

Supplementary Material

Mechanisms of the formation of imines in aqueous solution and the effect of the pH: a theoretical analysis

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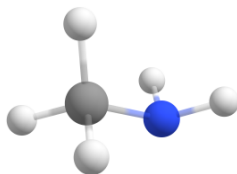
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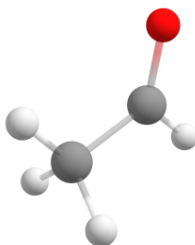
Coordinates of the optimized structures, obtained with the X3LYP functional and the def2-SVP basis set for C and H, and ma-def2-SVP basis set for O and N. Solvent effect obtained with the continuum SMD method in water.

MS1



N	-5.26401235692409	0.91593659814520	0.35683571776014
C	-6.56273604653515	0.38120743444600	-0.06020356853919
H	-4.81362887472060	1.38499691255716	-0.43023861348805
H	-4.64270743912648	0.14721450288601	0.61286546055630
H	-7.23837768610955	1.20538062589453	-0.33359799634405
H	-7.03192546943695	-0.16026126283105	0.77567539353788
H	-6.51724212714717	-0.31115481109786	-0.92133639348303

MS2



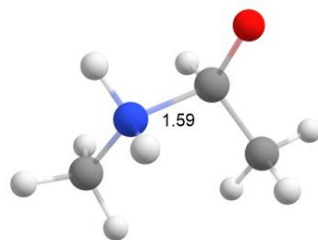
C	-7.31062737115367	2.42800733671458	0.00001106115704
O	-7.37379390996936	3.64769892925866	0.00009158285348
H	-8.25259952170799	1.83126692629228	0.00011174928397
C	-6.04628940659186	1.64463862993460	-0.00009262748713
H	-5.16236977912815	2.29652581191849	-0.00011003611831
H	-6.03896950444979	0.97983350820800	-0.88159576957270
H	-6.03948050699918	0.98004885767340	0.88158403988366

H2O



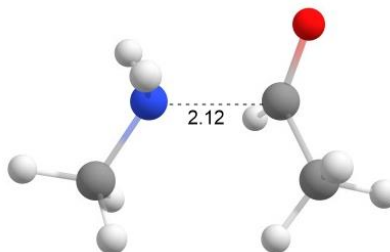
O	-3.60363949944461	1.19013489923631	-0.01540395682791
H	-2.63580610204266	1.16306703451380	0.02084240860864
H	-3.88309439851273	0.63549806624989	0.72732154821927

MSZ

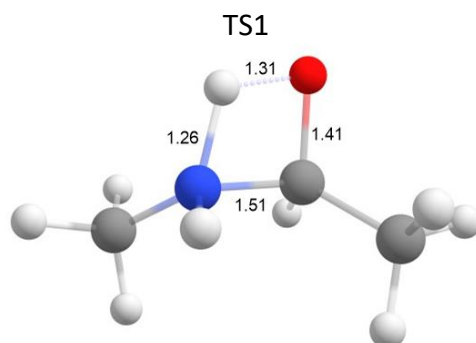


N	-5.24386212945786	0.81875139167039	0.09475476356660
C	-6.55599174377969	0.18447666757816	-0.17081220116242
H	-4.90873030931800	1.31533756298109	-0.74007631505435
H	-4.54219536940981	0.09845682127442	0.29701498880896
H	-7.24645084790429	0.92526246375442	-0.58900359082596
H	-6.95847221149655	-0.21592406602601	0.76892877152133
H	-6.42717810009399	-0.63563349394235	-0.88836845885810
C	-5.12016136077313	1.83992608535353	1.30894214760573
O	-3.83923272607184	2.20145686899726	1.40815319533751
C	-6.10423066167099	2.97798266827887	1.05622933647625
H	-5.49555408480371	1.20760293327965	2.14978499731596
H	-5.83767611834390	3.52284451192977	0.13456554009905
H	-6.03643003350591	3.68165678730600	1.90010000818789
H	-7.14865430337031	2.63578279756478	0.98645681698155

