091764	3.598997111109389	-1.75813878417622
N	4.37005890301843	5.97076874874521	-2.35551914039402
H	3.88274280860485	6.84077441347629	-2.10331624510724
H	5.32239580993958	6.03166872009216	-1.97168327011930
H	4.46071072487894	5.96285127342555	-3.38269716565676

PrNH₃⁺



N	4.23011650422479	5.60722529732583	-2.38896121903451
C	3.37532253193686	4.54733959887600	-1.77279983797069
H	5.13690182162632	5.68652650402193	-1.91230811297723
H	3.77507408629726	6.52755864442984	-2.34423527753258
C	4.07220360375828	3.19862819295978	-1.79157550137032
H	2.43631216786886	4.53006431802202	-2.34120059078520
H	3.15172547010630	4.87728190449511	-0.74960068197906
C	3.18922124274181	2.10885934745919	-1.19164891798677
H	4.33744747230292	2.93919655996410	-2.83099018543366
H	5.01921914350057	3.27049349583083	-1.23032486752844
H	2.24311449105747	2.00838238780624	-1.74682418640921
H	2.93548197546140	2.33055973964739	-0.14167389643945
H	3.70010471546877	1.13414092175922	-1.21714188279629
H	4.42308477364840	5.40567308740253	-3.37887484175659

PyridineH⁺

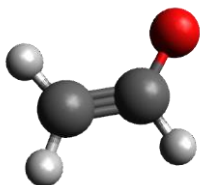


H	-0.24649092888731	4.96527394517997	-2.55566290918922
C	-0.03972392094022	4.38168650617815	-1.65920525467372
C	0.32216120622934	4.93006371544447	-0.43987930277556
H	0.42080916231730	6.01133834234120	-0.34468140122966
C	0.55824871070628	4.07654817160023	0.64178108118293
H	0.85183488899031	4.49281551501430	1.60736254522259
C	0.42676562656583	2.69324504220051	0.48433276344553

H	0.60859533096259	2.00584439305660	1.30980650813504
C	0.06261223954588	2.19123728571111	-0.75421133862282
H	-0.06684185319812	1.13098249787566	-0.97159451959297
N	-0.15588753106143	3.04481600654786	-1.77250857405407
H	-0.43087293123045	2.65654857884996	-2.67753959784808

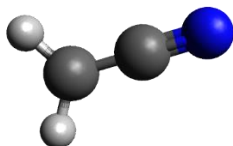
ANIONS

CH₂CHO⁻



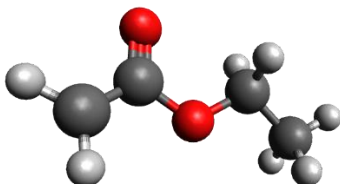
C	-6.89892301250380	4.13592854662754	-1.64528297798561
O	-6.73981552831611	4.48873768630204	-0.39215571131396
C	-7.88032962401289	4.51352521547082	-2.50881933136064
H	-6.12815277280401	3.44064754237821	-2.05591566966663
H	-8.69071230637206	5.18642495256135	-2.20304626562893
H	-7.89019675599114	4.12127605666004	-3.53020004404423

CH₂CN⁻



C	-7.00393013372671	1.12245312093306	-0.20397852016239
C	-5.70867499784008	0.74049310409774	-0.00592109480188
H	-7.50612453382903	1.74863772434914	0.53869825004641
H	-7.61007396478454	0.62197550020405	-0.96401751933623
N	-4.56193636981963	0.42599055041601	0.15333888425408

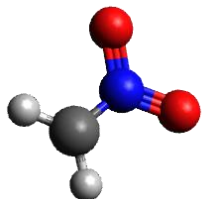
CH₂COOEt⁻



C	-7.00006349197201	4.52472182650670	-1.70913862173307
O	-6.60185217992552	5.20671523901608	-0.70139247881068
C	-8.18344598977791	4.61302297032628	-2.39162591993905
O	-6.10253086079796	3.56110822651282	-2.22153802446146
H	-8.91043573601535	5.37893080972408	-2.11382756584967
H	-8.41119792666744	3.93766982882185	-3.21835433829581

