Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Neutral species from "non-protic" N-heterocyclic ionic liquids†

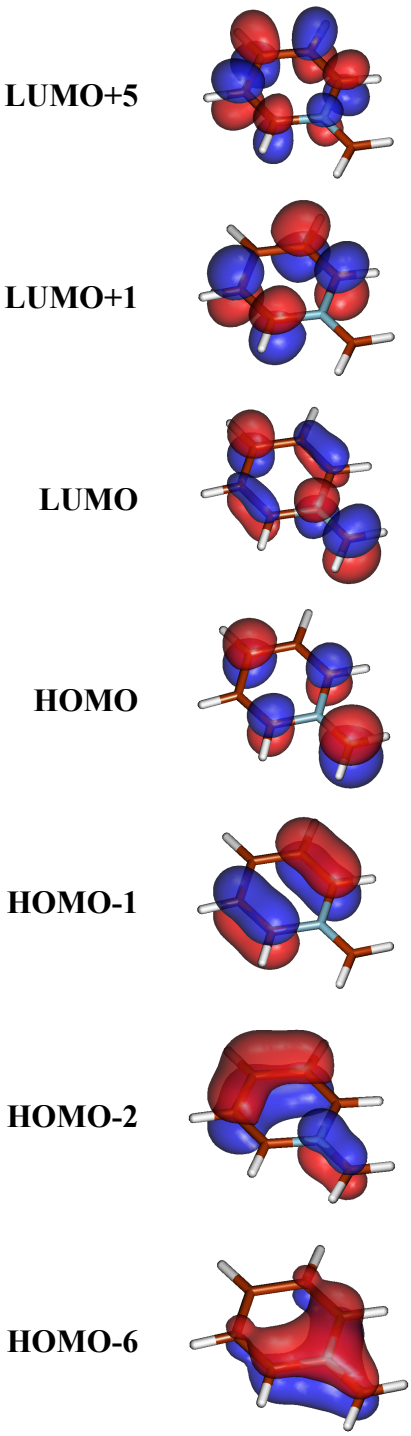
Supporting information

Oldamur Hollóczki and László Nyulászi*

Budapest University of Technology and Economics, Department of Inorganic and Analytical Chemistry, Szent Gellért tér 4. Budapest H-1111, Hungary. Tel: +36 1 463 3281; E-mail: nyulaszi@mail.bme.hu
Materials Structure and Modeling Research Group of the Hungarian Academy of Sciences, Budapest University of Technology and Economics, Szt. Gellért tér 4.,Budapest, H-1111, Hungary.

Table of contents

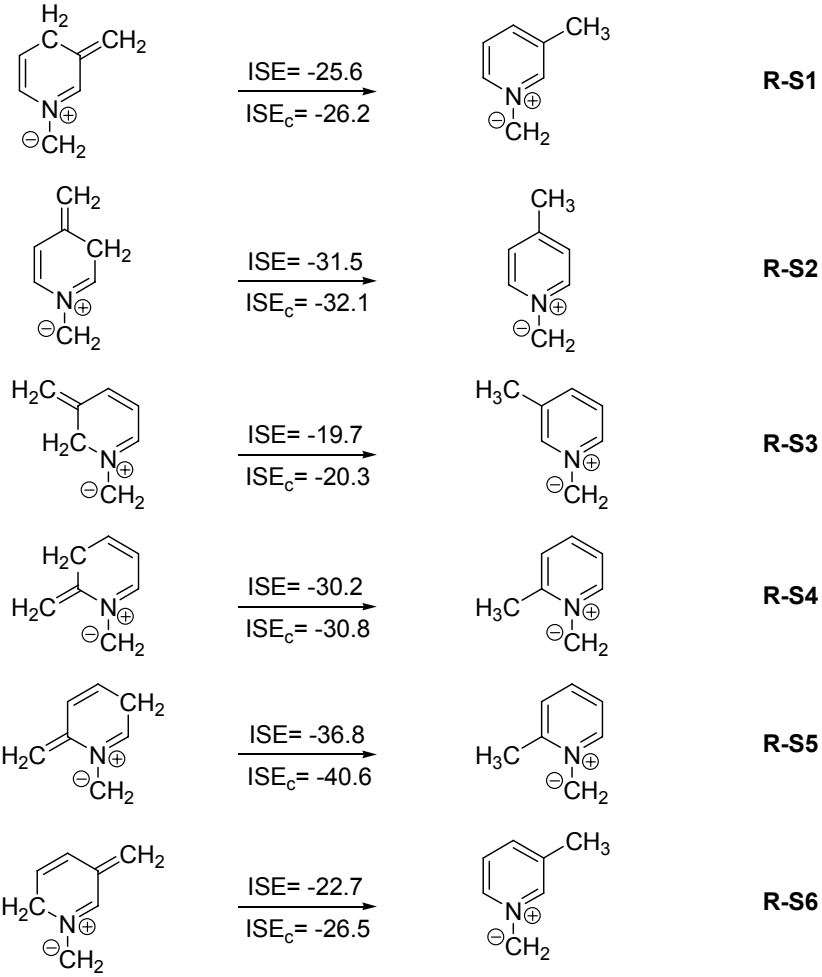
π-orbital of pyridinium-ylide 7



Scheme S1. π-orbitals of pyridinium-ylide **7**.

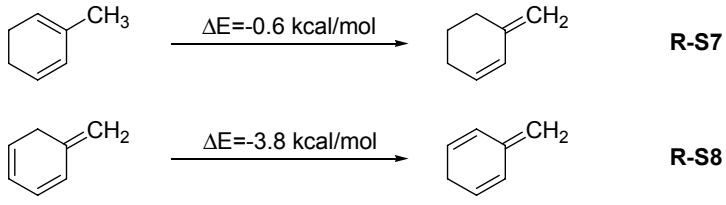
Detailed discussion of the ISE_c values of pyridinium-ylide 7

ISE reactions for **7** (**Scheme S2.**) have been constructed according to the analogue reactions for pyridine.[1]



Scheme S2. ISE reactions for **7**, their energies (ISE) and the corrected values (ISE_c) in kcal mol^{-1}

In order to cancel out the *anti-syn* mismatches (similarly to the case of pyridine),[1] the energies of the reactions **R-S1** – **R-S4** in **Scheme S2** have been corrected with the energy of reaction **R-S7**, while reactions **R-S5** and **R-S6** have been corrected with the energy of reaction **R-S8** (**Scheme S3.**).

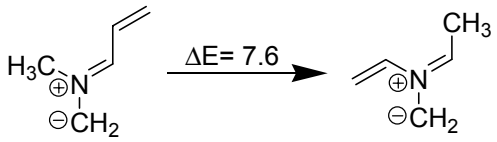


Scheme S3.

In the substrate of reactions **R-S4** and **R-S5** the two methylene moieties are bent out of the ring plane, due to steric repulsion. This destabilizing interaction results in the overestimation

[1] P. v. R. Schleyer, and F. Pühlhofer, *Org. Lett.* 2002**, 4**, 2873-2876.

of aromaticity, hence these two reactions should be excluded for further discussion. However, the remaining reactions also scatter significantly, which can partly be attributed to the different stabilizing effect of the C=C-N=C and C=C-C=N units in the substrates. To evaluate the extent of this error reaction **R-S9** has been investigated (**Scheme S4**).



Scheme S4.

Apparently, type C=C-C=N conjugation provides higher stability for the substrate of reactions **R-S3** and **R-S6**, resulting in lower ISE values.

XYZ coordinates and total energies of cations 1, 3 and 5 at the B3LYP/6-31+G* level

1

E(B3LYP/6-31+G*) = -305.235160

C	1.367145	0.116034	1.794736
N	0.056328	-0.011290	1.371402
C	0.049697	-0.086151	0.034306
N	1.310166	-0.011334	-0.411801
C	2.152034	0.116035	0.678521
C	-1.127729	-0.056524	2.244303
C	1.731068	-0.056634	-1.821372
H	0.847131	-0.161231	-2.451408
H	2.251224	0.869718	-2.073911
H	2.391499	-0.912654	-1.974780
H	-2.019643	-0.161169	1.625614
H	-1.048718	-0.912493	2.917765
H	-1.189461	0.869864	2.819166
H	3.223335	0.194732	0.568984
H	1.626583	0.194730	2.839911
H	-0.829727	-0.190127	-0.584153

3

E(B3LYP/6-31+G*) = -344.562477

C	-0.023144	0.001218	-0.149062
N	-0.051742	-0.031394	1.198870
N	1.271908	0.033425	-0.525217
C	1.749200	0.069040	-1.914687
C	2.074831	0.020244	0.601805
C	-1.260294	-0.071448	2.037208
C	1.246575	-0.019919	1.680841
H	1.463996	-0.041048	2.737677
H	3.152004	0.040784	0.537727
H	1.348855	0.947592	-2.426008
H	2.837385	0.128558	-1.901613
H	1.445248	-0.839829	-2.439783
H	-1.840242	-0.970875	1.819197
H	-0.946922	-0.095091	3.080828
H	-1.866366	0.821140	1.867363
C	-1.191386	0.001685	-1.072068
H	-2.130050	-0.027053	-0.516409
H	-1.196277	0.902143	-1.697582
H	-1.165261	-0.869172	-1.737644

5

E(B3LYP/6-31+G*) = -287.978828

C	-0.002704	-0.003232	-0.004065
N	-0.004259	-0.002222	1.351041
C	1.160681	0.000750	2.045550
C	2.378529	0.004157	1.385887
C	2.398883	0.004212	-0.012087
C	1.189457	0.000212	-0.711336
C	-1.291895	-0.048640	2.091474
H	1.076425	0.000308	3.126375
H	3.294310	0.009347	1.967049
H	3.343382	0.009174	-0.547602
H	1.159844	0.002237	-1.795551
H	-0.972326	-0.006626	-0.488205
H	-2.087134	0.325723	1.447304
H	-1.501878	-1.081303	2.381406
H	-1.216506	0.582276	2.977870

XYZ coordinates and total energies of the deprotonated cations at the B3LYP/6-31+G* level

2

E(B3LYP/6-31+G*) = -304.809082

C	-0.017511	-0.094819	-0.014922
N	0.070026	-0.011561	1.349372
N	1.296286	-0.011555	-0.393023
C	1.727434	-0.054724	-1.781913
C	2.162502	0.117490	0.688306
C	-1.091811	-0.054700	2.224045
C	1.380299	0.117103	1.799820
H	0.835755	-0.159593	-2.401178
H	2.251995	0.868331	-2.054074
H	2.392328	-0.908620	-1.955265
H	-1.975730	-0.159466	1.593738
H	-1.030586	-0.908652	2.908359
H	-1.170868	0.868317	2.809755
H	3.234971	0.196658	0.580992
H	1.641317	0.195821	2.845596

4

E(B3LYP/6-31+G*) = -344.129408

C	-0.017720	0.050114	-0.027526
N	-0.026674	-0.027396	1.367646
C	1.280890	-0.083864	1.846268
N	2.078059	-0.049109	0.703784
C	1.271856	0.036889	-0.434273
C	3.518727	-0.074075	0.747284
C	1.690133	-0.154082	3.146264
C	-1.181918	-0.026780	2.229850
H	3.908320	-0.037220	-0.272930
H	3.908610	0.787155	1.307510
H	3.878682	-0.992327	1.231134
H	-2.085539	0.023719	1.617572
H	-1.216103	-0.941539	2.837274
H	-1.163926	0.837624	2.908129
H	-0.932925	0.102545	-0.596989
H	2.741645	-0.193831	3.398044
H	0.972719	-0.175442	3.955891
H	1.695716	0.075455	-1.425989

3 deprotonated at position 1

E(B3LYP/6-31+G*) = -344.087737

C	0.216586	0.078332	0.201110
N	0.109029	-0.002359	1.564223
C	1.384840	0.043612	2.102099
N	2.280881	0.106162	1.081401
C	1.546063	0.153753	-0.109752
C	3.660864	0.010156	1.184268
C	1.786878	-0.168337	3.509281
C	-1.122928	-0.030005	2.326959
H	4.184620	0.310513	0.283642
H	4.070105	0.347669	2.129520
H	-1.963258	-0.037508	1.629638
H	-1.180909	-0.930048	2.949809
H	-1.206870	0.853722	2.971533
H	-0.651792	0.097355	-0.440105
H	2.464519	-1.037855	3.577703
H	2.343606	0.690466	3.914780
H	0.922136	-0.343028	4.155604
H	2.042824	0.208558	-1.065060

3 deprotonated at position 4

E(B3LYP/6-31+G*) = -344.100516

N	-0.088648	-0.004824	0.167340
C	-0.126263	0.010496	1.520111
N	1.153929	0.011184	1.932790
C	1.219438	-0.012552	-0.368439
C	1.970691	-0.003575	0.791833
C	1.611511	0.009932	3.315771
C	-1.285111	-0.007437	-0.664983
H	-0.944665	-0.066393	-1.698672
H	-1.922234	-0.870621	-0.439114
H	-1.866098	0.912379	-0.526388
H	2.701983	0.056445	3.310020
H	1.229894	0.881060	3.858577
H	1.302953	-0.904041	3.834454
H	3.044425	-0.002630	0.922494
C	-1.341331	-0.001088	2.386258
H	-2.070087	0.748469	2.055461
H	-1.846792	-0.977064	2.368235
H	-1.088081	0.220260	3.427143

6

E(B3LYP/6-31+G*) = -287.535985

C	-0.103469	0.056836	-0.054727
N	-0.003669	-0.013437	1.314089
C	1.157608	-0.067411	2.038032
C	2.374711	-0.053867	1.401905
C	2.383010	0.016740	-0.005786
C	1.177527	0.069130	-0.685705
C	-1.260096	-0.033334	2.089402
H	1.062379	-0.120306	3.118890
H	3.290645	-0.096896	1.982185
H	3.331809	0.029227	-0.539708
H	1.188604	0.123551	-1.772437
H	-2.076993	0.015103	1.371885
H	-1.328040	-0.956766	2.674669
H	-1.300963	0.828429	2.764364

7

E(B3LYP/6-31+G*) = -287.544686

C	0.007284	0.037654	-0.090979
N	-0.100099	-0.089983	1.297608
C	1.107247	-0.148368	2.001017
C	2.329226	-0.084440	1.368225
C	2.434723	0.043391	-0.023354
C	1.225934	0.102114	-0.730051
C	-1.289153	-0.152617	1.917211
H	1.002390	-0.247142	3.074093
H	3.216504	-0.137270	1.993535
H	3.394650	0.093922	-0.523617
H	1.215431	0.201095	-1.812252
H	-0.938247	0.081125	-0.616641
H	-2.188648	-0.102510	1.322672
H	-1.311016	-0.250791	2.991905

XYZ coordinates and total energies of 4, 7 and their rotational transition state at the B3LYP/6-311+G** level