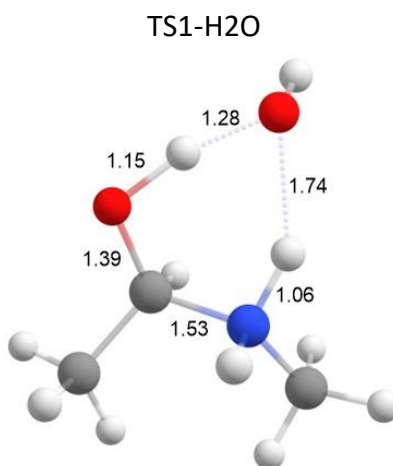
TSZ



N	-5.25047641443792	0.57598941836087	-0.15554903152412
C	-6.54597412613162	-0.04293659331175	-0.43644680416687
H	-4.89096860405602	1.08259421755220	-0.96718789438852
H	-4.55253948829342	-0.12235173754391	0.10442815431800
H	-7.24144908127002	0.70951866911992	-0.83418104233393
H	-6.97328617515892	-0.45247551886107	0.49216403471408
H	-6.47829126478701	-0.86407724704105	-1.17110190031584
C	-5.01483765940439	1.95306249380302	1.43244469405726
O	-3.79934889580632	2.26092137838654	1.41662649145434
C	-6.07744179371912	2.94129157121822	1.03141484100705
H	-5.36147927112356	1.16260290135140	2.13173879330653
H	-5.77323251603555	3.51736069349256	0.14419441053033
H	-6.20861655749246	3.64799741693090	1.87003014100816
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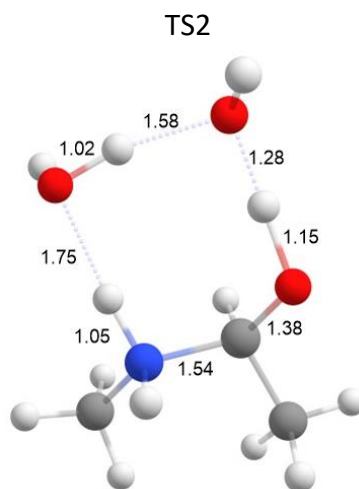


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H	-5.08075067501989	1.77707087619296	-1.03350477064228
H	-3.71252699821028	1.51417743357605	0.33355782442297
H	-6.23589649449229	-0.33845170471490	-0.47931386377874
H	-4.74518591633134	-0.79429913183617	0.40778592371816
H	-4.69494670716993	-0.56266321845328	-1.35786723155608
C	-5.14927755416097	1.86564840737943	1.08629155213345
O	-3.82357118205065	2.07293780739081	1.51691250113522
C	-5.96835541138644	3.12705946610304	0.90978733643008
H	-5.45312114230274	3.83133117364330	0.23668748021478
H	-6.10267720721689	3.61921338587755	1.88485640982247
H	-6.96497515377828	2.90066176791906	0.49748049421788
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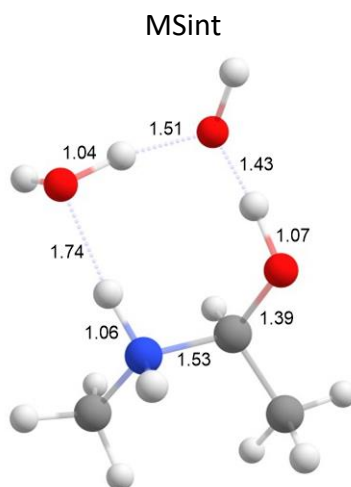


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H	-4.53805956841097	0.09099316328754	0.12397636515616
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H	-6.84966173143051	-0.46907822636503	0.52839999116442
H	-6.54187575654847	-0.15791339370168	-1.20596200861661
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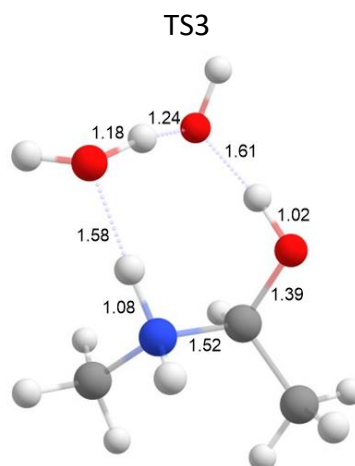
O	-3.95767429114078	2.37274921230080	1.35721833819129
H	-6.02802944551757	2.26541685346144	1.42312420803185
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O	-3.94227313836957	2.93783791257347	-0.99204053241151
H	-3.89615337050345	2.77546400388251	0.27973178256650
H	-4.39907110331712	3.76823574896504	-1.18634391368248
H	-4.26814591674002	0.01813285584684	2.59375324056723
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H	-5.10291896782259	1.28519063247702	3.53741191629950