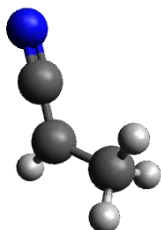
C	-5.11822455213600	3.03096188257605	-1.33238930328915
C	-4.27854234219276	2.02679447810117	-2.09526099767740
H	-5.61891999854763	2.54925502164909	-0.47244929823797
H	-4.48701019243778	3.84204187345475	-0.93448934991115
H	-4.90178452728344	1.21763586959850	-2.50855981092382
H	-3.53159451994760	1.57287304929164	-1.42494697837209
H	-3.74137768229859	2.50902892442100	-2.92801731249867

CH₂NO₂



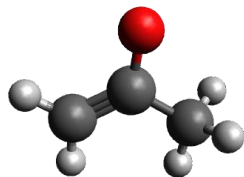
N	-7.17281531317300	4.29476683004891	-1.50291148740291
O	-7.11436616222345	4.87510193026858	-0.34048627589202
C	-8.07117814740505	4.63392184604624	-2.39434475859873
H	-8.77304611491009	5.42553366318240	-2.14162554177619
H	-8.06753834015310	4.11692513687565	-3.35121864464046
O	-6.29241592213532	3.36483059357822	-1.73940329168969

CH₃CHCN⁻



C	-5.20334232010727	6.42128126412473	-2.18323370348163
C	-4.91781911971468	4.95674712857095	-1.93238651077936
H	-5.39374764023788	7.01592667587628	-1.26346863381181
H	-6.09277982446842	6.57387241358885	-2.82434944832315
H	-4.36152442490150	6.91128295755901	-2.70241643012222
C	-3.65454722241168	4.44587316054059	-1.89202214940952
H	-5.71901322209422	4.32429462207071	-1.53264093232786
N	-2.54218622606435	3.98684177766889	-1.90369219174445

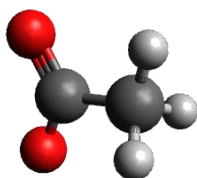
CH₃COCH₂



C	-5.51077616625207	5.43196468817379	-1.99751421403969
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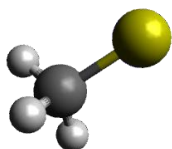
O	-4.97665176273235	6.47847430390667	-1.39505047287768
C	-6.84601752453996	5.68383171163215	-2.68261743066611
H	-6.73755627370843	6.45059020266227	-3.46987551670635
H	-7.57464023968180	6.08131391551989	-1.95433641494385
H	-7.26914569061642	4.77703330024219	-3.14152148885156
C	-4.95636062912192	4.18447273935433	-2.03726544936527
H	-5.44633947130535	3.35951328521240	-2.56041183013134
H	-3.99232224204168	3.98196585329630	-1.55664718241815

CH₃COO⁻



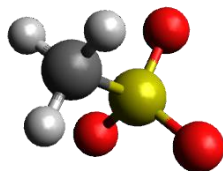
C	-5.41412357922854	5.34925614585977	-2.29858541179346
O	-4.53552179920640	6.26062497466666	-2.31404786447835
C	-6.85844302344851	5.72164955604454	-2.61207475625722
H	-6.94844001113820	6.74931597475928	-2.99151089489785
H	-7.45841950404704	5.62662102234569	-1.69180451341413
H	-7.28681694114534	5.02371661907550	-3.34701784530706
O	-5.17463514178596	4.13606570724855	-2.02012871385194

CH₃S⁻



S	-5.12230555626336	5.33300211888912	-2.24640429695578
C	-6.87775034154717	5.71774308783799	-2.60538367664759
H	-7.04491864054833	6.76718689876354	-2.93128570008381
H	-7.54811962735890	5.57185202474898	-1.73138569845269
H	-7.31604583428224	5.09281586976037	-3.41148062786013