4

E(B3LYP/6-311+G**) = -344.213323

C	-0.095826	0.087533	-0.139201
N	-0.065207	-0.004473	1.249402
N	1.242064	0.065549	-0.522782
C	1.671160	0.135447	-1.897420
C	2.057184	-0.041203	0.605933
C	-1.252876	-0.021898	2.066535
C	1.257346	-0.084107	1.690194
H	1.503388	-0.161894	2.734876
H	3.130037	-0.074758	0.529730
H	1.331532	1.066187	-2.365764
H	2.759938	0.101226	-1.934514
H	1.271826	-0.705997	-2.475130
H	-1.890205	-0.876538	1.812269
H	-0.964737	-0.098590	3.114901
H	-1.836123	0.895435	1.927515
C	-1.190053	0.177630	-0.942755
H	-2.184733	0.185403	-0.525042
H	-1.086136	0.244211	-2.014527

4 (rotational TS)

E(B3LYP/6-311+G**) = -344.168262

C	0.016388	0.249242	0.016112
N	0.052675	0.052015	1.379960
C	1.346229	-0.074565	1.835735
N	2.103029	0.054598	0.684567
C	1.302080	0.251070	-0.421429
C	1.726492	-0.287045	3.192630
C	-1.108630	-0.018750	2.257355
C	3.555325	-0.011228	0.664354
H	-0.904156	0.370898	-0.528451
H	1.698745	0.374705	-1.415013
H	3.876803	-0.173952	1.693835
H	3.890659	-0.839404	0.036345
H	3.974147	0.924983	0.289109
H	-1.669602	0.917197	2.215929
H	-1.753205	-0.849510	1.962798
H	-0.699147	-0.181657	3.258833
H	2.194585	-1.253862	3.383446
H	2.279487	0.539892	3.640552

7

E(B3LYP/6-311+G**) = -287.612090

C	0.008536	0.037635	-0.090357
N	-0.098268	-0.089967	1.296708
C	1.107416	-0.148247	1.999627
C	2.325145	-0.084308	1.367508
C	2.429533	0.043079	-0.020633
C	1.224175	0.101674	-0.726307
C	-1.285605	-0.152526	1.915331
H	1.004614	-0.247108	3.070090
H	3.211046	-0.136843	1.989928
H	3.386701	0.093651	-0.519489
H	1.215338	0.200373	-1.805735
H	-0.933766	0.081177	-0.616081
H	-2.182060	-0.102337	1.321728
H	-1.306577	-0.250073	2.987055

7 (rotational TS)

E(B3LYP/6-311+G**) = -287.567292

C	0.011398	-0.010226	-0.003935
N	-0.017668	-0.018404	1.349765
C	1.147660	-0.012101	2.023842
C	2.374417	0.002679	1.371843
C	2.406908	0.011415	-0.017501
C	1.199905	0.004605	-0.714886
C	-1.288193	-0.034119	2.179447
H	1.016941	-0.019394	3.097248
H	3.283842	0.007137	1.958575
H	3.350734	0.023512	-0.549517
H	1.173233	0.011052	-1.797322
H	-0.958805	-0.015958	-0.480595
H	-1.847842	0.844434	1.823418
H	-1.830895	-0.919652	1.814451

XYZ coordinates and total energies of the structures involved in the ISE reactions of 4 and 7 at the B3LYP/6-311+G** level

Substrate of the ISE reaction of 4

E(B3LYP/6-311+G**) = -383.536684

C	-0.077265	0.039916	-0.017632
N	0.002250	0.323066	1.413328
C	1.295118	0.052340	1.864438
N	2.110789	0.014093	0.726095
C	1.372636	0.033095	-0.447589
C	1.692880	-0.133230	3.138975
C	-1.143485	0.007593	2.239235
C	3.553930	-0.023734	0.756081
H	-0.665167	0.795834	-0.545029
C	1.834161	0.019611	-1.706905
H	3.908052	0.352141	1.714790
H	3.940093	-1.038517	0.604619
H	3.950920	0.622486	-0.030993
H	-1.061565	0.510120	3.204021
H	-2.045887	0.377773	1.748807
H	-1.253878	-1.073793	2.415559
H	0.989305	-0.072368	3.954447
H	2.724599	-0.333827	3.381940
H	1.139915	0.054346	-2.535300
H	2.888114	-0.036372	-1.941117
H	-0.534379	-0.944968	-0.208068

Product of the ISE reaction of 4

E(B3LYP/6-311+G**) = -383.542996

C	0.005093	-0.026422	0.011258
N	0.002330	-0.014953	1.409945
C	1.308281	0.008992	1.878845
N	2.098007	0.007657	0.731008
C	1.285684	-0.012620	-0.415981
C	1.728238	0.030198	3.173476
C	-1.151240	-0.017530	2.273343
C	3.539168	0.033819	0.790378
H	-0.909694	-0.044637	-0.556083
C	1.833321	-0.019007	-1.801023
H	3.921547	-0.839906	1.330723
H	3.948867	0.026744	-0.218351
H	3.891014	0.934861	1.306309
H	-1.173361	0.879892	2.902658
H	-2.054031	-0.039123	1.662873
H	-1.149013	-0.896098	2.928901
H	1.017311	0.028803	3.985114
H	2.778986	0.047838	3.416502
H	1.010860	-0.036923	-2.517742
H	2.438068	0.870684	-2.010128
H	2.461160	-0.896650	-1.992524

Substrate of reaction R-S1

E(B3LYP/6-311+G**) = -326.899604

C	-0.118150	0.133836	-0.016139
C	-0.040484	0.096495	1.407023
N	1.113054	0.049195	2.108509
C	2.357457	0.035627	1.384148
C	2.402096	0.056365	0.059060
C	1.182022	0.091495	-0.806280
C	1.223560	0.015101	3.447331
H	3.231204	0.007809	2.017232
H	3.375643	0.043558	-0.419057
H	1.241655	0.958751	-1.474506
C	-1.303871	0.200458	-0.671309
H	0.326377	0.022503	4.044198
H	2.204525	-0.020459	3.885717
H	-1.348057	0.227033	-1.753181
H	-2.245958	0.228216	-0.136792
H	-0.942692	0.112443	2.003039
H	1.189041	-0.785539	-1.465167

Product of reaction R-S1, R-S3 and R-S6

E(B3LYP/6-311+G**) = -326.940380

C	-0.002258	-0.010921	0.012111
C	0.024760	0.046144	1.387405
N	1.209117	0.036658	2.128952
C	2.392723	-0.035111	1.395798
C	2.385961	-0.092779	0.023091
C	1.199742	-0.082838	-0.710887
C	1.203210	0.093559	3.468480
H	3.297316	-0.041422	1.985156
H	3.346061	-0.147012	-0.477393
H	1.202679	-0.128592	-1.791826
C	-1.333437	0.005101	-0.697871
H	-0.875581	0.102183	1.982311
H	0.258166	0.147634	3.980781
H	2.144189	0.082951	3.990936
H	-1.400376	0.862056	-1.374493
H	-1.460466	-0.898188	-1.301670
H	-2.167509	0.062648	0.004006

Substrate of reaction R-S2

E(B3LYP/6-311+G**) = -326.888045

C	-0.120910	0.092598	-0.022643
C	-0.034819	-0.113221	1.474624
C	1.296634	0.088100	2.030076
C	2.390196	0.144205	1.263663
N	2.347429	-0.054081	-0.159163
C	1.152455	-0.258953	-0.731232
C	-1.087140	-0.412742	2.248576
C	3.556381	-0.030683	-0.769324
H	-0.944785	-0.492665	-0.439324
H	1.413902	0.180279	3.104286
H	3.383772	0.307791	1.651551
H	4.437664	-0.104262	-0.156368
H	3.591201	-0.185216	-1.835890
H	-0.989477	-0.498669	3.325459
H	-2.072485	-0.579992	1.828545
H	1.160971	-0.441888	-1.796265
H	-0.389500	1.152927	-0.194187

Product of reaction R-S2

E(B3LYP/6-311+G**) = -326.938276

C	0.006491	-0.012935	0.023565
C	0.004209	-0.004641	1.398707
N	1.181708	0.003303	2.143920
C	2.362162	-0.004350	1.401379
C	2.364426	-0.012741	0.027861
C	1.185682	-0.015601	-0.731319
C	1.181866	0.012634	3.487379
H	3.269039	-0.006191	1.987983
H	3.332795	-0.019080	-0.461952
C	1.191638	0.010329	-2.236938
H	-0.960070	-0.019468	-0.469518
H	-0.904715	-0.006749	1.982044
H	0.237980	0.014899	4.004407
H	2.125841	0.015007	4.004188
H	0.235544	-0.331853	-2.641030
H	1.368022	1.019279	-2.630074
H	1.973540	-0.636066	-2.646928

Substrate of reaction R-S3

E(B3LYP/6-311+G**) = -326.908950

C	-0.038583	0.126938	-0.056158
C	-0.023553	-0.277713	1.404823
N	1.249470	0.036154	2.129984
C	2.392650	-0.100280	1.413592
C	2.359597	-0.176424	0.001968
C	1.219152	-0.046211	-0.740796
C	1.151801	0.313252	3.426578
H	3.317446	-0.035014	1.968427
H	3.318100	-0.283451	-0.493959
H	1.254068	-0.004229	-1.822091
C	-1.196646	0.517134	-0.623822
H	-0.841415	0.179866	1.956748
H	0.178602	0.333926	3.886206
H	2.053583	0.476580	3.996414
H	-1.259440	0.705661	-1.689298
H	-2.104265	0.645800	-0.045527
H	-0.124182	-1.366779	1.467107

Substrate of reaction R-S4

E(B3LYP/6-311+G**) = -326.894567

C	-0.026928	-0.389798	-0.031774
C	-0.046923	0.129246	1.379531
N	1.200257	-0.082601	2.119376
C	2.343094	0.076947	1.399551
C	2.322884	0.268476	-0.012999
C	1.211191	0.080942	-0.756643
C	1.127367	-0.332856	3.433227
H	3.263602	0.027029	1.962673
H	3.264272	0.540291	-0.478575
H	1.199237	0.192425	-1.832476
H	-0.041003	-1.492764	-0.006435
C	-1.056801	0.792741	1.936049
H	0.166842	-0.517240	3.876884
H	2.046420	-0.420283	3.990756
H	-1.962586	0.955473	1.365554
H	-1.013292	1.197450	2.937013
H	-0.944953	-0.075831	-0.531316

Product of reaction R-S4 and R-S5

E(B3LYP/6-311+G**) = -326.942678

C	0.022935	0.020075	-0.003946
C	-0.009941	0.005559	1.378702
N	1.191406	-0.011073	2.108203
C	2.378005	-0.012252	1.370149
C	2.395394	0.002159	0.000788
C	1.207307	0.019013	-0.737040
C	1.224562	-0.024930	3.453671
H	3.277682	-0.025217	1.967433
H	3.361751	0.000137	-0.489689
H	1.205878	0.030306	-1.817891
H	-0.933617	0.032681	-0.514142
C	-1.276892	0.007200	2.163908
H	0.313238	-0.025667	4.017945
H	2.188553	-0.038692	3.933059
H	-2.133088	0.020279	1.489693
H	-1.356343	-0.880014	2.806126
H	-1.342923	0.882487	2.823775

Substrate of reaction R-S5

E(B3LYP/6-311+G**) = -326.884057

C	-0.017434	0.039268	-0.050485
C	-0.057313	0.126956	1.403938
N	1.219875	0.056530	2.118749
C	2.344046	-0.054027	1.384163
C	2.429992	0.126690	-0.088711
C	1.108170	0.059981	-0.769196
C	1.209054	0.105198	3.468978
H	3.251119	-0.182075	1.958111
H	3.101274	-0.637757	-0.505901
H	1.076873	0.050892	-1.852956
H	-0.986439	0.014135	-0.536178
C	-1.216833	0.302967	2.052047
H	0.313905	-0.159183	3.998590
H	2.167524	0.073123	3.963104
H	-2.132376	0.332141	1.475966
H	-1.299147	0.448499	3.116522
H	2.912948	1.086669	-0.352707

Sustrate of reaction R-S6

E(B3LYP/6-311+G**) = -326.904226

C	0.005952	-0.044081	-0.003159
C	0.004063	-0.011108	1.329544
C	1.260690	-0.015165	2.082379
C	2.472134	-0.003000	1.323737
N	2.525422	0.017295	-0.023645
C	1.261546	-0.107218	-0.812188
C	1.239022	-0.019907	3.441881
C	3.635575	0.109016	-0.763628
H	1.322303	-1.057745	-1.353494
H	-0.916767	-0.044499	-0.573803
H	-0.925978	0.022518	1.885516
H	4.590915	0.177485	-0.268605
H	3.549093	0.075219	-1.835869
H	0.300746	-0.020748	3.981530
H	2.150391	-0.023750	4.027728
H	3.430224	0.041605	1.824172
H	1.279566	0.689554	-1.561080

Substrate of reaction R-S7

E(B3LYP/6-311+G**) = -272.812813

C	0.114701	-0.223773	-0.445111
C	0.297316	-0.407132	1.038222
C	1.332328	0.109455	1.721473
C	1.441810	-0.052325	3.219290
H	2.079374	0.709747	1.209795
C	0.809948	-1.367766	3.698665
H	2.487070	-0.000871	3.537028
H	0.933418	0.796301	3.703902
C	-0.510071	-1.623154	3.013915
H	1.486243	-2.207676	3.474527
H	0.688502	-1.356345	4.785514
C	-0.725883	-1.175055	1.769293
H	-1.258808	-2.222022	3.523003
H	-1.660149	-1.395875	1.260749
H	-0.833327	0.281057	-0.663787
H	0.922926	0.369842	-0.877087
H	0.086509	-1.189343	-0.962390

Product of reaction R-S7

E(B3LYP/6-311+G**) = -272.813754

C	-0.147005	0.245271	-0.235389
C	0.211445	-0.294332	0.939033
C	1.543748	-0.004150	1.600237
C	1.414250	0.047321	3.129792
H	2.245502	-0.805768	1.331983
C	0.817770	-1.257734	3.675217
H	2.389376	0.240463	3.586634
H	0.760377	0.882312	3.405269
C	-0.382918	-1.697410	2.879720
H	1.575756	-2.054573	3.661579
H	0.538265	-1.136926	4.727700
C	-0.658271	-1.233881	1.650751
H	-1.054128	-2.416441	3.341146
H	-1.560306	-1.559761	1.140179
H	-1.092962	-0.002920	-0.705204
H	0.494004	0.945091	-0.760199
H	1.964078	0.926833	1.210885

Substrate of reaction R-S8

E(B3LYP/6-311+G**) = -271.584870

C	-0.033294	0.089384	-0.005177
C	-0.053347	0.105344	1.517262
C	1.243617	0.116047	2.188295
C	2.383299	0.394953	1.522511
C	2.371384	0.708402	0.096708
C	1.244670	0.598010	-0.620353
C	-1.202455	0.091416	2.213512
H	1.259978	-0.052759	3.260391
H	3.328247	0.430176	2.053784
H	3.293075	1.037290	-0.371090
H	1.237165	0.824165	-1.681712
H	-0.895576	0.634325	-0.401450
H	-1.201781	0.043780	3.296895
H	-2.169187	0.124729	1.723232
H	-0.169201	-0.951145	-0.341723