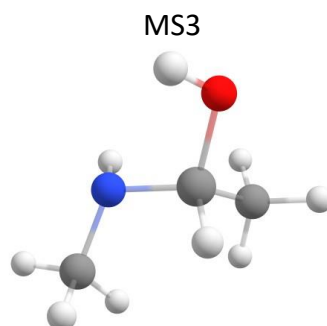
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H	-4.53863258708197	0.78735084119318	-0.42749680133365
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H	-7.47320305535170	0.81650323543781	0.06696218021775
H	-6.38710107837421	-0.56854420056828	0.44235706543338
C	-5.04905101122256	1.62955874825650	1.43573692821679
O	-4.00359673967658	2.52224460130011	1.41541378650399
C	-6.27129184468890	2.22358815441159	2.11300770951609
H	-4.77327030083928	0.66474794495862	1.90409171491945
O	-3.06596649077067	0.02505532531628	-0.97643728499712
H	-2.92939575970561	-0.90363964453968	-0.73725951801439
H	-2.48100264147621	0.56915607026523	-0.34262732951272
H	-2.99263723628126	2.07166614028071	1.08788320329994
O	-1.87596642361060	1.57749830507780	0.70838635204778
H	-1.39862401503349	2.28227579157969	0.24875383527130
H	-6.63246919971706	3.10122469328156	1.55332413235580
H	-5.98102923355751	2.55266370646733	3.12062051677527
H	-7.09070454377747	1.49893914110498	2.21492531607469



N	-5.52514337185785	1.56168679939380	-0.20664081743269
C	-6.72106676127694	0.69296243925327	-0.32022535181593
H	-5.67340588331396	2.42607972848293	-0.74223246078862
H	-4.70111884227126	1.06922340927767	-0.64438808067058
H	-6.82084433892515	0.36234513774702	-1.36127304331880
H	-7.61813972178544	1.24970835530834	-0.02804573263071
H	-6.58737847142616	-0.18173379317487	0.32841912897742
C	-5.11866711978200	1.96013101261597	1.21250019018581
O	-3.96522497918823	2.72229910753392	1.12852713895586
C	-6.23695098504142	2.72158768086806	1.89304350343674
H	-4.93397074901794	0.99796891410744	1.72248549592474
O	-3.24231260191460	0.30459134360725	-1.20300690067501
H	-3.24264825576742	-0.66184481164282	-1.25606464135261
H	-2.68416000092183	0.55211934848451	-0.36635955345012
H	-3.12301798009844	2.07287272364828	1.05214746321441
O	-2.09230105932965	1.08726244035959	0.92083248413040
H	-1.25217692563032	1.52620232041004	0.72750732711352
H	-6.51778160178387	3.61194238782578	1.30791647889187
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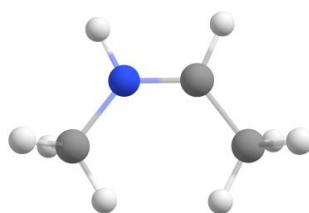


N	-5.42766494045413	1.36497502272644	-0.06618880582976
C	-6.27337716881758	0.15172078609490	0.02824448779332
H	-5.90387140317807	2.07238523620341	-0.63870775863548
H	-4.52308993270930	1.10142676097994	-0.60045569970227
H	-6.50854189394597	-0.19907259532929	-0.98419578288098
H	-7.20540558073213	0.37509212524629	0.56131109647718
H	-5.71940493882049	-0.62892537373666	0.56523118338299
C	-5.06950982646879	1.98838644746341	1.27635068123360
O	-3.88382780423502	2.71042660673163	1.15561021366917
H	-4.94139761290019	1.13186431072678	1.95856053787897
O	-3.16465843947335	0.72919767749312	-1.31959072466560
H	-3.12731308860003	-0.17969588338239	-1.64998333683205
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O	-2.01169737296142	0.92206398982671	0.79382225025415
H	-1.12842157221469	1.29708900505022	0.67099351588415
C	-6.18819283401481	2.89542121301355	1.73813313882804
H	-6.31281355480301	3.73194897767118	1.03257064767103
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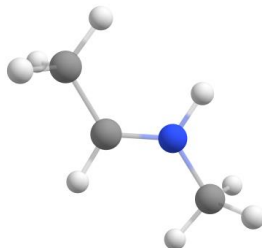