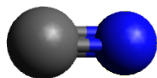
CH₃SO₃⁻



S	-5.37556917835362	5.02695834088013	-2.32801246330592
C	-6.91110605634121	5.93181313641765	-2.48788143255482
H	-6.67182292324628	6.98407062150696	-2.68950209023986

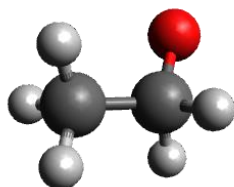
H	-7.46222002678808	5.83311011956469	-1.54284695012906
H	-7.48604796122157	5.49769961165789	-3.31578823400146
O	-4.61814000968790	5.22247354300576	-3.61147311541786
O	-4.65838042723524	5.61731124266918	-1.14781208491336
O	-5.75499341712610	3.59011338429774	-2.10616362943766

CN⁻



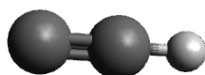
C	-6.66526831367756	2.24487392055595	0.94855809235265
N	-5.62385168632244	2.69004607944405	1.27420190764735

EtO⁻



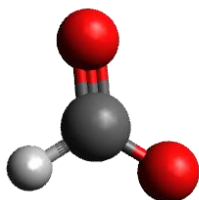
C	-6.32285599543338	1.18773376333951	0.41371041750000
C	-5.15791393888931	2.08193640153035	0.84431722167518
H	-6.22467221900767	0.89539859123041	-0.64718859885389
H	-7.29175063618982	1.70557064854509	0.53658230399242
H	-6.35593757699805	0.25961896289710	1.00994839148713
O	-3.89995045974113	1.49582010778219	0.67898720597248
H	-5.34603437787699	2.37942820493083	1.90761387500794
H	-5.24400479586365	3.03923331974453	0.27244918321874

HCC⁻



C	-7.94820845943289	2.49542373242551	0.11325045712915
C	-6.72919281625970	2.72775042307696	0.05963540693328
H	-9.00261872430741	2.26560584449753	0.16045413593756

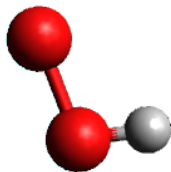
HCOO⁻



C	-4.18022874661894	2.04385490355348	2.45220695319593
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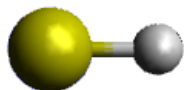
O	-4.43921666872617	0.86608776202389	2.08917010116883
O	-3.10142405682632	2.66936959644229	2.27451698640108
H	-4.99655052782856	2.59410773798034	2.99073595923416

HO₂⁻



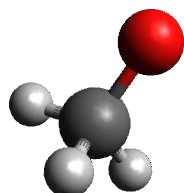
O	-10.47610929782990	-2.07860103031874	3.30276218915402
O	-9.08621512314413	-1.78674556272680	2.87092696638120
H	-10.74634557902596	-1.25348340695446	3.73487084446478

HS⁻



S	-10.31332376133084	-2.11470810579772	3.22443601021599
H	-10.99464623866916	-1.13660189420228	3.87874398978401

MeO⁻

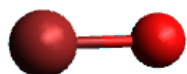


C	-4.84797428677519	1.18674136715400	2.81461193635869
O	-5.15795224371670	2.53955837752645	2.66660496971878
H	-3.90356879308668	0.88284477775894	2.29842346148243
H	-5.63171053111166	0.50149244658282	2.40751925929437
H	-4.71284414530977	0.87469303097779	3.87989037314573

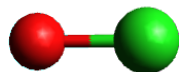
N₃⁻



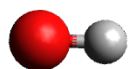
N	-4.72717001565941	-0.97333999215352	0.61498000703168
N	-4.38988087053328	-1.79012713746034	1.39797297016922
N	-5.06445911380730	-0.15655287038614	-0.16801297720089

OBr⁻

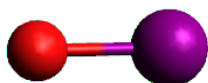
O	-5.16881290513731	1.81590996168867	-2.01481894586070
Br	-5.06519709486269	0.44874003831133	-0.73280105413930

OCI⁻

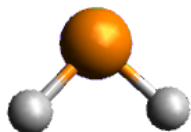
O	-5.16504637563532	1.76621208414478	-1.96821642257343
Cl	-5.06896362436468	0.49843791585522	-0.77940357742657