Product of reaction R-S8

E(B3LYP/6-311+G**) = -271.590882

C	-0.004590	0.001855	-0.010570
C	-0.010542	-0.103454	1.451684
C	1.290832	-0.344569	2.082151
C	2.421801	-0.462646	1.374753
C	2.463549	-0.359335	-0.122278
C	1.115583	-0.112923	-0.735302
C	-1.143439	0.013521	2.172262
H	3.363080	-0.641386	1.886009
H	3.160667	0.438619	-0.421418
H	2.904261	-1.274524	-0.547099
H	1.070948	-0.027259	-1.816983
H	-0.955980	0.180129	-0.502646
H	-2.100696	0.191277	1.695815
H	-1.136761	-0.066455	3.253245
H	1.314177	-0.427095	3.164609

Substrate of reaction R-S9

E(B3LYP/6-311+G**) = -250.684770

N	0.177171	-0.339630	0.049227
C	0.013572	-0.127654	1.504428
C	1.391481	-0.014943	-0.450779
C	-0.873648	-0.881564	-0.576183
H	-1.028266	0.106104	1.715044
H	0.300692	-1.035179	2.037105
H	0.639913	0.703752	1.820942
H	-0.796637	-1.172638	-1.609167
H	-1.790119	-1.003692	-0.025970
C	1.742143	-0.126450	-1.825745
H	2.113003	0.333336	0.273209
C	2.975646	0.076727	-2.339681
H	0.943957	-0.373039	-2.521652
H	3.154885	0.013013	-3.404964
H	3.826203	0.314591	-1.709244

Product of reaction R-S9

E(B3LYP/6-311+G**) = -250.672728

C	0.329561	-0.058075	-0.002488
N	0.464358	-0.585456	1.234518
C	1.519242	-0.008084	2.033828
C	1.421337	0.245672	3.331211
C	-0.269948	-1.569642	1.775791
C	-1.383601	-2.161720	1.000250
H	0.915828	0.809775	-0.249166
H	-0.432088	-0.437480	-0.659510
H	0.083632	-1.981062	2.705706
H	-1.895556	-2.926119	1.586192
H	-2.122615	-1.400808	0.703393
H	-1.037958	-2.630136	0.062287
H	2.405439	0.220930	1.455882
H	2.267180	0.670771	3.856412
H	0.518158	0.049900	3.894249

XYZ coordinates and total energies of the anions at the B3LYP/6-31+G* level

CF_3SO_3-
E(B3LYP/6-31+G*)= -961.553353

S	0.000000	0.000000	-0.169887
C	0.000000	0.000000	1.722755
F	1.257383	0.000000	2.230901
F	-0.628691	1.088926	2.230901
F	-0.628691	-1.088926	2.230901
O	-1.447908	0.000000	-0.485191
O	0.723954	1.253925	-0.485191
O	0.723954	-1.253925	-0.485191

Cl-
E(B3LYP/6-31+G*)= -460.2747235

$ClCH_2COO$-
E(B3LYP/6-31+G*)= -688.147116

C	0.013677	-0.003490	-0.144203
C	-0.115455	-0.004677	1.415241
H	0.716993	-0.556973	1.853882
Cl	-0.116249	1.636104	2.284350
H	-1.053133	-0.480179	1.706964
O	-0.005110	-1.198933	-0.550256
O	0.112680	1.069911	-0.766643

CH_3COO-
E(B3LYP/6-31+G*)= -228.539310

C	-0.022500	-0.022240	-0.104414
C	-0.004476	-0.023851	1.459059
H	1.022469	0.007166	1.844629
H	-0.525314	0.875699	1.820201
H	-0.532060	-0.898391	1.860533
O	-1.024678	-0.572024	-0.639299
O	0.951559	0.555700	-0.661708

SH-
E(B3LYP/6-31+G*)= -398.827370

S	0.000000	0.000000	-0.205450
H	0.000000	0.000000	1.155450

CN-
E(B3LYP/6-31+G*)= -92.865429

C	0.000000	0.000000	0.128224
N	0.000000	0.000000	1.311776

F-
E(B3LYP/6-31+G*)= -99.8596977

CH_3O^-

E(B3LYP/6-31+G*)= -115.111531

O	0.000000	0.000000	0.010105
C	0.000000	0.000000	1.350103
H	1.030414	0.000000	1.842931
H	-0.515207	0.892365	1.842931
H	-0.515207	-0.892365	1.842931

OH^-

E(B3LYP/6-31+G*)= -75.796681

O	0.000000	0.000000	-0.012437
H	0.000000	0.000000	0.962437

H^-

E(B3LYP/6-31+G*)= -0.4618167

XYZ coordinates and total energies of the protonated anions at the B3LYP/6-31+G* level

CF_3SO_3H

E(B3LYP/6-31+G*)= -962.034482

C	0.054594	-0.017084	-0.009344
F	0.006584	0.046243	1.320074
S	1.840980	0.078640	-0.604867
O	2.458715	1.207143	0.056816
O	2.417559	-1.271739	0.104422
O	1.819537	-0.113375	-2.047499
F	-0.626486	1.002372	-0.533872
F	-0.484217	-1.172628	-0.420595
H	2.367537	-2.013074	-0.531456

HCl

E(B3LYP/6-31+G*)= -460.798000

H	0.000000	0.000000	-0.141217
Cl	0.000000	0.000000	1.149217

$ClCH_2COOH$

E(B3LYP/6-31+G*)= -688.681150

C	0.079891	-0.042282	-0.068688
C	0.017954	0.001548	1.446813
H	1.012750	0.222338	1.829014
Cl	-1.107001	1.283471	2.044190
H	-0.342349	-0.952694	1.837500
O	-1.109114	-0.355290	-0.623305
O	1.091011	0.146246	-0.708135
H	-0.989404	-0.360996	-1.592061

CH_3COOH

E(B3LYP/6-31+G*)= -229.096146

C	0.083954	-0.034897	-0.052155
C	-0.002944	-0.009464	1.451551
H	0.966377	0.265195	1.868957
H	-0.764928	0.710108	1.770044
H	-0.305943	-0.993504	1.825352
O	-1.105832	-0.373854	-0.617811
O	1.068932	0.208925	-0.715981
H	-0.974281	-0.369872	-1.584961

H_2S

E(B3LYP/6-31+G*)= -399.387272

S	-0.209133	0.000000	-0.146535
H	-0.013146	0.000000	1.189240
H	1.115119	0.000000	-0.408372

HCN

E(B3LYP/6-31+G*)= -93.428617

C	0.000000	0.000000	0.088424
N	0.000000	0.000000	1.245960
H	0.000000	0.000000	-0.983384

HF

E(B3LYP/6-31+G*)= -100.443376

H	0.000000	0.000000	0.035168
F	0.000000	0.000000	0.972832

CH_3OH

E(B3LYP/6-31+G*)= -115.725194

O	0.022046	0.000000	0.013673
C	-0.018460	0.000000	1.438290
H	1.020657	0.000000	1.776007
H	-0.516339	0.895824	1.836775
H	-0.516339	-0.895824	1.836775
H	-0.884406	0.000000	-0.328186

H_2O

E(B3LYP/6-31+G*)= -76.422572

O	-0.022110	0.000000	-0.014344
H	0.012946	0.000000	0.953818
H	0.902004	0.000000	-0.305141

H_2

E(B3LYP/6-31+G*)= -1.175482

H	0.000000	0.000000	0.132545
H	0.000000	0.000000	0.875455

XYZ coordinates and total energies of type 3a species at the B3LYP/6-31+G* level

A = CF_3SO_3-

E(B3LYP/6-31+G*)= -1306.241999

C	0.369033	-0.784771	0.096735
N	0.205442	-0.298407	1.378768
C	1.346141	0.299093	1.776522
N	2.221910	0.215145	0.756162
C	1.631107	-0.463348	-0.293361
C	-0.950077	-0.549049	2.245828
C	3.634219	0.608047	0.814215
O	1.263560	-2.175746	3.906447
S	2.421155	-2.586605	3.063709
O	2.055835	-3.083642	1.717517
C	3.102104	-4.095803	3.952380
F	3.476980	-3.787132	5.207782
O	3.555103	-1.623481	3.085864
F	2.174767	-5.069322	4.020866
F	4.175668	-4.586962	3.304929
H	4.137789	-0.028113	1.547619
H	4.066286	0.454377	-0.175275
H	3.721341	1.663912	1.080807
H	-1.295078	0.389047	2.687700
H	-1.747851	-0.972753	1.634798
H	-0.649837	-1.257395	3.024197
H	2.169773	-0.689340	-1.199567
H	-0.404490	-1.345490	-0.403072
C	1.562122	0.941573	3.100316
H	1.351457	0.215928	3.892880
H	2.600288	1.255414	3.210952
H	0.909980	1.816376	3.220227

A = Cl- (isomer 1)

E(B3LYP/6-31+G*)= -804.976472

C	0.038052	0.011117	0.021384
N	0.047955	0.107657	1.368819
N	1.321169	0.064350	-0.397774
C	2.154897	0.056220	0.708995
C	1.361450	0.083314	1.809947
C	1.741774	-0.237750	-1.763819
H	1.457700	-1.273301	-1.984416
H	1.271490	0.451680	-2.468886
H	2.825037	-0.122488	-1.824754
H	3.228664	0.029538	0.611853
H	1.608669	0.084719	2.859702
C	-1.119869	-0.140494	2.210903
H	-1.920711	0.562477	1.970136
H	-1.445343	-1.173807	2.043185
H	-0.828695	-0.001426	3.253203
C	-1.162797	0.129111	-0.850368
H	-2.027749	-0.320997	-0.362967
H	-1.374210	1.185058	-1.077497
H	-1.008145	-0.421696	-1.778465
Cl	-0.175244	-2.774949	-0.065921

A = Cl- (isomer 2)

E(B3LYP/6-31+G*)= -804.965968

C	0.006925	0.115549	0.016791
N	-0.004538	0.131702	1.406661
C	1.269110	0.078085	1.850952
N	2.070934	0.025140	0.772919
C	1.307416	0.048232	-0.383341
C	1.698186	0.050758	3.277079
C	-1.197810	0.204803	2.247344
C	3.543605	-0.053370	0.783970
Cl	3.621172	-0.157776	-2.607010
H	3.954257	0.848095	1.247007
H	3.857547	-0.942553	1.336488
H	3.868467	-0.119308	-0.266601
H	1.815244	0.005349	-1.359922
H	-0.906368	0.153563	-0.556420
H	-1.218806	-0.627946	2.955227
H	-1.228076	1.152625	2.792936
H	-2.074464	0.140826	1.601839
H	1.053479	0.682696	3.895436
H	1.667115	-0.967833	3.686547
H	2.723427	0.416293	3.371899

A = Cl- (isomer 3)

E(B3LYP/6-31+G*)= -804.954695

C	0.022389	0.098849	0.032534
N	0.026599	0.132667	1.417811
C	1.298965	0.072559	1.866507
N	2.096934	-0.003873	0.779646
C	1.320147	0.013333	-0.367571
C	1.737910	0.051597	3.290365
C	-1.171330	0.223346	2.252972
C	3.557455	-0.087232	0.796753
Cl	-0.211305	0.027773	-3.111279
H	3.989671	0.835436	1.194771
H	3.884318	-0.939826	1.397593
H	3.896477	-0.224222	-0.230255
H	1.686490	-0.032553	-1.386199
H	-0.855305	0.134923	-0.600901
H	-1.209597	-0.610772	2.958327
H	-1.188509	1.171910	2.797358
H	-2.040517	0.174820	1.596772
H	1.028903	0.591685	3.923979
H	1.818407	-0.974131	3.675638
H	2.715742	0.528643	3.403691

A = $ClCH_2COO^-$

E(B3LYP/6-31+G*)= -1032.850141

N	0.009081	-0.013630	-0.109298
C	-0.105680	0.036078	1.268398
C	1.155563	0.061092	1.775776
N	2.025434	0.035016	0.699696
C	1.314309	0.026402	-0.442646
C	3.483181	0.179663	0.768999
C	1.902928	-0.014011	-1.805644
C	-1.095961	0.192439	-1.046805
O	0.794478	2.626209	-0.942196
C	1.871159	3.269092	-0.942015
C	1.867201	4.800747	-1.145506
O	3.043500	2.814117	-0.795701
H	3.744888	1.137069	0.301393
H	3.774921	0.169005	1.820264
H	3.965899	-0.655942	0.254638
H	-1.019273	1.208643	-1.443987
H	-1.053597	-0.546732	-1.849936
H	-2.032791	0.067026	-0.501745
H	-1.066255	0.059289	1.758305
H	1.510078	0.097190	2.793749
H	2.332833	5.280453	-0.282936
H	2.448916	5.048233	-2.035125
Cl	0.232991	5.575339	-1.356405
H	1.134974	0.149913	-2.561786
H	2.636477	0.795506	-1.887855
H	2.389377	-0.981263	-1.992648

A = CH_3COO^- (isomer 1)

E(B3LYP/6-31+G*)= -573.252304

N	0.000240	-0.000338	0.001195
C	0.001232	-0.004064	1.384655
C	1.300620	-0.004981	1.784900
N	2.077636	0.007657	0.639607
C	1.273841	0.051482	-0.438917
C	3.537198	0.141575	0.592350
C	1.746253	0.046806	-1.846558
C	-1.172890	0.257536	-0.833463
O	0.729927	2.664534	-0.823009
C	1.829295	3.292734	-0.904416
C	1.763034	4.816011	-1.092955
O	2.982435	2.767792	-0.872569
H	3.763161	1.107581	0.122199
H	3.913329	0.108348	1.616128
H	3.969830	-0.686882	0.024177
H	-1.100250	1.283978	-1.205001
H	-1.215216	-0.456857	-1.659043
H	-2.064471	0.135722	-0.216134
H	-0.914897	0.003763	1.953797
H	1.739299	-0.011500	2.770170
H	0.781950	5.210575	-0.811729
H	2.550547	5.308500	-0.512560
H	1.942215	5.052501	-2.150246
H	0.916853	0.221097	-2.532143
H	2.464222	0.867029	-1.964105
H	2.221526	-0.912548	-2.094738

A = CH_3COO^- (isomer 2)

E(B3LYP/6-31+G*)= -573.242036

C	-0.000981	-0.031017	0.018864
N	-0.014118	0.039104	1.407458
C	1.259104	-0.024477	1.852238
N	2.057145	-0.137313	0.775843
C	1.297266	-0.142081	-0.383319
C	3.526368	-0.232574	0.798877
C	-1.212374	0.151642	2.236227
O	2.491460	-0.484408	-2.972282
C	3.558239	-1.171666	-2.903885
C	4.173251	-1.612017	-4.240029
O	4.150289	-1.511901	-1.838625
H	-1.206686	1.088908	2.800035
H	-2.081510	0.143798	1.577497
H	-1.285299	-0.693816	2.925624
H	3.832442	-0.881078	1.623367
H	3.844492	-0.669861	-0.166139
H	3.954057	0.766522	0.931333
H	1.764757	-0.249407	-1.392184
H	-0.913945	-0.001641	-0.555530
C	1.706229	0.002927	3.273391
H	4.485836	-0.725942	-4.806909
H	5.037127	-2.264562	-4.085021
H	3.419923	-2.129850	-4.845553
H	0.906657	0.353998	3.930044
H	2.011989	-0.994534	3.614885
H	2.564362	0.671699	3.394840