C	-7.25893150570495	1.86477210340954	0.37879341157903
O	-6.21583458948172	0.94101564463249	0.68481786495950
N	-8.54841876994701	1.23706204136803	0.62618304102649

C	-6.99142261811526	3.11771190191638	1.19407665259960
H	-7.22409961358897	2.11357534363381	-0.69746731762994
H	-6.40261912739297	0.11792128794503	0.20760685550238
C	-9.67631542895325	1.88113809522165	-0.04103972217805
H	-8.71696219364676	1.23978509654308	1.63475984892274
H	-9.78032871321015	2.96074137953371	0.18504852982911
H	-10.60874668076544	1.38720781939570	0.26690545499036
H	-9.58743946339665	1.76968767637333	-1.13362774256720
H	-6.00347258695003	3.53971502844436	0.95292182845370
H	-7.02385187559828	2.88408591848062	2.27183331532449
H	-7.74709683324856	3.88765066310227	0.97764797918780

MS4H⁺

C	-6.89167826707524	2.03744024590900	-0.05751238402216
N	-7.90736321314775	1.39715090448686	-0.52197801032025
H	-6.46097332171341	1.61984834790796	0.85826493227547
C	-6.27457762972347	3.24590280939228	-0.62111393735833
H	-6.73758382470374	3.61832530732309	-1.54050472014390
H	-5.20559315106655	3.03385346698307	-0.79507742408618
H	-6.30673379731837	4.02738973589851	0.15823818593673
C	-8.69234451510649	1.67893419964460	-1.71702973966895
H	-8.25757586143625	2.50598980265921	-2.28396026209355
H	-9.71822271504664	1.93227965930896	-1.41544105373303
H	-8.71628069887212	0.77378933884479	-2.33868015177926
H	-8.21276300478998	0.57859618164167	0.01103456499342

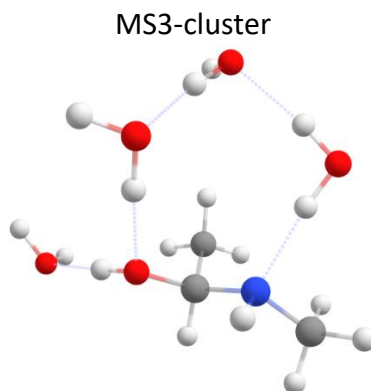
MS5H⁺

C	-7.03361476137244	2.00518097615613	-0.11150955666186
N	-8.05474877307409	1.38461670438986	-0.58164572536420
H	-6.61250140255134	1.61927609070843	0.82355654249347
C	-6.41867877455543	3.17767791602959	-0.74845208439195
C	-8.69745313234459	0.21827351146736	0.01221823103632

H	-8.19177567003981	-0.04547130770492	0.94700631530559
H	-8.64259039911173	-0.61938737517396	-0.69616007656849
H	-9.75250527641715	0.45375220884602	0.20871027755759
H	-6.90817690785364	3.46456881936890	-1.68776265517656
H	-5.35201300763054	2.95622257260307	-0.92521723351878
H	-6.44435350854352	4.01603375478642	-0.03123437594172
H	-8.46642838650573	1.72524612852310	-1.45654965876942