OH⁻

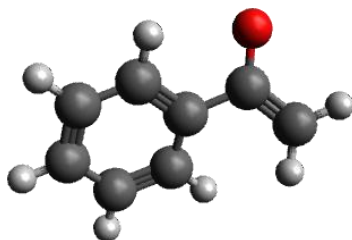
O	-5.14370762939576	1.48465570791241	-1.70419634307486
H	-5.09030237060424	0.77999429208759	-1.04342365692514

OI⁻

O	-5.17274288059637	1.86776444444561	-2.06344375359209
I	-5.06126711940363	0.39688555555439	-0.68417624640791

PH₂

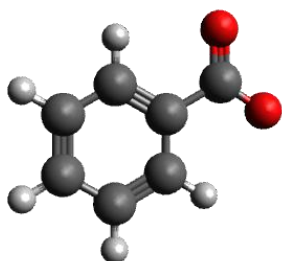
P	-4.88848015970551	0.24552972322619	-0.53224740291402
H	-3.67096392332364	-0.27130304387350	0.02547613431355
H	-4.20145591697085	1.18788332064731	-1.36886873139953

PhCOCH₂

H	-2.88687312946137	-3.12579691470618	3.82415252839596
C	-3.55960481426617	-2.83436767604172	3.01503586531727
C	-4.89762010804538	-3.27665552618848	3.02312374615125
C	-5.73621344807889	-2.83390527892715	1.98394771255107

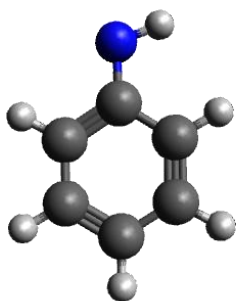
H	-6.77771786494124	-3.16076583195969	1.98033899329879
C	-5.25960327779454	-2.00133316476406	0.96637019128880
H	-5.93559761780679	-1.67641961727001	0.17082663859062
C	-3.92605197269234	-1.57998069288338	0.96826579363393
H	-3.54960098979430	-0.92473396285823	0.17823946929671
C	-3.08062400111443	-2.00014737741548	2.00160369403519
H	-2.04140648493731	-1.66147278630301	2.02565600825206
C	-5.45733736169111	-4.17972554007523	4.10187307081140
O	-6.75878825890570	-4.13825670302810	4.27807870282759
C	-4.60981862095420	-4.98955562377074	4.81071665962669
H	-3.54047060144669	-5.04267841446940	4.59792937001019
H	-5.00698144806954	-5.64624488933914	5.59202155591245

PhCOO⁻



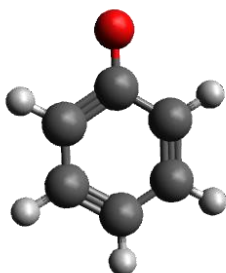
H	-2.89320327384034	-3.23883561558791	3.77464666952200
C	-3.56039263048675	-2.87793028168260	2.98988664826535
C	-4.90854990061077	-3.27202579407909	3.00526476712921
C	-5.75747300195704	-2.80411693638578	1.98877521048608
H	-6.80489916303692	-3.11114498721808	1.98953424841373
C	-5.27465723486376	-1.96010185562495	0.98459359771311
H	-5.94975326261834	-1.60260323137745	0.20311520866219
C	-3.93052417021968	-1.57030569958269	0.98237132607311
H	-3.55025989292620	-0.90870319363144	0.19945581144716
C	-3.07522378022564	-2.03286445961389	1.98813462649440
H	-2.02612741131813	-1.72643402184493	1.99336829819146
C	-5.43594882669036	-4.18202277643191	4.10653761469184
O	-6.66244912257159	-4.49279419647498	4.08175386741403
O	-4.61724832863448	-4.57696695046430	4.98673210549632