A = CH_3COO^- (isomer 3)

E(B3LYP/6-31+G*)= -573.235938

N	-0.009013	-0.048578	-0.008291
C	-0.022099	-0.004605	1.379707
C	1.272480	0.024616	1.801555
N	2.054130	-0.002049	0.657510
C	1.270069	-0.044531	-0.440410
C	3.517374	0.011399	0.667885
C	-1.198365	-0.089882	-0.857210
O	1.812245	0.107917	4.592597
C	0.602359	0.102463	4.997060
C	0.401891	0.137993	6.520548
O	-0.422473	0.069621	4.260313
H	3.896069	0.905984	0.164803
H	3.837920	0.023444	1.709955
H	3.912378	-0.883121	0.178201
H	-1.262892	0.810125	-1.475805
H	-1.184980	-0.977112	-1.496049
H	-2.072299	-0.134649	-0.206814
H	-0.913977	0.004996	1.989213
H	1.653205	0.061456	2.849141
C	1.730716	-0.114785	-1.855923
H	0.884964	-0.734899	6.977165
H	0.889303	1.027692	6.938097
H	-0.660460	0.145408	6.781430
H	0.970291	0.281897	-2.534097
H	2.643010	0.472641	-1.997813
H	1.947946	-1.147296	-2.162321

A = SH-

E(B3LYP/6-31+G*)= -743.531502

C	0.428426	-0.732044	0.339637
C	0.280355	-0.423161	1.651137
N	1.403734	0.297687	2.040801
C	2.317619	0.268205	1.017840
N	1.643266	-0.202027	-0.080607
C	1.763624	0.581427	3.422353
C	2.300428	-0.538108	-1.335116
S	3.715106	-1.840848	1.672361
H	2.536783	-0.132045	3.736331
H	2.130705	1.606763	3.521631
H	0.873332	0.468417	4.044189
H	3.086319	-1.277319	-1.131864
H	1.557073	-0.957653	-2.015906
H	2.730357	0.355645	-1.795872
H	-0.226562	-1.257010	-0.338165
H	-0.528390	-0.627361	2.335415
C	3.453863	1.239272	0.917460
H	4.950088	-1.284710	1.681778
H	4.173582	0.908597	0.167451
H	3.078685	2.237307	0.640491
H	3.981829	1.308967	1.869472

A = CN-

E(B3LYP/6-31+G*)= -437.566177

C	0.313654	-0.546436	0.212653
C	0.231774	-0.312367	1.549245
N	1.415156	0.294754	1.930064
C	2.225584	0.385242	0.856493
N	1.546232	-0.081908	-0.207942
C	1.855447	0.468925	3.314440
C	2.150395	-0.358788	-1.512805
N	3.699190	-2.232942	0.537246
C	3.480841	-2.045310	1.683031
H	2.571943	-0.332342	3.534895
H	2.309946	1.452920	3.447784
H	0.982725	0.389925	3.964408
H	2.622102	0.543627	-1.908312
H	2.885076	-1.162078	-1.366501
H	1.360503	-0.676856	-2.194867
H	-0.383327	-1.007012	-0.469334
H	-0.549959	-0.529951	2.259537
C	3.578353	1.002755	0.820957
H	4.211288	0.464180	0.114261
H	3.516987	2.063055	0.536678
H	4.057690	0.917459	1.796828

A = F-

E(B3LYP/6-31+G*)= -444.589135

C	-0.000417	0.206033	0.035158
N	0.018795	0.111469	1.382495
N	1.255145	-0.074556	-0.398290
C	2.067724	-0.354330	0.692192
C	1.291726	-0.230761	1.801686
C	1.669689	-0.126777	-1.797274
H	1.183166	-0.961330	-2.309904
H	1.416529	0.808914	-2.301857
H	2.751346	-0.266885	-1.829879
H	3.108521	-0.613740	0.577751
H	1.527041	-0.365383	2.845759
C	-1.174241	0.229167	2.238238
H	-1.967885	-0.399758	1.777340
H	-0.904991	-0.128620	3.233693
H	-1.479567	1.278830	2.298339
C	-1.194001	0.463144	-0.777353
H	-1.964476	-0.351926	-0.454238
H	-1.646632	1.429287	-0.522883
H	-0.973291	0.437189	-1.846138
F	-2.715827	-1.327532	0.442495

XYZ coordinates and total energies of type 3b species at the B3LYP/6-31+G* level

A = CH_3COO^-

E(B3LYP/6-31+G*)= -573.240633

C	0.562937	-0.638486	-0.147257
C	0.461216	-0.725747	1.199219
N	1.647687	-0.224951	1.741210
C	2.498372	0.164635	0.723625
N	1.809038	-0.088870	-0.444695
C	1.996571	-0.160115	3.143554
C	2.352694	0.159991	-1.768522
O	5.425618	-1.778580	0.814930
C	5.513521	-2.408693	-0.361029
O	4.915493	-2.062847	-1.368997
C	6.443179	-3.601195	-0.299718
H	2.199491	0.874528	3.446798
H	1.161339	-0.543053	3.734008
H	2.887245	-0.766774	3.349839
H	3.280142	-0.404542	-1.905896
H	1.620150	-0.163226	-2.511529
H	2.547565	1.231135	-1.906579
H	-0.131535	-0.916936	-0.924665
H	-0.338068	-1.091087	1.825111
C	3.797183	0.631567	0.852073
H	6.471964	-4.099881	-1.269908
H	7.450730	-3.273514	-0.020236
H	6.104415	-4.302339	0.470964
H	4.273243	1.087985	-0.009288
H	4.135237	0.972958	1.825074
H	4.811866	-0.965053	0.752426

A = SH-

E(B3LYP/6-31+G*)= -743.522463

C	-0.064880	0.150508	-0.009082
C	-0.011096	0.048902	1.338162
N	1.330148	-0.099911	1.700306
C	2.127511	-0.091000	0.563643
N	1.242453	0.065703	-0.494679
C	1.855880	-0.244450	3.038115
C	3.489553	-0.244302	0.497509
C	1.659344	0.125605	-1.876734
S	3.344537	-3.893157	0.177041
H	2.173205	-0.799053	-2.168922
H	0.777393	0.253754	-2.508373
H	2.339680	0.971596	-2.041726
H	2.388188	-1.198112	3.146587
H	2.550288	0.572825	3.274010
H	1.027574	-0.220147	3.749849
H	-0.907728	0.271158	-0.671951
H	-0.797962	0.064054	2.076371
H	3.407169	-2.528351	0.309660
H	4.009810	-0.134837	-0.445443
H	4.084136	-0.274697	1.401595
H	4.686162	-4.020260	0.105589

A = CN-

E(B3LYP/6-31+G*)= -437.566734

N	0.266960	-0.131172	-0.139653
C	0.148183	-0.556428	1.186404
C	1.313212	-0.278658	1.813156
N	2.164612	0.321491	0.881320
C	1.523295	0.421178	-0.345237
C	3.504698	0.806383	1.120837
C	2.035704	0.920127	-1.518815
C	-0.747537	-0.206310	-1.166081
C	3.393099	-1.893389	-2.816865
N	3.858655	-2.853421	-3.269654
H	4.229078	0.287756	0.479856
H	3.570366	1.883818	0.920671
H	3.766786	0.624557	2.165426
H	-1.001478	0.795453	-1.536544
H	-0.403684	-0.814436	-2.012516
H	-1.644909	-0.665424	-0.745536
H	-0.753846	-1.021884	1.552455
H	1.623512	-0.454944	2.831456
H	1.392895	1.055319	-2.380355
H	2.988487	1.435805	-1.521999
H	2.954334	-0.989973	-2.388416

A = F-

E(B3LYP/6-31+G*)= -444.594522

C	0.150803	-0.111199	0.064755
N	0.124304	-0.009642	1.456603
C	1.411211	0.073727	1.941662
N	2.224533	0.062232	0.829660
C	1.446581	-0.067883	-0.322130
C	1.809037	0.049483	3.275557
C	-1.044041	-0.115584	2.307791
C	3.672108	0.051340	0.898648
H	4.039005	0.945669	1.415274
H	4.025381	-0.838214	1.433990
H	4.073106	0.041179	-0.116929
H	1.890340	-0.103750	-1.304908
H	-0.755499	-0.192217	-0.514987
H	-0.969643	-1.000370	2.951204
H	-1.144206	0.775273	2.938584
H	-1.931698	-0.203490	1.678073
H	1.069908	0.299409	4.030853
H	2.829455	0.339475	3.506966
H	1.911405	-1.661382	3.546140
F	1.947898	-2.651880	3.673953

A = CH_3O-

E(B3LYP/6-31+G*)= -459.864414

C	0.269739	-0.637468	0.085521
N	0.032342	0.180257	1.180399
C	1.214739	0.827134	1.551671
C	2.192528	0.397843	0.722307
N	1.627623	-0.517674	-0.167247
C	-1.278191	0.381488	1.752048
C	2.281155	-1.118336	-1.311892
O	-0.354588	0.473066	-3.122385
C	-1.485046	1.172053	-3.616948
H	1.247585	1.513027	2.384019
H	3.242733	0.643352	0.688470
H	3.345574	-0.874965	-1.275669
H	2.170691	-2.209276	-1.287093
H	1.856133	-0.735598	-2.248480
H	-1.190541	1.037316	2.621260
H	-1.959108	0.843802	1.024159
H	-1.709953	-0.574663	2.073283
C	-0.655825	-1.358143	-0.634183
H	-1.165132	1.711255	-4.513785
H	-2.304611	0.491724	-3.895941
H	-1.869858	1.906054	-2.891564
H	-0.610229	-0.029229	-2.314232
H	-0.326066	-2.081715	-1.370232
H	-1.675315	-1.441307	-0.277861

A = OH-

E(B3LYP/6-31+G*)= -420.562289

C	0.187136	-0.453535	0.201652
N	0.179447	-0.043718	1.537972
C	1.419861	0.475339	1.875186
N	2.162596	0.427094	0.705993
C	1.406050	-0.164914	-0.307134
O	3.622810	-1.662322	3.308374
C	-0.887939	-0.232907	2.492236
C	3.571987	0.755738	0.644775
H	4.152183	0.096458	1.302808
H	3.917213	0.630556	-0.384087
H	3.735745	1.797925	0.944729
H	-0.586071	-0.930615	3.285248
H	-1.166579	0.722145	2.954822
H	-1.759449	-0.640178	1.974688
H	1.805256	-0.307601	-1.299383
H	-0.683828	-0.891292	-0.261006
C	1.843194	0.883621	3.120272
H	3.869293	-1.892099	4.216483
H	2.981006	-0.917323	3.388817
H	2.781205	1.415700	3.224851
H	1.133311	0.962825	3.934475

A = H-

E(B3LYP/6-31+G*)= -345.305231

C	-0.057866	0.015840	0.000555
C	-0.058794	0.015094	1.352729
N	1.271390	0.022224	1.781271
C	2.122432	0.051631	0.678168
N	1.272910	0.023513	-0.426131
C	1.742625	0.089370	3.142190
C	3.486228	0.107214	0.679149
C	1.746162	0.090769	-1.786335
H	4.299422	-4.005704	0.724429
H	2.301259	1.022755	-1.964255
H	2.410314	-0.754797	-2.009220
H	0.890306	0.053943	-2.464651
H	-0.876880	-0.005827	-0.701904
H	-0.878784	-0.007341	2.054027
H	2.406189	-0.756337	3.366270
H	2.297692	1.021233	3.320882
H	0.885714	0.052829	3.819188
H	4.042467	0.127261	1.606964
H	4.043780	0.128797	-0.247854
H	4.143112	-3.278349	0.712493

XYZ coordinates and total energies of type 3c species at the B3LYP/6-31+G* level

A = CN-

E(B3LYP/6-31+G*)= -398.255042

C	0.009634	0.023155	0.005381
N	-0.034394	-0.086196	1.418659
C	1.373753	-0.042792	1.827829
N	2.103936	-0.534739	0.654364
C	1.249824	-0.236844	-0.437873
C	1.637824	-0.848772	3.039943
C	-0.928944	0.782322	2.170650
C	3.505981	-0.148010	0.585561
H	4.052766	-0.593643	1.422359
H	3.935696	-0.533845	-0.342988
H	3.640577	0.948655	0.612792
H	-0.964487	0.458900	3.215601
H	-0.614826	1.841328	2.133650
H	-1.937300	0.698121	1.756093
H	1.597895	-0.376141	-1.452177
H	-0.905084	0.148606	-0.557577
H	1.677157	1.012749	2.057183
N	1.858586	-1.444613	4.011042

A = F-

E(B3LYP/6-31+G*)= -444.600790

C	-0.029455	-0.306084	-0.014078
N	-0.027021	0.099228	1.347049
N	1.239977	0.117180	-0.489828
C	2.078458	0.307292	0.629728
C	1.315593	0.296496	1.735714
C	1.768825	-0.380663	-1.750534
H	1.038140	-0.229139	-2.549217
H	2.664638	0.194774	-2.003255
H	2.024431	-1.447294	-1.701516
H	3.130901	0.516129	0.507035
H	1.572898	0.494072	2.765792
C	-1.013022	-0.419966	2.282550
H	-2.020506	-0.272620	1.885036
H	-0.866511	-1.488070	2.490230
H	-0.936451	0.144137	3.217109
C	-1.242529	0.063934	-0.847167
H	-2.149467	-0.357907	-0.406932
H	-1.338729	1.152273	-0.902934
H	-1.149495	-0.343838	-1.856800
F	-0.066579	-1.841601	-0.054723

A = CH_3O-

E(B3LYP/6-31+G*)= -459.860231

C	0.078794	-0.078060	0.011336
C	0.101319	-0.075223	1.355061
N	1.431365	0.093388	1.812409
C	2.303417	0.177293	0.628419
N	1.375094	0.073635	-0.490532
C	1.633449	0.959264	2.966541
O	3.156557	-0.993661	0.515719
C	3.905974	-1.357918	1.663598
C	1.633874	0.663112	-1.787540
H	2.623015	0.364546	-2.147779
H	0.893905	0.275831	-2.495374
H	1.567087	1.765125	-1.795005
H	2.650299	0.857191	3.356289
H	1.437002	2.024974	2.758783
H	0.945094	0.637290	3.755070
H	-0.748151	-0.276344	-0.657809
H	-0.697589	-0.277755	2.055446
C	3.179591	1.435303	0.581304
H	4.416529	-2.290318	1.408477
H	4.667602	-0.607275	1.928469
H	3.251844	-1.533646	2.527419
H	3.789260	1.424964	-0.325691
H	2.563807	2.341887	0.584189
H	3.860120	1.482979	1.435455

