Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

Carbenes in Ionic Liquids

Oldamur Hollóczki[†] Dirk Gerhard,[‡] Klemens Massone,[‡,] László Szarvas,[‡] Balázs Németh,[†] Tamás Veszprémi[†,]* and László Nyulászi[†,]**

[†]Department of Inorganic and Analytical Chemistry Budapest Univerity of Technology and Economics Szt. Gellért tér 4., Budapest, H-1111, Hungary; [‡]BASF AG D-67056 Ludwigshafen, Germany

E-mail: klemens.massonne@basf.com; nyulaszi@mail.bme.hu; veszpremi@mail.bme.hu

Table of Contents

1. XYZ coordinates and total energies of the optimized structures at the B3LYP/6-31+G* level

1,3-dimethylimidazol-2-ylidene

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

1,3-dimethylimidazolium cation (MeMIM)

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

1-ethyl-3-methylimidazol-2-ylidene (EMIM)

E(B3LYP/6-31+G*) = -344.126422

C	0.109961	-0.530703	0.395117
N	0.185076	0.254146	1.542277
C	1.451460	0.713932	1.787944
N	2.159353	0.184368	0.742420
C	1.368367	-0.572960	-0.116705
C	-0.944384	0.526160	2.429597
C	3.585010	0.405629	0.554659
H	3.932761	1.032508	1.376666
H	4.129638	-0.545396	0.567398
H	3.776944	0.915304	-0.396535
C	-1.285257	-0.656664	3.339196
H	-0.659872	1.397909	3.023298
H	-1.809615	0.803248	1.814361
H	1.753938	-1.058606	-1.001839
H	-0.808568	-0.977052	0.041481
H	-2.128572	-0.399539	3.991500
H	-1.564378	-1.543500	2.758112
H	-0.426336	-0.914488	3.967926

1-butyl-3-methylimidazol-2-ylidene

E(B3LYP/6-31+G*) = -422.755912

C	-0.009926	0.040931	-0.041885
C	-0.016094	0.057236	1.317135
N	1.318731	0.034970	1.710772
C	2.183579	-0.000751	0.649427
N	1.329084	0.004372	-0.420380
C	1.767051	-0.004275	3.100779
C	1.677274	-1.403297	3.723065
C	1.785161	-0.013569	-1.801697
H	2.875235	-0.048111	-1.788634
H	1.399905	-0.895824	-2.325614
H	1.457102	0.888422	-2.331040
H	2.802487	0.346493	3.098834
H	1.168982	0.712062	3.679185
H	-0.824879	0.060767	-0.751383
H	-0.838936	0.089195	2.017031
C	2.167658	-1.431684	5.176767
H	0.637872	-1.759615	3.677266
H	2.273434	-2.093608	3.111432
C	2.089579	-2.827149	5.807496
H	3.205623	-1.071066	5.216331
H	1.574922	-0.725943	5.777514
H	2.447207	-2.816756	6.844023
H	1.058249	-3.202770	5.814065
H	2.701424	-3.547682	5.250237

Anions:

$(CF_3SO_2)_2N^-$

E(B3LYP/6-31+G*) = -1827.2821948

C	0.219722	-0.147707	0.151505
F	0.303372	0.535775	1.304793
S	1.740648	0.093739	-0.940743
O	1.820541	1.549770	-1.129921
N	2.800174	-0.488780	0.141966
O	1.483771	-0.748170	-2.119565
F	-0.862904	0.304468	-0.518510
F	0.011252	-1.443736	0.440659
S	4.291513	-0.958233	-0.227530
C	4.132173	-2.830241	-0.457165
F	5.352089	-3.365169	-0.687302
F	3.629855	-3.417574	0.646903
F	3.340812	-3.143961	-1.493618
O	4.811633	-0.486627	-1.519343
O	5.130272	-0.858869	0.972708

$CF_3SO_3^-$

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_3CCOO^-

E(B3LYP/6-31+G*)= -1607.329643

C	-0.026650	-0.015119	-0.198477
C	0.002689	-0.038063	1.452013
Cl	1.688669	-0.009717	2.132115
Cl	-0.866722	1.455974	2.055437
Cl	-0.840520	-1.490159	2.150727
O	-1.046129	-0.542488	-0.663827
O	0.953663	0.561630	-0.687988

Cl_2CHCOO^-

E(B3LYP/6-31+G*)= -1147.743359

C	-0.043000	-0.025933	-0.159546
C	-0.034553	0.013639	1.427355
H	0.969704	0.173456	1.809571
Cl	-1.037011	1.390017	2.098617
Cl	-0.594152	-1.562951	2.169742
O	-1.138169	-0.203438	-0.718520
O	1.118983	0.137268	-0.607552