PhNH⁻



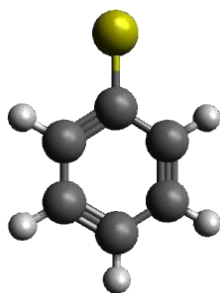
H	-2.97969947343840	-3.25451805292142	3.83967154280453
C	-3.63700892252850	-2.90280141471698	3.03586887927672
C	-5.00788524022499	-3.33615312501636	3.04535121809701
C	-5.79650039086202	-2.83935013166759	1.95180038127114
H	-6.84640872550000	-3.14675913453268	1.89526184581698
C	-5.27422329913949	-1.99572389235686	0.97630217379964
H	-5.93183065749036	-1.64726499644524	0.17233983012346
C	-3.93075901676157	-1.58126393992506	1.00397574740778
H	-3.52521535695664	-0.91785230837808	0.23620777734026
C	-3.12894092785170	-2.05526310358499	2.05472075565246
H	-2.07830637331214	-1.74964996106652	2.11201651192083
N	-5.55007174050493	-4.14300993457540	3.98746955892040
H	-4.82429987542925	-4.38050000481281	4.66961377756879

PhO⁻



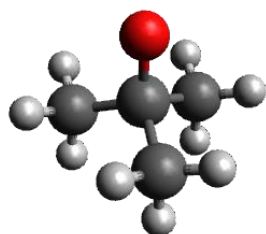
H	-3.00309894973980	-3.27097850583877	3.85434487486579
C	-3.64871713333957	-2.90898018008581	3.04773336029683
C	-5.01371624037780	-3.32659473700420	3.03819526964779
C	-5.80518464496757	-2.84204032109312	1.95321617894496
H	-6.85319499327427	-3.15509671357816	1.90137719389252
C	-5.27825549541699	-1.99754823866362	0.97544035229216
H	-5.92861980456857	-1.64576216505520	0.16804016385001
C	-3.93631277211105	-1.59209523993408	1.01617601129293
H	-3.52663485380274	-0.92890500333446	0.25034422613905
C	-3.13374037600940	-2.06305818880454	2.06474017342170
H	-2.08341446248269	-1.75888448967212	2.11977813338006
O	-5.50900027390954	-4.10755621693593	3.97012406197620

PhS⁻



H	-2.99626314915840	-3.24283840905162	3.83012152689452
C	-3.64054427342968	-2.88540353676533	3.02101806231779
C	-5.00153833638842	-3.31081972073131	3.01403172682250
C	-5.78708615662884	-2.81860607540383	1.93078602207525
H	-6.83546869617126	-3.12829203078715	1.88153103958415
C	-5.26436092991363	-1.97432470894612	0.95028742524433
H	-5.91764015356609	-1.62289978853688	0.14495218570265
C	-3.92105839010707	-1.57073492990605	0.98837899653289
H	-3.50998214627351	-0.91085940617556	0.22001461098540
C	-3.11987857650951	-2.04057038093232	2.03960832358876
H	-2.06920517354582	-1.73703399960475	2.09714862906018
S	-5.65686401830777	-4.35511701315908	4.24163145119157

Tert-Buo⁻



C	-4.84235830513223	-1.62192110313009	0.09736545770173
C	-6.36751428797601	-1.59065801353759	-0.13984240397363
H	-6.68064686596958	-2.23007636921286	-0.98289430590765
H	-6.70617039262964	-0.56278273829010	-0.35655556894578
H	-6.90403145920950	-1.94036967445662	0.75881680971427
C	-4.42287049025056	-3.08291785788857	0.37667384318859
H	-4.93481885383676	-3.46618198633143	1.27549245308543
H	-3.33589253957288	-3.14266154788937	0.55654184573047
H	-4.66414184327589	-3.76233088990477	-0.45904750174439
C	-4.13669091404698	-1.14540977404334	-1.19129999837525
H	-4.38929327832034	-1.76506439255222	-2.06878209112876
H	-3.04079032046627	-1.17099797543567	-1.06293042745613
H	-4.42354817980464	-0.10473533355305	-1.42149804248398
O	-4.49426226950874	-0.79567234377432	1.17792993059507