A = OH-

E(B3LYP/6-31+G*)= -420.567217

C	-0.010385	0.042788	-0.013014
C	-0.008825	0.049849	1.331679
N	1.318760	-0.038175	1.797549
C	2.217910	0.214361	0.655835
N	1.316061	-0.050495	-0.480965
C	1.664064	0.478325	3.110882
O	3.319740	-0.678425	0.659359
C	2.834924	1.619383	0.647473
C	1.658617	0.451520	-1.800622
H	2.692498	0.181983	-2.034862
H	1.010651	-0.031734	-2.539511
H	1.540249	1.543746	-1.899908
H	2.698722	0.212162	3.345579
H	1.545020	1.571460	3.198701
H	1.018334	0.002492	3.856524
H	-0.844413	-0.036893	-0.696873
H	-0.841248	-0.022460	2.018303
H	2.940147	-1.575178	0.664191
H	3.463457	1.754921	-0.236436
H	2.042626	2.376294	0.644281
H	3.465451	1.764585	1.528422

A = H-

E(B3LYP/6-31+G*)= -345.338004

C	-0.079372	-0.287697	-0.048310
N	-0.103079	0.198099	1.345163
N	1.210291	0.216649	-0.558927
C	2.017755	0.403247	0.588930
C	1.255011	0.392475	1.694736
C	1.777157	-0.530614	-1.670302
H	1.126590	-0.453234	-2.547154
H	2.748461	-0.101821	-1.935799
H	1.917928	-1.601589	-1.429154
H	3.064599	0.657204	0.487113
H	1.529433	0.635524	2.712756
C	-0.933715	-0.568901	2.259847
H	-1.985154	-0.497181	1.964172
H	-0.648546	-1.637837	2.291650
H	-0.840714	-0.152514	3.267695
C	-1.277091	0.174960	-0.869945
H	-2.210819	-0.210749	-0.444209
H	-1.318760	1.268137	-0.888037
H	-1.207354	-0.196577	-1.899007
H	-0.048526	-1.409249	-0.037959

XYZ coordinates and total energies of type 5a species at the B3LYP/6-31+G* level

A = CF_3SO_3- (isomer 1)

E(B3LYP/6-31+G*)= -1249.655918

C	-0.154102	0.269456	0.144125
C	-0.080503	0.359513	1.530602
N	1.072936	0.075557	2.173524
C	2.186835	-0.290895	1.489193
C	2.166986	-0.380688	0.110872
C	0.976683	-0.099461	-0.576767
C	1.111922	0.169493	3.656632
H	1.639368	1.084367	3.939544
O	-3.065480	0.153304	1.595843
S	-3.281029	-0.033286	3.056769
C	-3.365205	-1.906105	3.229921
F	-2.219413	-2.477407	2.770793
O	-2.053993	0.296757	3.851833
O	-4.552132	0.443761	3.609617
F	-3.512598	-2.276863	4.514416
F	-4.385507	-2.421872	2.524033
H	3.066318	-0.506365	2.085107
H	3.068462	-0.677753	-0.413937
H	0.940528	-0.179927	-1.659185
H	-1.113201	0.471142	-0.320125
H	-0.934762	0.613796	2.150764
H	0.083557	0.190504	4.023853
H	1.636715	-0.703647	4.048718

A = CF_3SO_3- (isomer 2)

E(B3LYP/6-31+G*)= -1249.656918

C	-0.004818	0.066198	0.013018
C	-0.046712	0.057970	1.402509
N	1.104154	-0.007018	2.112218
C	2.306599	-0.079049	1.493963
C	2.396109	-0.076402	0.113316
C	1.221622	-0.002249	-0.643509
C	1.015222	-0.066393	3.592950
H	0.436281	0.788675	3.945669
O	-2.575922	-0.455786	2.909540
S	-2.395894	-1.898581	3.257225
C	-2.602046	-1.896131	5.127394
F	-2.431626	-3.127695	5.638918
O	-0.981394	-2.345316	3.084264
O	-3.432446	-2.816966	2.773467
F	-1.677961	-1.083380	5.703269
F	-3.816475	-1.453447	5.490439
H	3.175168	-0.141507	2.138389
H	3.372540	-0.136182	-0.354675
H	1.268096	-0.003461	-1.728467
H	-0.942512	0.111101	-0.529990
H	-0.980686	0.068131	1.972203
H	0.494523	-0.993489	3.850776
H	2.022980	-0.037137	4.007348

A = CF_3SO_3- (isomer 3)

E(B3LYP/6-31+G*)= -1249.657513

C	-0.030131	-0.014744	0.072590
C	-0.012228	0.140078	1.459112
C	1.203158	0.133753	2.123633
N	2.362320	0.012299	1.439291
C	2.361420	-0.175110	0.102501
C	1.174758	-0.175579	-0.612114
C	3.634926	-0.003486	2.195403
H	3.883175	1.018847	2.494382
O	1.919872	-2.395046	3.205316
S	2.434517	-3.412640	2.240826
O	3.203134	-4.519742	2.823060
C	0.852661	-4.224130	1.620871
F	1.111328	-5.151667	0.682894
F	0.026007	-3.299647	1.060414
F	0.176085	-4.814066	2.620991
O	2.995876	-2.800206	1.002800
H	3.325650	-0.336721	-0.359811
H	1.204567	-0.334004	-1.684068
H	-0.973307	-0.032519	-0.464966
H	-0.926809	0.231394	2.033732
H	1.288678	0.207451	3.199271
H	3.497380	-0.653895	3.060082
H	4.414249	-0.420884	1.560604

A = CF_3SO_3- (isomer 4)

E(B3LYP/6-31+G*)= -1249.642988

C	0.012013	0.043363	0.009152
C	0.001024	0.014534	1.387660
N	1.161991	-0.015065	2.093628
C	2.359241	-0.031836	1.448331
C	2.420853	-0.003306	0.072098
C	1.235554	0.071101	-0.672094
C	1.128367	0.052556	3.567418
H	1.184333	1.096551	3.888358
O	1.322960	2.642537	-1.076363
S	1.641372	2.842953	-2.525406
C	3.482941	3.237139	-2.469100
F	3.728532	4.358439	-1.765927
O	1.601191	1.573197	-3.299153
O	1.040310	4.024756	-3.155845
F	4.171289	2.226500	-1.867106
F	3.996418	3.394753	-3.699889
H	3.240148	-0.050563	2.079562
H	3.386359	0.018883	-0.419888
H	1.272782	0.144752	-1.756359
H	-0.927502	0.094885	-0.529234
H	-0.911752	0.028579	1.971912
H	0.200682	-0.394061	3.927580
H	1.974235	-0.504181	3.973475

A = Cl- (isomer 1)

E(B3LYP/6-31+G*)= -748.399753

C	0.081602	0.187021	-0.028367
N	0.016204	0.003897	1.324315
C	1.152266	-0.176925	2.061356
C	2.367308	-0.366236	1.456583
C	2.433528	-0.357743	0.040460
C	1.299194	-0.101582	-0.691249
C	-1.260744	0.299268	1.987477
H	-1.468520	1.367220	1.862440
Cl	-0.156959	2.631842	-0.277466
H	1.020760	-0.186874	3.136896
H	3.248442	-0.532638	2.065689
H	3.378862	-0.546853	-0.459505
H	1.314396	-0.049791	-1.773600
H	-0.862082	0.181316	-0.550704
H	-2.057074	-0.286548	1.521038
H	-1.190571	0.036269	3.043850

A = Cl- (isomer 2)

E(B3LYP/6-31+G*)= -748.395325

C	-0.011372	-0.270486	0.044320
N	0.015495	-0.006725	1.373895
C	1.187578	0.135173	2.041780
C	2.397032	-0.002618	1.389137
C	2.399960	-0.283914	0.014486
C	1.187428	-0.407419	-0.653865
C	-1.277670	0.134806	2.088329
H	-1.125670	0.763667	2.966650
Cl	-2.708633	1.033984	-0.841817
H	1.110773	0.357547	3.099761
H	3.319061	0.114774	1.947873
H	3.339842	-0.395949	-0.518273
H	1.140640	-0.599221	-1.720499
H	-1.004741	-0.252396	-0.428873
H	-1.994062	0.588415	1.385653
H	-1.627594	-0.856780	2.387964

A = Cl- (isomer 3)

E(B3LYP/6-31+G*)= -748.391556

C	-0.040557	-0.420954	-0.035337
N	0.010411	0.135305	1.222146
C	1.224578	0.192951	1.866894
C	2.381582	-0.183514	1.259479
C	2.393951	-0.564023	-0.137427
C	1.081463	-0.814391	-0.695271
C	-1.223535	0.455589	1.938125
H	-1.027761	1.248769	2.663293
Cl	3.212748	1.125840	-1.227624
H	1.192929	0.542416	2.893326
H	3.313369	-0.118327	1.809847
H	3.203557	-1.202108	-0.469991
H	0.988735	-1.246507	-1.685254
H	-1.034049	-0.538181	-0.454855
H	-1.972900	0.816225	1.229582
H	-1.619569	-0.422435	2.464346

A = $ClCH_2COO^-$

E(B3LYP/6-31+G*)= -976.268751

C	0.055776	0.077321	-0.060508
N	-0.000814	0.084499	1.293234
C	1.117320	-0.040869	2.048462
C	2.352132	-0.192577	1.422727
C	2.434545	-0.210919	0.033101
C	1.262485	-0.070004	-0.719811
C	-1.297813	0.254381	1.994590
O	0.851477	0.448784	4.878875
C	0.312128	1.580836	4.959601
C	0.331666	2.364473	6.288246
O	-0.293630	2.208229	4.041714
H	0.991169	0.033059	3.150096
H	3.234285	-0.284956	2.047387
H	3.393374	-0.327798	-0.463701
H	1.278393	-0.070769	-1.804253
H	-0.887621	0.193235	-0.580743
H	-2.054909	0.543522	1.264700
H	-1.567529	-0.694988	2.463772
H	-1.151317	1.031158	2.765440
H	-0.693616	2.495335	6.640032
Cl	1.262662	1.603596	7.649458
H	0.766359	3.350446	6.116559

A = CH_3COO^- (isomer 1)

E(B3LYP/6-31+G*)= -516.672649

N	0.134222	-0.267508	0.078085
C	0.122824	-0.554499	1.532451
C	1.301305	-0.442462	-0.588313
C	1.357242	-0.152384	-1.950140
C	0.228173	0.316500	-2.614695
C	-0.959662	0.496604	-1.894363
C	-0.975678	0.197406	-0.544684
H	2.183666	-0.766361	0.013042
H	2.302403	-0.293316	-2.463838
H	0.264153	0.545242	-3.676042
H	-1.862634	0.867052	-2.367319
H	-1.857639	0.317760	0.073246
H	-0.825225	-0.214123	1.950878
H	0.238599	-1.630826	1.679095
H	0.987524	-0.017489	1.961478
C	3.665118	0.078739	1.742563
O	2.700360	0.879713	1.925312
O	3.629471	-0.951746	0.998513
C	4.985030	0.358884	2.470176
H	4.923452	1.271972	3.068309
H	5.233208	-0.489347	3.119684
H	5.797751	0.450191	1.739617

A = CH_3COO^- (isomer 1)

E(B3LYP/6-31+G*)= -516.655832

N	-0.054023	0.013269	-0.011261
C	0.272885	-0.027310	1.427512
C	0.961173	-0.006066	-0.922016
C	0.705804	-0.000402	-2.278085
C	-0.628616	0.025897	-2.714563
C	-1.659245	0.045820	-1.769468
C	-1.347034	0.038131	-0.419928
H	1.963721	-0.025467	-0.506631
H	1.504184	-0.014489	-3.055898
H	-0.767049	0.029589	-3.803472
H	-2.703532	0.068829	-2.065019
H	-2.096963	0.051794	0.362631
H	-0.622670	0.195991	2.007829
H	0.641922	-1.021616	1.693000
H	1.038656	0.719836	1.645564
C	1.518840	-0.019939	-5.594921
O	0.257587	0.001674	-5.482715
O	2.356233	-0.032387	-4.638293
C	2.109613	-0.017707	-7.013063
H	1.328358	-0.130411	-7.770177
H	2.641054	0.927513	-7.182890
H	2.847082	-0.822550	-7.114302

A = CN^- (isomer 1)

E(B3LYP/6-31+G*)= -380.982632

C	-0.009513	-0.118669	0.026629
N	0.014412	-0.006679	1.375403
C	1.180281	0.110087	2.060324
C	2.391809	0.118565	1.397635
C	2.401602	0.004288	-0.000234
C	1.193793	-0.114138	-0.678899
C	-1.272414	-0.011744	2.126053
H	-1.359442	0.929970	2.673323
N	-2.814919	-0.318832	-0.639778
C	-3.995018	-0.373657	-0.577598
H	1.094017	0.194104	3.137990
H	3.310135	0.212970	1.966901
H	3.343448	0.008742	-0.541424
H	1.154488	-0.204890	-1.759286
H	-1.023801	-0.208444	-0.425387
H	-2.091528	-0.114662	1.405148
H	-1.265745	-0.854161	2.821883

A = CN- (isomer 2)

E(B3LYP/6-31+G*)= -380.976062

C	0.155834	-0.028721	-0.036571
N	0.054802	0.017724	1.307473
C	1.163027	0.062543	2.097274
C	2.421071	0.061365	1.530806
C	2.547956	0.013332	0.131028
C	1.403216	-0.032123	-0.655010
C	-1.288075	0.021052	1.931636
H	-1.417686	0.941127	2.506549
C	-1.528997	-0.150329	-2.487984
N	-0.514818	-0.157131	-3.094436
H	0.991627	0.097994	3.167296
H	3.291399	0.097408	2.177364
H	3.533934	0.011855	-0.324833
H	1.386513	-0.071959	-1.745036
H	-0.756154	-0.065191	-0.652722
H	-2.036236	-0.028466	1.140624
H	-1.384507	-0.847527	2.587400

A = CN- (isomer 3)

E(B3LYP/6-31+G*)= -380.967400

C	-0.032151	-0.001053	0.033631
N	-0.029787	-0.009275	1.396908
C	1.138421	-0.033715	2.084338
C	2.351578	-0.052430	1.415645
C	2.367681	-0.044017	0.017811
C	1.149997	-0.017684	-0.675822
C	-1.319666	0.040804	2.114530
H	-1.767107	1.031063	1.995478
C	2.806036	-0.016509	-3.264070
N	3.775428	-0.035342	-2.586718
H	1.058184	-0.037749	3.165235
H	3.269621	-0.074620	1.993934
H	3.278335	-0.056513	-0.595967
H	1.185056	-0.011709	-1.771386
H	-1.009334	0.018993	-0.437079
H	-1.989637	-0.718992	1.707029
H	-1.150948	-0.158411	3.172853

A = CN- (isomer 4)

E(B3LYP/6-31+G*)= -380.967377

C	-0.008603	-0.003066	0.031531
N	-0.023517	-0.009662	1.394753
C	1.135017	-0.032480	2.097913
C	2.356818	-0.051215	1.444585
C	2.387983	-0.044530	0.047662
C	1.181874	-0.019719	-0.665145
C	-1.322658	0.040883	2.095721
H	-1.766016	1.032692	1.974305
N	2.667275	-0.016659	-3.212155
C	3.747329	-0.031021	-2.730171
H	1.040814	-0.035304	3.177618
H	3.267947	-0.072153	2.033767
H	3.311340	-0.057254	-0.543255
H	1.243726	-0.014971	-1.761800
H	-0.980143	0.015758	-0.450728
H	-1.988913	-0.715616	1.676311
H	-1.168568	-0.162844	3.155437