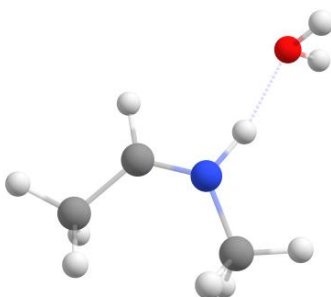


O	-3.60381467095367	1.18978075977902	-0.01492585257951
H	-3.88291532904633	0.63584924022098	0.72684585257951

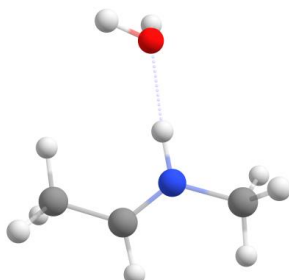


C	-6.85436798777879	2.38577437876243	-0.24217138383505
O	-6.67508739142301	3.58314743689223	-0.99536818865435
N	-8.02563634369791	1.71975176715059	-0.81797440722760
C	-7.02781108104515	2.68227595440822	1.24058609921324
H	-5.95327213457606	1.75384880562021	-0.39137745295513
H	-5.90526528345093	4.08046409900401	-0.62983075220216
C	-8.07348340433355	0.28234868098116	-0.53701777453298
H	-7.96209506575951	1.84671778754413	-1.82991673507773
H	-8.21480109681132	0.10313893601215	0.53912945336640
H	-7.15657027543135	-0.24933814374000	-0.85553065803639
H	-8.92696852752782	-0.16542719607528	-1.06435469289052
H	-7.23587801962044	1.76279489608192	1.80720851726408
H	-7.85765383109311	3.38839599793258	1.39900648281515
H	-6.11121715557723	3.12765123804675	1.65653584034491
O	-4.54633420238985	5.02576740573336	0.03605896225256
H	-4.32914713117373	4.84506192181629	0.96355742393976
H	-4.77884476989214	5.96767722361157	0.02697880835752
O	-8.83273313045728	5.25918469544492	-1.30899719373276
H	-8.03071928246858	4.68994733354762	-1.21490149607132
H	-8.50296489674980	6.13938628393622	-1.54003876530124

O	-10.41614388430552	5.00386387036542	0.89280851630618
H	-9.79526532482238	5.19913482834214	0.14822790163948
H	-9.93262372595489	5.24141731921821	1.69764620340931
O	-10.57825816070802	2.25758159441353	0.28275437891205
H	-10.58966254745128	3.19316173451072	0.57610697932511
H	-9.66565534550026	2.13528115043878	-0.09000606662848

MS4H⁺-cluster

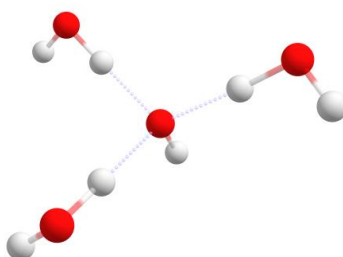
C	-6.99836948316842	2.08915791682175	0.03039846754361
N	-7.99245691097021	1.43757869319059	-0.46094201477410
H	-6.66598177735971	1.76265539961878	1.02132349261147
C	-6.27915497459342	3.17847340706848	-0.65181761862323
H	-6.92023096387644	3.75627837437206	-1.33187375515102
H	-5.47184050721857	2.72057067282630	-1.25482885450267
H	-5.80161931888980	3.83828045030976	0.08473475577048
C	-8.57913828753048	1.65341360458540	-1.78212742444437
H	-8.91366427825771	2.69455322413909	-1.89026953626291
H	-9.43812055436680	0.98477193513651	-1.89456574951225
H	-7.83861044378313	1.42780953097200	-2.56230610719385
H	-8.38014169585126	0.67366661168992	0.13806901834213
O	-8.78613138404282	-0.45359641921975	1.39992768352007
H	-8.76769269612688	-1.36572520212762	1.06911937097188
H	-9.68846672396430	-0.33915819938331	1.73692827170479

MS5H⁺-cluter

C	-7.08625819486478	2.00503797692355	-0.08628772492638
N	-8.01391096566191	1.26825088473974	-0.57860911333406
H	-6.73812960891989	1.76258536306497	0.92433861472666
C	-6.47429500050410	3.13849334669694	-0.79839702351404

C	-8.64244852082759	0.14204363377494	0.09873863313503
H	-8.21209621679001	0.01929057966956	1.09936061436912
H	-8.48266361213535	-0.76935050729123	-0.49375692079762
H	-9.72309166906375	0.32829366603317	0.17652516015644
H	-6.91351639259399	3.31311245870048	-1.78947793800459
H	-5.39154652869086	2.94577168790643	-0.89363350143000
H	-6.57479914041780	4.04189553200376	-0.17408828718226
H	-8.34633119116805	1.46825947996378	-1.54968674510045
O	-8.91694914026089	1.66992267067077	-3.20906009555013
H	-8.29791818339904	2.06363681911889	-3.84343624981995
H	-9.71148563470199	2.22292640802424	-3.27181942272776

OH-cluster



O	-3.94060499622666	1.23110304913552	0.21070292272186
H	-4.75000871818598	1.70592384202131	-0.02576123578365
O	-4.35934099525508	-0.67514372196435	1.96580371221892
H	-4.23679090468130	0.07106613217783	1.28594346830522
H	-5.20386563971290	-1.08587372803963	1.73431445305110
O	-3.15048855585745	-0.20082414369423	-1.83147931036684
H	-3.48886803277339	0.35324522114229	-1.04641215844217
H	-3.91655592268456	-0.71544770077137	-2.12115126107321
O	-2.13120164438510	2.94867506224449	0.94045583727589
H	-2.84871576203568	2.29285151312879	0.62863647500808
H	-1.77894882820195	3.33793447461934	0.12779709708482