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

$CH_3CH_2COO^-$

E(B3LYP/6-31+G*)= -267.854773

C	0.000784	0.059608	0.042933
C	0.025451	-0.025840	1.608331
O	1.105463	-0.464179	2.092953
O	-1.018924	0.338314	2.214939
H	0.890850	0.625101	-0.270345
H	0.151790	-0.961551	-0.339554
C	-1.264419	0.670926	-0.566943
H	-1.220527	0.682182	-1.668934
H	-2.153672	0.109250	-0.258674
H	-1.408360	1.700335	-0.217039

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

PhO-

E(B3LYP/6-31+G*)= -306.920996

C	-0.001843	0.000000	0.005007
C	0.009167	0.000000	1.396905
C	1.212436	0.000000	2.126279
C	2.415705	0.000000	1.396905
C	2.426714	0.000000	0.005007
C	1.212436	0.000000	-0.784897
O	1.212436	0.000000	-2.060613
H	3.370669	0.000000	-0.540318
H	3.367010	0.000000	1.934939
H	1.212436	0.000000	3.215164
H	-0.942139	0.000000	1.934939
H	-0.945798	0.000000	-0.540318

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

Protonated anions:

$(CF_3SO_2)_2NH$

E(B3LYP/6-31+G*)= -1827.756993

C	0.256250	-0.617262	0.116666
F	0.320010	-0.336952	1.423100
S	1.630671	0.315542	-0.791910
O	1.467371	1.712962	-0.425171
N	2.979188	-0.282169	0.077539
O	1.674563	-0.186878	-2.149960
F	-0.913724	-0.211477	-0.373472
F	0.390172	-1.930697	-0.063133
S	4.387487	-1.062570	-0.517041
H	3.187691	0.256762	0.919977
C	3.889044	-2.879283	-0.342052
F	4.946077	-3.622540	-0.667389
F	3.532064	-3.130442	0.918576
F	2.874095	-3.150801	-1.160162
O	4.577329	-0.810227	-1.930001
O	5.384871	-0.796090	0.508938

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

Cl_3CCOOH

E(B3LYP/6-31+G*)= -1607.842157

C	0.087944	-0.067201	-0.087455
C	0.013878	-0.021186	1.467602
Cl	1.638923	0.240601	2.140695
Cl	-1.073302	1.330005	1.949173
Cl	-0.647403	-1.588365	2.056006
O	-1.129500	-0.264595	-0.614019
O	1.104569	0.058560	-0.718277
H	-1.030248	-0.285457	-1.584783

$Cl_2CHCOOH$

E(B3LYP/6-31+G*)= -1148.266087

C	0.057099	-0.062198	-0.070036
C	-0.031316	0.002937	1.454404
H	0.966223	0.196103	1.840040
Cl	-1.080363	1.366284	1.972647
Cl	-0.575319	-1.568758	2.129184
O	-1.123991	-0.296722	-0.658984
O	1.105158	0.087449	-0.655245
H	-0.975827	-0.322732	-1.623397

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_3CH_2COOH

E(B3LYP/6-31+G*)= -268.409955

C	-0.054057	-0.061816	0.037757
C	0.033996	0.077516	1.540264
O	0.915882	0.641364	2.154252
O	-1.025660	-0.501147	2.168657
H	0.914915	0.235994	-0.371134
H	-0.222480	-1.118244	-0.203699
C	-1.185657	0.792864	-0.564152
H	-0.906073	-0.353614	3.125971
H	-1.199990	0.678369	-1.653349
H	-2.161742	0.487750	-0.174404
H	-1.039541	1.855110	-0.338491

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

PhOH

E(B3LYP/6-31+G*)= -307.480312

C	0.013689	0.000000	-0.005332
O	-0.043107	0.000000	1.366395
H	0.855010	0.000000	1.733370
C	-1.203226	0.000000	-0.695398
C	-1.202070	0.000000	-2.090687
C	0.001050	0.000000	-2.805549
C	1.210893	0.000000	-2.106762
C	1.223314	0.000000	-0.709076
H	-2.130408	0.000000	-0.130190
H	-2.150374	0.000000	-2.622378
H	-0.005091	0.000000	-3.891796
H	2.154272	0.000000	-2.647060
H	2.168890	0.000000	-0.168870

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

Ion pairs (type 2 structures)