A = F-

E(B3LYP/6-31+G*)= -388.019084

N	0.040144	0.008417	0.038495
C	-0.001613	-0.035626	1.394015
C	1.214136	-0.041527	2.088464
C	2.424429	-0.003382	1.407556
C	2.419548	0.041694	0.004198
C	1.207247	0.046491	-0.654619
H	-1.097168	-0.063278	1.820752
H	1.182011	-0.076693	3.172917
H	3.367162	-0.008071	1.948367
H	3.340192	0.072616	-0.568499
H	1.122178	0.080060	-1.735464
C	-1.250824	0.014495	-0.707273
H	-2.054250	-0.017903	0.046717
H	-1.302147	0.927537	-1.306677
H	-1.280280	-0.863155	-1.358856
F	-2.512945	-0.081676	1.874407

XYZ coordinates and total energies of type 5b species at the B3LYP/6-31+G* level

A = SH-

E(B3LYP/6-31+G*)= -686.933706

C	-0.029509	-0.030898	0.137503
C	-0.030264	-0.042576	1.558499
N	1.227722	-0.045577	2.100240
C	2.396201	-0.039273	1.389305
C	2.376302	-0.029715	0.014986
C	1.124681	-0.025169	-0.629906
C	1.349774	-0.050066	3.574242
H	1.864122	0.856955	3.907657
H	3.318359	-0.041815	1.962923
H	3.308951	-0.025199	-0.539398
H	1.076584	-0.016450	-1.717069
H	-0.997911	-0.025029	-0.358080
H	0.345427	-0.079361	3.993163
H	1.914999	-0.929623	3.898592
H	-1.683841	0.020147	2.683161
S	-2.805499	0.055032	3.527485
H	-3.031256	-1.271481	3.408186

A = CN-

E(B3LYP/6-31+G*)= -380.979981

C	-0.038558	-0.016947	0.027671
N	-0.010853	0.024211	1.398518
C	1.117476	0.047395	2.171423
C	2.362527	0.028517	1.590006
C	2.435832	-0.014749	0.185008
C	1.261391	-0.035555	-0.550638
C	-1.299656	0.051840	2.120738
H	-1.392040	0.984191	2.686948
C	-2.548882	-0.058605	-1.975567
N	-3.450695	-0.074665	-2.705334
H	0.973423	0.080754	3.247227
H	3.250874	0.046435	2.212589
H	3.406586	-0.031296	-0.306297
H	1.319695	-0.068505	-1.636623
H	-1.696494	-0.043072	-1.268856
H	-2.095462	-0.009487	1.381393
H	-1.363818	-0.798882	2.806493

A = CH_3O-

E(B3LYP/6-31+G*)= -403.279056

C	0.011117	0.066922	-0.012570
C	-0.000118	0.078727	1.408744
N	1.255918	0.035860	1.958035
C	2.425681	-0.012903	1.252810
C	2.414894	-0.025087	-0.121886
C	1.168379	0.015549	-0.773829
C	1.375302	0.064162	3.434017
H	1.822340	1.013089	3.747680
O	-1.981989	0.238755	3.518798
H	3.344029	-0.040365	1.831607
H	3.350371	-0.065597	-0.670040
H	1.125206	0.006777	-1.861181
H	-0.952324	0.100594	-0.516301
H	-1.407502	0.193791	2.698113
H	0.377609	-0.028884	3.860764
H	2.007305	-0.764249	3.768870
C	-3.212959	-0.408214	3.268435
H	-3.790715	-0.402523	4.199324
H	-3.806518	0.108573	2.495934
H	-3.079337	-1.457328	2.955537

A = OH-

E(B3LYP/6-31+G*)= -363.976857

C	-0.005362	0.004313	-0.005800
N	-0.006736	0.029956	1.365395
C	1.107727	0.033895	2.156804
C	2.363710	0.008698	1.598483
C	2.463019	-0.019408	0.194879
C	1.302344	-0.020034	-0.562700
C	-1.311911	0.074058	2.064579
H	-1.418719	1.033282	2.581399
O	-2.745165	0.096771	-0.957449
H	0.943997	0.058210	3.229977
H	3.240364	0.010717	2.237799
H	3.442683	-0.039560	-0.278563
H	1.379236	-0.038963	-1.647609
H	-1.757151	0.054937	-0.785171
H	-2.102686	-0.033725	1.323775
H	-1.366305	-0.740333	2.793813
H	-2.899088	-0.399340	-1.774712

A = H-

E(B3LYP/6-31+G*)= -288.712351

C	-0.021666	0.068897	-0.203681
N	-0.170941	0.000417	1.156268
C	0.843699	-0.074308	2.079569
C	2.131637	-0.074988	1.463454
C	2.342511	-0.010187	0.096503
C	1.231065	0.064825	-0.766839
C	-1.557720	0.009929	1.663412
H	1.783929	-0.051070	5.653140
H	1.527290	-0.046956	4.952649
H	2.992786	-0.131800	2.126325
H	3.348827	-0.016779	-0.319020
H	1.341482	0.118301	-1.844986
H	-0.930404	0.125527	-0.796219
H	-1.500977	-0.063421	2.747825
H	-2.058094	0.941043	1.376156
H	-2.113864	-0.841846	1.257375

XYZ coordinates and total energies of type 5c species at the B3LYP/6-31+G* level

A = CH_3COO^-

E(B3LYP/6-31+G*)= -516.654787

C	-0.034407	0.092656	0.000756
N	-0.330711	0.142459	1.343879
C	0.679794	-0.155232	2.230897
C	1.947766	-0.494967	1.799155
C	2.252823	-0.548869	0.435494
C	1.222120	-0.249252	-0.460827
C	-1.630013	0.387660	1.794583
H	0.390214	-0.156457	3.272820
H	2.694441	-0.725007	2.552849
H	3.245162	-0.814210	0.087416
H	1.384472	-0.268934	-1.534260
H	-0.856893	0.333444	-0.661312
H	-1.659049	0.820261	2.790621
H	-2.251877	0.879711	1.051301
H	-2.296427	-1.159338	2.185617
O	-2.706776	-2.086279	2.459992
C	-2.071841	-2.580226	3.520983
O	-1.103343	-2.047816	4.050231
C	-2.682230	-3.877290	4.009426
H	-2.098856	-4.274291	4.842028
H	-3.714632	-3.701181	4.332251
H	-2.717876	-4.607729	3.193916

A = SH^-

E(B3LYP/6-31+G*)= -686.936624

C	-0.005462	-0.052257	0.118012
N	-0.022803	0.149707	1.494859
C	1.215227	0.197143	2.128956
C	2.398629	0.040510	1.438941
C	2.415468	-0.170825	0.054587
C	1.170366	-0.210688	-0.584796
C	-1.185710	0.237407	2.189283
H	-1.126275	0.565915	3.217669
H	1.173413	0.357190	3.198941
H	3.321606	0.089765	2.009751
H	3.342766	-0.293063	-0.492950
H	1.095532	-0.365924	-1.657370
H	-0.980940	-0.082345	-0.350731
H	-2.094063	0.376449	1.619463
H	-1.540580	-1.843609	2.564695
S	-1.782909	-3.190489	2.743060
H	-0.650456	-3.556187	2.105135

A = CN-

E(B3LYP/6-31+G*)= -380.980068

C	0.011059	0.010404	-0.009232
N	0.010199	0.007981	1.379504
C	1.252890	-0.008065	1.999421
C	2.431421	0.000557	1.282173
C	2.431486	0.015356	-0.117269
C	1.179678	0.018379	-0.742721
C	-1.148988	0.079798	2.096341
H	-1.079255	-0.145825	3.152669
C	-1.212266	3.367470	2.035373
N	-1.171204	4.522889	1.953016
H	1.223554	-0.018440	3.081750
H	3.361279	-0.008313	1.843388
H	3.353370	0.023694	-0.687151
H	1.093270	0.024733	-1.825382
H	-0.970240	0.015096	-0.466909
H	-1.257472	2.276840	2.115163
H	-2.063065	-0.141154	1.560424

A = F-

E(B3LYP/6-31+G*)= -388.008226

C	-0.003567	0.031878	0.041312
N	-0.034280	0.052980	1.414206
C	1.167572	0.019153	2.077935
C	2.373206	-0.048216	1.405905
C	2.408455	-0.076653	0.008705
C	1.183324	-0.035323	-0.663296
C	-1.250129	-0.002965	2.112998
H	1.097066	0.028350	3.158334
H	3.285493	-0.076771	1.993521
H	3.347298	-0.130107	-0.531477
H	1.134193	-0.053431	-1.747563
H	-0.972721	0.050894	-0.441061
H	-1.167467	0.388053	3.124178
H	-2.080445	0.397426	1.536404
H	-1.558521	-1.582107	2.281163
F	-1.689172	-2.595119	2.350151

A = CH_3O-

E(B3LYP/6-31+G*)= -403.277117

C	0.029488	-0.148705	-0.112034
C	-0.051521	-0.145449	1.265005
N	1.070794	-0.022966	2.069825
C	2.292804	0.069859	1.421122
C	2.395506	0.068747	0.045528
C	1.261394	-0.039980	-0.767318
C	0.972235	0.060427	3.432175
H	1.889341	-0.098745	3.985305
O	0.632142	3.081856	3.698083
H	3.150884	0.163414	2.074641
H	3.389010	0.152710	-0.385297
H	1.333534	-0.039766	-1.848893
H	-0.897388	-0.240923	-0.670676
H	-0.990799	-0.216329	1.798668
H	0.757189	2.103184	3.651073
H	0.034065	-0.269694	3.860609
C	0.398149	3.446810	5.047600
H	0.259060	4.532055	5.069090
H	-0.509583	2.975114	5.456764
H	1.247921	3.195412	5.702179

A = OH-

E(B3LYP/6-31+G*)= -363.974771

C	-0.007380	-0.059634	-0.044025
N	-0.044539	-0.006099	1.340724
C	1.176399	0.077059	1.991918
C	2.372193	0.128885	1.306115
C	2.409379	0.087340	-0.092249
C	1.177284	-0.009098	-0.748920
C	-1.228430	0.022290	2.027268
H	-1.166345	-0.188997	3.087436
O	-1.589475	3.055309	1.996158
H	1.115974	0.119443	3.072019
H	3.285042	0.201197	1.890176
H	3.344490	0.129564	-0.638884
H	1.120354	-0.048706	-1.832826
H	-0.975319	-0.121762	-0.524914
H	-1.532530	2.069920	2.047795
H	-2.103666	-0.297514	1.475804
H	-2.402499	3.288788	2.468455

A = H-

E(B3LYP/6-31+G*)= -288.720661

C	0.003752	-0.045846	0.066993
C	-0.012013	0.133420	1.433050
N	1.162310	0.243354	2.183343
C	2.357830	0.146393	1.465434
C	2.381365	-0.032828	0.099485
C	1.203122	-0.133467	-0.652125
C	1.143139	0.422773	3.514188
H	1.159912	-3.223276	3.439331
H	3.255268	0.227586	2.065598
H	3.355917	-0.094569	-0.377384
H	1.218575	-0.274363	-1.726476
H	-0.956670	-0.118180	-0.436320
H	-0.926352	0.204708	2.008448
H	2.081457	0.514344	4.039734
H	0.189865	0.504009	4.013880
H	1.155213	-2.491096	3.576990

XYZ coordinates and total energies of type 5d species at the B3LYP/6-31+G* level

A = $ClCH_2COO^-$ (isomer 1)

E(B3LYP/6-31+G*)= -976.264549

N	0.000962	-0.004778	0.008205
C	0.004974	0.040875	1.388670
C	1.143658	0.058335	2.116908
C	2.474496	-0.115005	1.482281
C	2.399934	0.065844	0.009147
C	1.216754	0.047313	-0.645485
O	2.912649	-1.559378	1.803515
C	4.210476	-1.816993	1.754003
O	5.089007	-1.027729	1.445406
C	-1.241982	-0.180088	-0.731084
C	4.580051	-3.267699	2.053998
Cl	3.453716	-4.165130	3.141222
H	-1.486462	-1.241350	-0.871988
H	-0.975108	0.107907	1.851189
H	1.080821	0.155469	3.195720
H	3.261502	0.483303	1.943933
H	3.320945	0.175271	-0.552890
H	1.155919	0.119046	-1.727354
H	-2.062395	0.300422	-0.189938
H	-1.155233	0.294189	-1.712990
H	4.619513	-3.815003	1.108088
H	5.569304	-3.278444	2.510786

A = $ClCH_2COO^-$ (isomer 2)

E(B3LYP/6-31+G*)= -976.260939

C	-0.039370	0.139376	-0.067461
C	-0.060111	0.073112	1.283226
C	1.194371	-0.061453	2.060766
C	2.377995	0.322242	1.254849
C	2.313677	0.381112	-0.094995
N	1.131444	0.238801	-0.787397
O	1.344048	-1.501961	2.638977
C	1.400653	-2.558796	1.834052
C	1.482387	-3.860337	2.631263
C	1.130238	0.079962	-2.236453
O	1.417741	-2.557005	0.616433
H	1.230637	-0.974498	-2.521635
H	-0.949156	0.157262	-0.659885
H	-1.012317	0.065593	1.803446
H	1.153381	0.446602	3.025865
H	3.322553	0.515429	1.753214
H	3.186782	0.584500	-0.707812
H	0.195552	0.472281	-2.647790
H	1.960881	0.646028	-2.668161
H	2.264318	-3.804541	3.390656
Cl	-0.068907	-4.216219	3.501597
H	1.664038	-4.684866	1.943617

A = CH_3COO^- (isomer 1)

E(B3LYP/6-31+G*)= -516.676519

C	-0.003682	-0.003538	-0.018095
C	-0.022003	0.015989	1.471028
C	1.362857	0.050645	2.022707
C	2.440327	-0.224335	1.255617
N	2.357003	-0.428053	-0.110425
C	1.122568	-0.275063	-0.713137
O	-0.721184	-1.260131	1.908328
C	-1.269224	-1.267456	3.136412
O	-1.229674	-0.328557	3.913069
C	3.510184	-0.886877	-0.870488
H	3.584743	-1.983012	-0.882459
C	-1.932813	-2.594895	3.436137
H	1.128051	-0.342320	-1.797111
H	-0.929086	0.168616	-0.558437
H	-0.651692	0.807480	1.882602
H	1.497715	0.267107	3.076914
H	3.446052	-0.255976	1.664528
H	3.436130	-0.529818	-1.902108
H	4.426000	-0.478419	-0.432518
H	-2.645604	-2.853306	2.646104
H	-1.176305	-3.387386	3.465658
H	-2.442877	-2.540155	4.399572

A = CH_3COO^- (isomer 2)