Pyridine



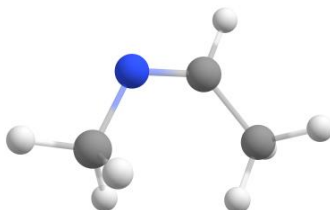
C	-10.44284436674023	4.90327076200995	0.00021710273203
C	-9.19886237296036	5.53700329715143	0.00008780254449
C	-10.47943783565055	3.50806958687788	0.00007661069285
H	-11.37190677994311	5.47622938133689	-0.00004215425212

C	-8.04666063641891	4.74918935375683	-0.00012735808797
H	-9.12584207011121	6.62759128238044	0.00003972971730
C	-8.18902302448812	3.36086719317896	-0.00011574374898
H	-7.05203380308522	5.19914367438430	-0.00017441065107
N	-9.37811009590932	2.74209318253854	-0.00002454687840
H	-11.43959929322736	2.98311435129653	-0.00019262465262
H	-7.30456972146560	2.71692793508825	0.00025559258451

PyridineH⁺

C	-10.44985538069542	4.90155043666397	-0.00042173333900
C	-9.19850718377402	5.52559128419317	0.00270443278024
C	-10.50820291693143	3.51785057374655	-0.00717601048152
H	-11.37388444552511	5.47907640387158	0.00202266992489
C	-8.03142365085546	4.75582245110503	-0.00071422716482
H	-9.13036671063350	6.61560222410053	0.00798179720564
C	-8.13993720148193	3.37539802094007	-0.00751620902310
H	-7.04471663457354	5.21867705969440	0.00201779607401
N	-9.36220877103876	2.80937624602120	-0.01091654373825
H	-11.43502014966864	2.94470305246839	-0.01093673963827
H	-7.28836777213156	2.69596072855235	-0.00947642234891
H	-9.42460918269063	1.78879151864278	-0.01613881025090

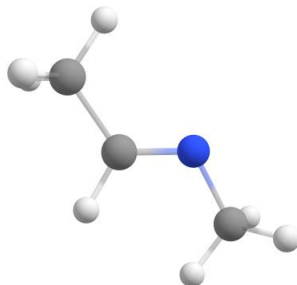
MS4



C	-7.04832767966448	2.02943608850922	-0.32731290908620
N	-7.99423957083117	1.38949253047210	-0.90203937730521
C	-6.47055097512466	1.82774592164347	1.03750792634403
H	-6.59284257673867	2.84588266662730	-0.91040256846133
C	-8.64894710787218	0.29716876285284	-0.19055680167868
H	-7.93508219610853	-0.42293520171039	0.24262472417713
H	-9.30404207274126	-0.25319024094982	-0.87991047834974
H	-9.27954637864099	0.67795486952210	0.62979295593490

H	-6.94898145686808	1.02407526246827	1.60967416244674
H	-6.55531889912226	2.76879060692481	1.60815433310753
H	-5.39095108628774	1.61164873364009	0.95155803287084

MS5



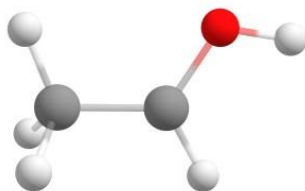
C	-7.09756553122744	1.98480071940775	-0.14381948794781
N	-8.11594038314187	1.41881536145150	-0.66371887387479
H	-6.66210006190608	1.59395470761751	0.79723401614866
C	-6.41679937039100	3.17927502347603	-0.72113645553434
C	-8.67090272851470	0.26335822315921	0.01500803779907
H	-8.13054036995623	-0.00986140307181	0.93920341151549
H	-8.66585502409788	-0.60437905407317	-0.66334323230160
H	-9.72510742848491	0.45436118929378	0.27318057323325
H	-6.89027898728289	3.52041249883447	-1.65204201139726
H	-5.35649314343736	2.94471261105839	-0.92017462699816
H	-6.42281697155964	4.00448012284634	0.01179864935751