MeMIM - $(CF_3SO_2)_2N$-

E(B3LYP/6-31+G*) = -2132.639052

C	0.454754	0.643353	-0.317902
N	-0.192647	0.611103	0.852189
N	1.157955	-0.486783	-0.450679
C	1.918081	-0.866491	-1.647287
C	0.948289	-1.270625	0.668141
C	-1.181768	1.605603	1.283781
C	0.099979	-0.582811	1.485403
H	1.688588	-0.150399	-2.436238
H	2.988018	-0.867600	-1.424154
H	1.582917	-1.852552	-1.972386
H	-1.069827	2.496810	0.665625
H	-2.183023	1.195099	1.135848
H	-1.009118	1.853137	2.333380
H	1.398885	-2.244970	0.775681
H	-0.327838	-0.843673	2.440981
H	0.365774	1.438412	-1.053443
S	-1.962433	-0.555765	-2.404835
C	-3.364286	-1.132219	-3.529778
F	-4.119944	-2.020639	-2.863908
F	-4.130716	-0.105674	-3.904849
F	-2.864442	-1.726208	-4.622073
N	-1.057789	0.430037	-3.304409
O	-2.627565	0.093077	-1.259467
O	-1.181306	-1.777764	-2.162033
S	-1.275810	2.043006	-3.354848
C	-0.255208	2.340423	-4.912078
F	-0.256828	3.656251	-5.168765
F	1.018464	1.942506	-4.740882
F	-0.773943	1.693959	-5.959286
O	-0.506956	2.729945	-2.286940
O	-2.624291	2.527266	-3.650302

MeMIM - CF_3SO_3-

E(B3LYP/6-31+G*) = -1266.918087

C	-0.077233	0.119418	-0.236102
N	-0.224984	-0.171207	1.061396
N	1.210571	-0.032721	-0.564999
C	1.750622	0.196298	-1.913317
C	1.911522	-0.433875	0.560084
C	-1.507832	-0.118014	1.777981
C	1.010108	-0.520844	1.581341
H	0.922318	0.490462	-2.561206
H	2.498814	0.991822	-1.873634
H	2.205028	-0.726614	-2.281901
H	-2.278473	0.182012	1.064912
H	-1.736683	-1.106867	2.182830
H	-1.440072	0.611662	2.588657
H	2.974240	-0.620679	0.537472
H	1.139212	-0.797725	2.616448
H	-0.870704	0.426966	-0.909607
S	-2.739942	1.012867	-2.514923
C	-3.483202	-0.526156	-3.301511
F	-4.790396	-0.638875	-3.008508
F	-3.351753	-0.500237	-4.639177
F	-2.860972	-1.640906	-2.847315
O	-1.299331	0.916857	-2.902280
O	-3.499228	2.126536	-3.090372
O	-2.930658	0.759821	-1.053943

MeMIM - $CCl_3CO_2^-$

E(B3LYP/6-31+G*) = -1912.701917

C	-0.020589	0.000408	0.005086
C	-0.007486	-0.008706	1.369533
N	1.322799	-0.006486	1.755399
C	2.096260	0.003823	0.660666
N	1.299589	0.008110	-0.415062
C	1.851778	-0.013982	3.124178
C	1.781146	0.019449	-1.805609
O	4.909398	0.009249	1.207354
C	5.427897	0.015771	0.062467
O	4.871530	0.021712	-1.050434
C	7.021919	0.015725	0.075334
H	2.941824	-0.009431	3.064365
H	1.506460	0.875852	3.656605
H	1.513286	-0.913726	3.644184
H	2.875579	0.021303	-1.778890
H	1.413879	-0.872410	-2.319864
H	1.410660	0.917596	-2.306473
H	-0.843584	0.001998	-0.693209
H	-0.815452	-0.016637	2.085103
H	3.202125	0.007837	0.693276
Cl	7.726646	0.029018	-1.574395
Cl	7.602033	1.482123	0.964671
Cl	7.600950	-1.466436	0.940114

MeMIM – $CHCl_2CO_2^-$

E(B3LYP/6-31+G*) = -1453.120345

C	-0.011499	-0.031504	0.001605
C	-0.002651	0.081677	1.361438
N	1.326539	0.101401	1.750463
C	2.103291	0.003384	0.662265
N	1.309765	-0.078577	-0.412526
C	1.853091	0.210370	3.115354
C	1.796323	-0.198287	-1.796656
O	4.927385	0.027128	1.270850
C	5.430816	-0.069685	0.111705
O	4.831128	-0.153683	-0.979448
C	6.987330	-0.079112	0.113021
H	2.943160	0.193659	3.056489
H	1.520228	1.149658	3.564417
H	1.500869	-0.633452	3.714193
H	2.890722	-0.205666	-1.761940
H	1.420282	-1.128995	-2.229298
H	1.437340	0.655212	-2.377587
H	-0.832397	-0.081929	-0.697351
H	-0.812705	0.148514	2.071544
H	3.207710	-0.004166	0.698142
Cl	7.646117	1.345101	-0.786322
H	7.368135	-0.006818	1.127722
Cl	7.630298	-1.625333	-0.569406