E(B3LYP/6-31+G*)= -516.672250

C	0.040824	0.080206	-0.098501
C	-0.005544	-0.078251	1.379497
C	1.359530	-0.025398	1.967313
C	2.457731	-0.222954	1.205015
N	2.399104	-0.331124	-0.168425
C	1.185356	-0.121082	-0.788222
O	-0.752727	-1.355236	1.791159
C	-0.296451	-2.570009	1.437577
O	0.708288	-2.788233	0.785253
C	3.551938	-0.795003	-0.928031
H	3.571140	-1.889988	-0.996088
C	-1.211455	-3.659215	1.965021
H	1.221212	-0.088758	-1.873258
H	-0.872363	0.314766	-0.636420
H	-0.688570	0.631806	1.851815
H	1.471991	0.127024	3.036146
H	3.456749	-0.267729	1.628797
H	3.518358	-0.376713	-1.938636
H	4.472111	-0.452837	-0.444683
H	-1.279736	-3.599997	3.056853
H	-2.223851	-3.527484	1.567469
H	-0.822631	-4.636030	1.670739

A = SH- (isomer 1)

E(B3LYP/6-31+G*)= -686.971434

C	0.011147	-0.035275	0.014109
C	0.009818	-0.052425	1.363870
N	1.174118	-0.058220	2.122817
C	2.373054	0.123725	1.443768
C	2.459850	0.147222	0.096899
C	1.275362	-0.099894	-0.780053
C	1.105328	0.214806	3.551604
H	1.015934	1.290742	3.765900
S	1.431645	-1.773086	-1.714813
H	3.245711	0.253826	2.076567
H	3.431983	0.283548	-0.365842
H	1.253721	0.580408	-1.639357
H	-0.937170	-0.042049	-0.513534
H	-0.913004	-0.056127	1.935959
H	0.242219	-0.301531	3.981493
H	2.006297	-0.166677	4.040531
H	1.451124	-2.538586	-0.602359

A = SH- (isomer 2)

E(B3LYP/6-31+G*)= -686.968547

C	0.006977	0.077382	-0.021162
C	-0.001261	0.182000	1.324427
N	1.159572	0.236632	2.081356
C	2.368411	0.255612	1.404451
C	2.459593	0.156350	0.060929
C	1.268244	-0.120283	-0.797624
C	1.112773	0.128486	3.530044
H	1.117760	-0.917723	3.868065
S	1.417877	-1.926371	-1.485659
H	3.244168	0.403714	2.029467
H	3.435605	0.230798	-0.407599
H	1.287630	0.474776	-1.715855
H	-0.940113	0.091492	-0.551754
H	-0.924308	0.267436	1.890141
H	0.205898	0.612452	3.906292
H	1.977373	0.639680	3.964696
H	0.748743	-1.714995	-2.642839

A = CN-

E(B3LYP/6-31+G*)= -381.020476

C	0.002747	0.104735	0.020876
C	0.010714	0.088614	1.365338
N	1.170937	0.107835	2.131806
C	2.375107	-0.038865	1.451931
C	2.482641	-0.028850	0.111655
C	1.282480	0.189195	-0.795745
C	1.101526	-0.214965	3.550763
H	1.036534	-1.298798	3.731166
C	1.378723	1.493294	-1.505238
H	3.246988	-0.169986	2.085679
H	3.460642	-0.136981	-0.345173
H	1.271014	-0.570496	-1.594476
H	-0.945317	0.100479	-0.506540
H	-0.914011	0.054451	1.933472
H	1.990339	0.173000	4.056408
H	0.224913	0.268104	3.991635
N	1.453904	2.512248	-2.059593

A = F-

E(B3LYP/6-31+G*)= -388.033693

C	0.000299	-0.000045	0.000043
C	0.000213	0.012672	1.352909
N	1.162098	0.026592	2.099663
C	2.363052	-0.086505	1.426811
C	2.446296	-0.102713	0.076546
C	1.256142	0.122348	-0.778672
C	1.109875	-0.138693	3.547513
H	1.056354	-1.197496	3.837509
F	1.330734	1.491867	-1.325676
H	3.239734	-0.183535	2.059960
H	3.419565	-0.206418	-0.391962
H	1.259753	-0.474590	-1.695250
H	-0.947106	-0.023132	-0.528537
H	-0.919299	-0.008963	1.929879
H	2.000703	0.306318	3.998740
H	0.233032	0.380530	3.943454

A = CH_3O- (isomer 1)

E(B3LYP/6-31+G*)= -403.305154

C	-0.026304	0.048188	0.042777
C	-0.007114	0.027719	1.392945
N	1.164134	-0.027195	2.129836
C	2.359762	0.082131	1.435394
C	2.427844	0.101600	0.088497
C	1.223423	-0.104854	-0.776925
C	1.134295	0.195229	3.568380
H	1.118146	1.265543	3.823253
O	1.342597	-1.441331	-1.358365
H	3.245727	0.167138	2.057779
H	3.398257	0.187557	-0.390130
H	1.225100	0.590935	-1.633312
H	-0.987405	0.117088	-0.457760
H	-0.918340	0.073379	1.982654
H	0.245947	-0.280209	3.993745
H	2.015346	-0.261762	4.028105
C	0.501850	-1.666133	-2.474432
H	0.764648	-2.648354	-2.877378
H	-0.564497	-1.673820	-2.200367
H	0.658716	-0.905782	-3.258285

A = CH_3O- (isomer 2)

E(B3LYP/6-31+G*)= -403.306220

C	-0.001586	0.036616	0.044232
C	-0.003411	0.039966	1.394030
N	1.159545	0.010218	2.151173
C	2.365614	0.115998	1.472331
C	2.453050	0.115404	0.125362
C	1.259067	-0.089208	-0.763289
C	1.103518	0.284435	3.580427
H	1.061972	1.362687	3.795382
O	1.323863	-1.355738	-1.493468
H	3.241469	0.214190	2.107623
H	3.431755	0.204947	-0.337263
H	1.264059	0.617913	-1.601084
H	-0.951363	0.064254	-0.482133
H	-0.923752	0.080506	1.969953
H	0.218553	-0.193324	4.010512
H	1.986805	-0.136857	4.069006
C	1.335674	-2.534855	-0.703723
H	1.385753	-3.370174	-1.407735
H	2.209975	-2.575366	-0.038065
H	0.423822	-2.632756	-0.097025

A = OH- (isomer 1)

E(B3LYP/6-31+G*)= -363.999286

C	-0.004713	-0.025054	0.002366
N	-0.006284	-0.050560	1.387076
C	1.223065	-0.032287	2.028199
C	2.397293	-0.123616	1.370215
C	2.468356	-0.362053	-0.105333
C	1.126635	-0.110193	-0.729860
C	-1.216977	0.284193	2.123321
H	-1.353091	1.371123	2.227504
O	2.897900	-1.752988	-0.289089
H	1.175876	0.076194	3.107747
H	3.323175	-0.107237	1.936334
H	3.246427	0.264858	-0.567697
H	1.050671	-0.063290	-1.813247
H	-0.982745	0.087174	-0.456630
H	-2.086405	-0.130188	1.605192
H	-1.173947	-0.161412	3.121277
H	3.137213	-1.876916	-1.223456

A = OH- (isomer 2)

E(B3LYP/6-31+G*)= -364.003519

C	0.004418	-0.081280	0.033563
N	-0.012071	-0.048397	1.420217
C	1.211379	-0.017665	2.073127
C	2.394278	-0.109109	1.426961
C	2.492974	-0.343152	-0.053003
C	1.142662	-0.175093	-0.688043
C	-1.227553	0.328395	2.127777
H	-1.360410	1.419505	2.172980
O	3.048435	-1.662720	-0.340500
H	1.152240	0.092805	3.152129
H	3.313075	-0.085326	2.005318
H	3.241376	0.310529	-0.516346
H	1.078040	-0.203114	-1.771692
H	-0.972251	-0.019191	-0.437813
H	-2.094794	-0.109667	1.625235
H	-1.193585	-0.063052	3.148654
H	2.439240	-2.317972	0.040311

A = H-

E(B3LYP/6-31+G*)= -288.778005

C	0.022727	-0.199803	0.079438
N	0.001191	-0.015838	1.465982
C	1.235663	-0.076313	2.121097
C	2.380068	-0.445966	1.520840
C	2.452541	-0.832325	0.059001
C	1.116967	-0.574614	-0.605221
C	-1.061740	0.787808	2.048822
H	1.201294	0.184213	3.175382
H	3.285598	-0.492341	2.120032
H	2.741421	-1.893794	-0.048377
H	1.028951	-0.722115	-1.678381
H	-0.930998	-0.032955	-0.413650
H	-2.020722	0.502252	1.605113
H	-1.117126	0.595095	3.124857
H	-0.912452	1.869329	1.894003
H	3.254135	-0.272015	-0.451159

XYZ coordinates and total energies of type 5e species at the B3LYP/6-31+G* level

A = $ClCH_2COO^-$ (isomer 1)

E(B3LYP/6-31+G*)= -976.267621

C	0.001953	-0.014049	0.173932
C	0.143855	0.135965	1.519112
C	1.475416	0.226962	2.050126
C	2.554122	0.038922	1.248467
C	2.376771	-0.377172	-0.157812
N	1.087388	-0.101048	-0.668252
O	2.552907	-1.946905	-0.257062
C	3.788921	-2.398128	-0.416289
C	3.849489	-3.915620	-0.563602
C	0.886341	-0.254607	-2.107873
O	4.801787	-1.716343	-0.416075
H	0.851768	-1.311018	-2.398840
H	-0.966314	-0.020320	-0.316163
H	-0.730121	0.239683	2.151281
H	1.615543	0.480832	3.098186
H	3.572660	0.125350	1.611193
H	3.155563	-0.025021	-0.833449
H	-0.047269	0.233678	-2.398576
H	1.710371	0.229868	-2.641457
Cl	2.919392	-4.508216	-2.002385
H	4.887322	-4.216539	-0.696842
H	3.416463	-4.399962	0.314220

A = $ClCH_2COO^-$ (isomer 2)

E(B3LYP/6-31+G*)= -976.266443

C	-0.007350	0.035156	-0.012838
C	-0.017261	0.016163	1.348157
C	1.245481	-0.017885	2.030502
C	2.401053	-0.165154	1.334746
C	2.372508	-0.416781	-0.120284
N	1.164649	-0.008067	-0.733890
O	2.534084	-1.986945	-0.281187
C	3.374678	-2.437087	-1.206503
C	3.580594	-3.945854	-1.106505
C	1.121062	0.063197	-2.193811
O	3.926577	-1.764943	-2.063344
H	1.003376	-0.929799	-2.645601
H	-0.911772	0.140288	-0.603724
H	-0.954397	0.088581	1.887467
H	1.273245	0.109773	3.109888
H	3.371113	-0.169082	1.820791
H	3.232525	-0.046429	-0.674703
H	0.286052	0.698938	-2.499312
H	2.051562	0.498549	-2.564969
Cl	4.634929	-4.363271	0.307409
H	2.630841	-4.461842	-0.957717
H	4.085299	-4.299942	-2.004151

A = CH_3COO^- (isomer 1)

E(B3LYP/6-31+G*)= -516.679175

C	-0.014040	0.032854	-0.001844
C	-0.036887	0.022161	1.436600
C	1.117778	0.017175	2.146533
C	2.426868	-0.104830	1.456763
N	2.365419	0.285021	0.089262
C	1.189571	0.177354	-0.619193
O	2.878767	-1.579252	1.473805
C	3.564077	-1.991419	2.553231
O	3.844451	-1.274706	3.499965
C	3.629724	0.457465	-0.617629
H	4.097839	-0.505435	-0.859386
C	3.931159	-3.456720	2.457201
H	1.286750	0.271577	-1.696354
H	-0.925473	-0.010199	-0.586515
H	-0.992939	0.052604	1.954229
H	1.135115	0.038529	3.231084
H	3.239496	0.411038	1.968612
H	3.458086	1.015109	-1.542287
H	4.319373	1.033179	0.008360
H	3.022212	-4.065407	2.528128
H	4.397274	-3.677284	1.491514
H	4.607733	-3.719388	3.272533

A = CH_3COO^- (isomer 2)

E(B3LYP/6-31+G*)= -516.679106

C	-0.007147	0.002845	0.031339
C	0.056748	-0.073701	1.465518
C	1.252469	-0.067698	2.104299
C	2.521530	-0.112622	1.335817
N	2.362649	0.347191	-0.004408
C	1.151900	0.226308	-0.646586
O	2.973994	-1.585311	1.319714
C	4.264137	-1.859940	1.586140
O	5.124761	-1.017721	1.782701
C	3.570544	0.622682	-0.778388
H	4.041244	-0.299153	-1.145015
C	4.513232	-3.352221	1.626250
H	1.180041	0.376842	-1.721518
H	-0.949767	-0.048469	-0.500814
H	-0.866444	-0.099281	2.039862
H	1.327703	-0.090669	3.186970
H	3.355691	0.401703	1.810833
H	3.317713	1.258420	-1.631267
H	4.293619	1.147580	-0.149170
H	4.008253	-3.782622	2.498827
H	4.095573	-3.836000	0.737540
H	5.585405	-3.545073	1.694983

A = CH_3COO^- (isomer 3)

E(B3LYP/6-31+G*)= -516.673105

C	-0.021415	0.335480	0.090438
C	0.019916	0.434693	1.444922
C	1.275575	0.200896	2.097321
C	2.362491	-0.196400	1.389530
C	2.277812	-0.475869	-0.062147
N	1.095010	0.041205	-0.659008
O	2.497370	-1.994152	-0.348757
C	1.579652	-2.913587	0.004005
C	2.097455	-4.318058	-0.240238
C	0.992103	-0.035814	-2.111197
O	0.478031	-2.664574	0.455804
H	0.729462	-1.046827	-2.448603
H	-0.924884	0.519213	-0.481993
H	-0.871443	0.698913	2.001228
H	1.360472	0.365729	3.169051
H	3.327883	-0.354574	1.860363
H	3.154351	-0.139315	-0.622616
H	0.230839	0.666103	-2.461946
H	1.952906	0.240246	-2.558638
H	2.485937	-4.416877	-1.259139
H	2.925634	-4.528158	0.446503
H	1.294434	-5.038390	-0.072179

A = SH- (isomer 1)

E(B3LYP/6-31+G*)= -686.972658

C	0.027005	0.007081	-0.004322
C	0.026375	0.024826	1.482089
N	1.361952	0.023324	2.012707
C	2.368548	-0.625904	1.336438
C	2.267645	-0.925398	0.011875
C	1.079883	-0.503459	-0.687836
S	-1.081204	-1.448026	2.180458
C	1.514582	0.341549	3.425386
H	1.038885	1.306070	3.637744
H	3.263797	-0.833566	1.914750
H	3.092444	-1.403703	-0.503319
H	1.043809	-0.574913	-1.772213
H	-0.878976	0.335215	-0.503960
H	-0.522695	0.873364	1.897579
H	1.050270	-0.424508	4.060248
H	2.576986	0.421626	3.668255
H	-0.470578	-2.395554	1.437326

A = SH- (isomer 2)

E(B3LYP/6-31+G*)= -686.969976

C	0.034449	-0.014372	-0.134871
C	-0.021937	-0.052778	1.349256
N	1.289404	-0.090208	1.930310
C	2.344773	0.525989	1.295118
C	2.307605	0.829942	-0.030032
C	1.129421	0.461011	-0.774631
S	-1.102158	1.498642	1.954070
C	1.376552	-0.379355	3.353619
H	0.997616	0.455542	3.959640
H	3.221186	0.704415	1.910618
H	3.167279	1.280983	-0.511490
H	1.134303	0.543075	-1.858812
H	-0.866059	-0.297310	-0.670506
H	-0.609332	-0.890808	1.729984
H	0.785966	-1.274025	3.581685
H	2.416878	-0.576711	3.624229
H	-1.688966	0.884310	3.007147