MS1H+

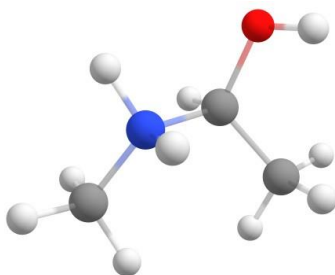


N	-5.29916304013977	0.89588632274845	0.33483748128405
C	-6.62253360668286	0.35566263630878	-0.08058664575834
H	-4.84613659743606	1.41216395435263	-0.42995644770039
H	-4.65984437006692	0.14358100233615	0.61984479816151
H	-7.26619198592099	1.19034334090569	-0.37956088694718
H	-7.06614819887331	-0.18098959643595	0.76591045733307
H	-6.47485052927503	-0.32680548916365	-0.92486157401877
H	-5.38844167160506	1.54074782894791	1.13008281764605

MS2H+

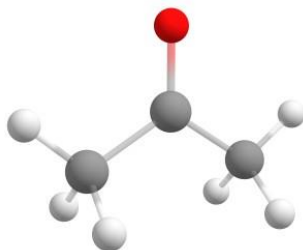


C	-7.31051429590657	2.36147855875897	-0.01894894474046
O	-7.35754281875187	3.62263388295464	-0.04303792684770
H	-8.26223976936234	1.80996061495406	-0.01475117300577
C	-6.04433830736081	1.66261306104447	0.00115905198727
H	-5.17861071865033	2.33406967089356	-0.00108154461135
H	-6.03728881628149	0.97123457339869	-0.86354166496053
H	-6.05279664419429	0.99422575608558	0.88352346843357
H	-8.27233862949230	3.97601388191004	-0.05320126625503

MS3H⁺

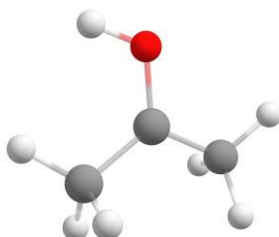
C	-7.00426536416539	2.32092779948802	-0.04768737365937
O	-6.96403177635802	3.71983812994782	-0.04176519710693
N	-8.46528498494103	1.90894232201349	0.03215262947484
C	-6.20557697495686	1.68368478652767	1.06277520716189
H	-6.66655571017741	1.98966986876187	-1.03895316268415
H	-6.96290252593017	4.04916878739598	0.87193417789541
C	-8.76073863124943	0.47732809277545	-0.24376735592206
H	-8.97612214441763	2.49729466965306	-0.63967183185363
H	-8.27395674704863	-0.14730338887858	0.51137723191796
H	-8.39220189431332	0.22568547667720	-1.24565369400998
H	-9.84632767325873	0.33356413323472	-0.19374528769983
H	-6.19457438819262	0.58857037851180	0.97352967666056
H	-6.61459867097466	1.96157447966911	2.04843669411890
H	-5.16854962787438	2.04025675945973	0.99536451632115
H	-8.82810288614173	2.16058770476267	0.96273376938521

Propanone



C	-7.17006485211425	2.50375092194796	-0.00070558546324
O	-7.13298845560209	3.73199968543485	0.00000840830878
C	-8.47826917533238	1.76372384391102	0.00069415485144
C	-5.91076805020633	1.68250677970386	-0.00059765528978
H	-5.02086091767742	2.32549079474357	0.00258010958288
H	-5.89456100929067	1.02453214096975	-0.88545095596101
H	-5.89775473839567	1.01981593612078	0.88072664817009
H	-9.32341758500883	2.46471823405301	-0.00179860515000
H	-8.53678623222940	1.10938179916435	0.88619260231463
H	-8.53561898414295	1.10428986395086	-0.88103912136381

PropanoneH+



C	-7.18895938671979	2.54883128238076	-0.06123703205430
O	-7.00899129333332	3.78843085282444	-0.30243559976281
C	-8.53923567360445	1.98265559200942	0.01361102191623
C	-5.98588033040631	1.73192342545071	0.12613006567774
H	-5.11384390799698	2.34057661368704	0.39478960693892
H	-5.79248955952629	1.24555356832579	-0.85073812061252
H	-6.17120295451656	0.92257761632762	0.84472906977116
H	-8.72434048127833	1.74750926342361	1.07873077844772
H	-8.56993037110511	1.02066231355388	-0.51977418412797
H	-9.30860084059467	2.67311801771257	-0.35366517500702
H	-7.84516520091820	4.27453145430418	-0.45738043118715

H3O⁺

O	-3.59003698975942	1.23517131145126	0.03723069069225
H	-2.61309337495162	1.16429559952026	-0.00359823033458
H	-3.91119045252630	0.61539519817902	0.72517897994947
H	-3.95076918276266	0.94306789084946	-0.82634144030714