A = CN-

E(B3LYP/6-31+G*)= -381.015856

C	0.025677	-0.015900	0.020541
C	0.021371	-0.049738	1.378292
N	1.187796	-0.025730	2.118676
C	2.382793	0.551083	1.507338
C	2.448678	0.195247	0.033857
C	1.306151	-0.007021	-0.653787
C	1.127426	0.014191	3.572455
H	0.251052	-0.542140	3.914792
C	2.443984	2.045177	1.712221
H	3.256419	0.147451	2.035846
H	3.427858	0.178814	-0.433573
H	1.345816	-0.211813	-1.721128
H	-0.904107	-0.085213	-0.531109
H	-0.891342	-0.169542	1.954660
H	2.020369	-0.464740	3.989709
H	1.070120	1.043546	3.958986
N	2.494097	3.194368	1.878073

A = F-

E(B3LYP/6-31+G*)= -388.038975

C	-0.003844	0.108733	0.000881
C	-0.002929	0.076300	1.361618
N	1.158182	-0.056322	2.087522
C	2.425051	0.161650	1.486883
C	2.417375	-0.050661	0.024358
C	1.255597	-0.012799	-0.676412
C	1.104262	-0.060814	3.547758
H	1.932996	-0.660736	3.937358
F	2.847888	1.560824	1.759321
H	3.198612	-0.393470	2.023459
H	3.380222	-0.162436	-0.463486
H	1.271607	-0.103149	-1.760041
H	-0.939084	0.174927	-0.542519
H	-0.915716	0.105023	1.948282
H	1.184412	0.952634	3.958181
H	0.164936	-0.513245	3.876625

A = CH_3O- (isomer 1)

E(B3LYP/6-31+G*)= -403.308940

C	0.159486	0.050672	-0.047261
C	-0.058469	0.222409	1.285419
N	0.963973	0.244397	2.202728
C	2.262632	-0.284377	1.871348
C	2.536373	-0.164287	0.402127
C	1.521748	-0.078104	-0.491700
C	0.663140	0.410347	3.619513
H	-0.219836	1.046112	3.733183
O	2.294492	-1.668178	2.340961
H	3.019393	0.249078	2.471041
H	3.572421	-0.205283	0.079055
H	1.736416	-0.062825	-1.558394
H	-0.668831	0.079370	-0.745373
H	-1.048616	0.406449	1.692159
H	0.485441	-0.550527	4.117961
H	1.507679	0.905078	4.112152
C	3.595077	-2.219407	2.436633
H	3.491510	-3.197246	2.914448
H	4.061619	-2.357201	1.450192
H	4.255143	-1.588343	3.056279

A = CH_3O- (isomer 2)

E(B3LYP/6-31+G*)= -403.311164

C	-0.032301	0.112596	-0.072872
C	-0.027192	0.015727	1.286142
N	1.131264	0.015457	2.021835
C	2.432242	-0.199186	1.405265
C	2.398409	0.157418	-0.050375
C	1.236038	0.243602	-0.741448
C	1.078953	-0.058076	3.476251
H	1.903790	0.527173	3.898722
O	2.936331	-1.538385	1.652344
H	3.173188	0.395800	1.952297
H	3.361606	0.285142	-0.536182
H	1.254473	0.447137	-1.810433
H	-0.970089	0.144062	-0.614913
H	-0.944633	-0.025856	1.866986
H	0.136024	0.367439	3.831272
H	1.170567	-1.088065	3.844257
C	2.187126	-2.605437	1.081092
H	2.737735	-3.521542	1.310360
H	1.181491	-2.671683	1.520215
H	2.093169	-2.501480	-0.007199

A = OH- (isomer 1)

E(B3LYP/6-31+G*)= -364.002988

C	-0.000881	-0.012431	-0.017661
N	-0.022309	0.095234	1.353308
C	1.207469	0.128013	2.123876
C	2.335018	0.674349	1.309098
C	2.298228	0.669207	-0.044273
C	1.113533	0.256118	-0.749679
C	-1.242225	-0.228257	2.077759
H	-1.274781	0.348839	3.010004
O	1.594117	-1.198547	2.591762
H	1.019454	0.734466	3.022287
H	3.216886	0.992364	1.856753
H	3.164946	1.003141	-0.610603
H	1.084321	0.200373	-1.831545
H	-0.947439	-0.282073	-0.477421
H	-2.113059	0.050041	1.477124
H	-1.313439	-1.296820	2.325425
H	1.226215	-1.349770	3.477839

A = OH- (isomer 2)

E(B3LYP/6-31+G*)= -364.008728

C	0.065156	-0.097668	0.052940
N	-0.016313	0.109949	1.405606
C	1.184039	0.244524	2.218671
C	2.313835	0.800995	1.408972
C	2.337458	0.675041	0.058093
C	1.204328	0.147324	-0.655141
C	-1.255137	-0.178114	2.118348
H	-1.371146	0.531683	2.945348
O	1.547977	-1.010187	2.851039
H	0.934365	0.871537	3.080992
H	3.146237	1.228422	1.960108
H	3.209239	1.007537	-0.501694
H	1.221045	0.008474	-1.729667
H	-0.852714	-0.429352	-0.424514
H	-2.104183	-0.057411	1.439787
H	-1.264269	-1.193760	2.533165
H	2.042803	-1.533639	2.197278

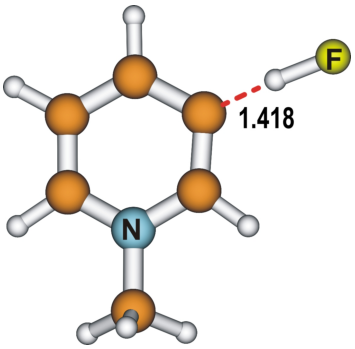
A = H-

E(B3LYP/6-31+G*)= -288.776593

N	0.003243	-0.185265	0.016278
C	0.029843	-0.061844	1.389503
C	1.191467	0.041195	2.088989
C	2.440548	-0.036162	1.352467
C	2.442376	0.029717	0.005593
C	1.158246	0.319284	-0.736418
H	-0.936130	-0.132737	1.883195
H	1.174203	0.070822	3.172339
H	3.368856	-0.192357	1.897941
H	3.357956	-0.060781	-0.572744
H	1.038734	1.413030	-0.921006
C	-1.262477	-0.095694	-0.684037
H	-1.215295	-0.674255	-1.613995
H	-2.064094	-0.508502	-0.064686
H	-1.517787	0.948180	-0.942559
H	1.154537	-0.161135	-1.723109

Structure, relative stability, XYZ coordinates and total energies of alternative H-bonded complexes between acids and the deprotonated 3 and 5

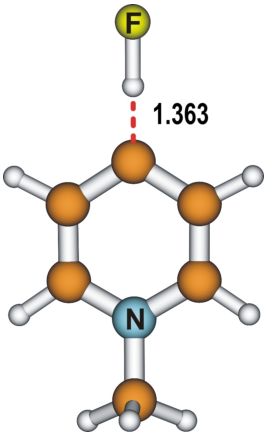
H-bonded complexes of acetic acid, HF and water with **3** deprotonated at position 4 or the N-methyl groups, and **5** deprotonated at position 3 and 4 were attempted to be optimized. The structures that could be optimized are listed below, together with the relative and total energies, and XYZ coordinates.



Relative stability compared to **5e**: 26.3 kcal mol^{-1}

E(B3LYP/6-31+G*)= -387.997050

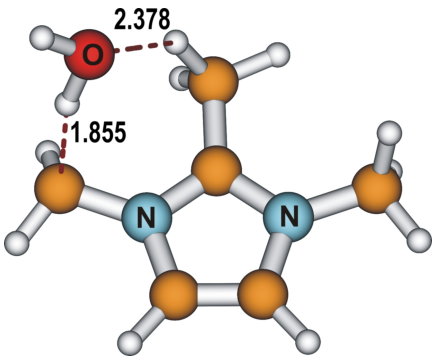
C	0.004015	0.009925	0.000474
C	0.002872	0.012547	1.402944
C	1.210297	0.003685	2.078459
N	2.372366	-0.012465	1.379858
C	2.357542	-0.021126	0.013015
C	1.194348	-0.009526	-0.750198
C	3.655913	0.034156	2.104964
H	3.939767	1.074072	2.291024
F	1.459386	-0.034038	-3.270281
H	3.345105	-0.039688	-0.442416
H	1.306408	-0.022150	-2.163571
H	-0.953642	0.021278	-0.518574
H	-0.918674	0.020321	1.978611
H	1.292699	0.008893	3.159349
H	4.424134	-0.449724	1.500450
H	3.558969	-0.496056	3.054148



Relative stability compared to **5e**: 27.8 kcal mol^{-1}

E(B3LYP/6-31+G*)= -387.994671

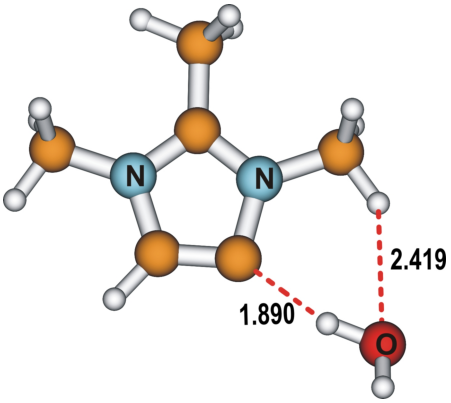
N	-0.033498	-0.032174	-0.000376
C	-0.125326	-0.016368	1.357650
C	1.013340	0.002721	2.138725
C	2.311020	0.008280	1.578249
C	2.342383	-0.006159	0.165101
C	1.190397	-0.025162	-0.596178
H	-1.133551	-0.021539	1.760733
H	0.886582	0.009574	3.219254
H	3.441100	0.024210	2.339315
H	3.295958	-0.006524	-0.358684
H	1.184732	-0.037042	-1.681930
C	-1.253893	0.010914	-0.822506
H	-2.064056	-0.493931	-0.293623
H	-1.537822	1.049003	-1.020456
H	-1.071545	-0.503556	-1.767516
F	4.400615	0.037754	2.985833



Relative stability compared to **3c**: 23.4 kcal mol^{-1}

E(B3LYP/6-31+G*)= -420.529950

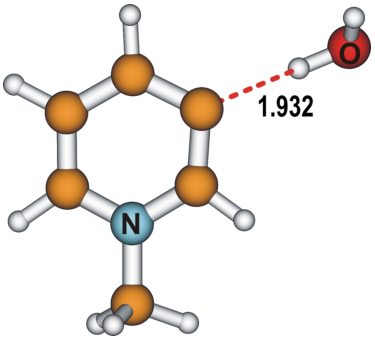
C	0.158971	0.628530	-0.119054
N	-0.046816	0.343664	1.225376
C	1.146229	0.022273	1.765704
N	2.101287	0.098409	0.783507
C	1.488244	0.468602	-0.390977
C	1.329968	-0.435185	3.164794
C	-1.317704	0.229253	1.876402
C	3.513939	-0.203911	0.949799
H	3.955751	0.425053	1.729371
H	3.660459	-1.257594	1.209480
H	4.023182	-0.000569	0.005927
H	2.041373	0.597096	-1.308732
H	-0.661211	0.911168	-0.759496
H	-1.255623	0.620941	2.894611
H	-2.067532	0.761847	1.289835
H	-1.342605	-1.608210	2.126503
H	1.053117	0.349009	3.883193
H	0.680053	-1.302943	3.352022
H	2.367618	-0.720366	3.356785
O	-1.050026	-2.565390	2.319733
H	-1.861886	-3.093732	2.334855



Relative stability compared to **3c**: 14.8 kcal mol^{-1}

E(B3LYP/6-31+G*)= -420.543625

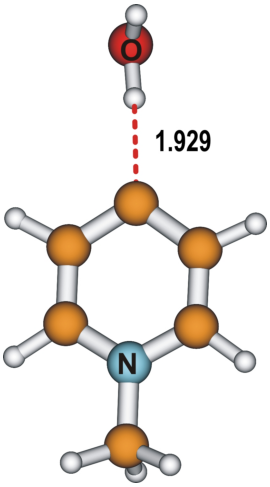
C	-0.403311	0.050663	0.154742
N	-0.188488	0.052237	1.539441
C	1.139535	-0.000188	1.749575
N	1.721506	-0.034255	0.531226
C	0.791815	-0.002773	-0.529413
C	3.169666	-0.087188	0.333217
C	-1.222697	0.102174	2.565218
H	3.353107	-0.144557	-0.740427
H	3.647465	0.812984	0.736246
H	3.594190	-0.969587	0.825195
H	-2.191823	0.138895	2.064874
H	-1.191313	-0.788880	3.200495
H	-1.117424	0.996708	3.187533
H	-1.416990	0.092683	-0.219136
C	1.835561	-0.019451	3.068961
H	1.670309	0.028440	-2.202874
O	2.358232	0.038315	-2.937598
H	1.987061	-0.499003	-3.652732
H	1.121284	0.042097	3.894170
H	2.419618	-0.939679	3.199970
H	2.531079	0.824013	3.164830



Relative stability compared to **5e**: 33.6 kcal mol^{-1}

E(B3LYP/6-31+G*)= -363.955075

C	0.046503	0.098245	0.003684
C	0.024082	0.112739	1.408167
C	1.219504	0.057064	2.101067
N	2.386011	-0.011310	1.413528
C	2.380250	-0.022943	0.040967
C	1.235859	0.030426	-0.756388
C	3.654310	-0.043092	2.163129
H	3.849975	0.936369	2.609474
O	1.628486	-0.319369	-3.644173
H	3.381027	-0.085157	-0.384649
H	1.494293	-0.199885	-2.657292
H	-0.915262	0.137813	-0.510474
H	-0.905001	0.162793	1.971155
H	1.290945	0.062487	3.183233
H	4.463728	-0.294881	1.477167
H	3.601333	-0.800512	2.949123
H	1.248656	0.478355	-4.041442



Relative stability compared to **5e**: 35.5 kcal mol^{-1}

E(B3LYP/6-31+G*)= -363.952121

C	0.000761	-0.007419	-0.003976
C	-0.001405	-0.006821	1.419733
C	1.315971	-0.006827	1.958254
C	2.460573	-0.010781	1.184367
N	2.377026	-0.015180	-0.174877
C	1.151216	-0.010438	-0.768756
C	3.596367	0.049273	-0.992412
H	3.875598	1.091569	-1.176903
O	-2.567148	0.390002	2.779330
H	1.158366	-0.009915	-1.855728
H	-0.943460	-0.005772	-0.548359
H	-1.673916	0.230787	2.350047
H	1.464281	-0.003863	3.038189
H	3.468614	-0.010833	1.591072
H	3.420249	-0.452823	-1.945657
H	4.410342	-0.456974	-0.469936
H	-2.790569	-0.449693	3.207614