MeMIM – Cl^-

E(B3LYP/6-31+G*) = -765.654219

N	-0.056800	0.000276	-1.566240
C	-0.089246	0.000044	-0.225251
N	1.174160	-0.000066	0.218619
C	2.037023	0.000158	-0.864638
C	1.264810	0.000349	-1.988944
C	1.533907	-0.000359	1.645209
C	-1.246094	0.000438	-2.420453
H	-0.972462	-0.000051	0.464954
H	3.109791	0.000140	-0.745444
H	1.535952	0.000536	-3.033749
H	0.600086	-0.000356	2.219200
H	2.117468	-0.896559	1.870499
H	2.117674	0.895630	1.870803
H	-1.251706	-0.894316	-3.048376
H	-2.127893	0.000319	-1.778160
H	-1.251701	0.895431	-3.048034
Cl	-2.032512	-0.000251	2.178772

MeMIM – $CH_2ClCO_2^-$

E(B3LYP/6-31+G*) = -993.530307

C	-0.008029	-0.080673	-0.005704
C	-0.019677	0.001217	1.356251
N	1.303480	0.060031	1.762417
C	2.098507	0.015576	0.683105
N	1.319653	-0.070117	-0.402702
C	1.808369	0.155782	3.136308
C	1.830486	-0.140126	-1.780894
O	4.867590	0.121295	1.215598
C	5.441046	0.072255	0.093191
O	4.887309	-0.008086	-1.037271
C	6.979133	0.109534	0.003315
H	2.898981	0.183274	3.092957
H	1.433384	1.069850	3.603974
H	1.482692	-0.715566	3.710378
H	2.925693	-0.105909	-1.728843
H	1.497173	-1.074625	-2.240112
H	1.446623	0.711131	-2.349445
H	-0.818102	-0.144507	-0.716147
H	-0.840242	0.022287	2.057139
H	3.213325	0.048145	0.736047
H	7.281213	0.970830	-0.595135
Cl	7.869814	0.225702	1.583121
H	7.330113	-0.797107	-0.492704

MeMIM – $CH_3CH_2CO_2^-$

E(B3LYP/6-31+G*) = -573.248182

C	-0.036597	-0.199111	-0.008395
C	-0.045427	-0.079047	1.350601
N	1.273665	0.084336	1.742265
C	2.064618	0.064899	0.658028
N	1.284303	-0.106774	-0.417008
C	1.780741	0.255151	3.106911
C	1.788010	-0.180491	-1.797793
O	4.803790	0.380448	1.164327
C	5.377377	0.340618	0.025152
O	4.780229	0.185994	-1.076473
C	6.907636	0.490241	-0.025569
H	2.866339	0.357786	3.050072
H	1.346409	1.153818	3.553048
H	1.522290	-0.619530	3.709774
H	2.879316	-0.067682	-1.752658
H	1.516682	-1.148935	-2.226879
H	1.340072	0.625152	-2.385906
H	-0.844721	-0.340209	-0.709925
H	-0.860713	-0.095483	2.057785
H	3.181600	0.178505	0.704846
H	7.124549	1.333311	-0.696011
C	7.601919	0.679861	1.324215
H	7.298659	-0.397193	-0.542240
H	8.688238	0.777284	1.193693
H	7.235889	1.577660	1.834419
H	7.411090	-0.169287	1.989649

MeMIM – $CH_3CO_2^-$

E(B3LYP/6-31+G*) = -533.933992

C	-0.006773	0.097868	-0.009758
N	-0.003429	0.000114	1.372440
C	1.263756	-0.051542	1.811747
N	2.070948	0.010816	0.744445
C	1.299553	0.104345	-0.403213
C	3.540052	-0.018542	0.820288
C	-1.166366	-0.043378	2.263594
O	1.567128	-0.247876	4.580492
C	2.824924	-0.270383	4.808228
C	3.249948	-0.379153	6.275385
O	3.718576	-0.214164	3.920844
H	-0.798801	-0.121164	3.288841
H	-1.754600	0.871089	2.149325
H	-1.783807	-0.913319	2.024242
H	3.810684	-0.092052	1.881771
H	3.910778	-0.885470	0.266487
H	3.940172	0.900479	0.383330
H	1.740271	0.166652	-1.386577
H	-0.919411	0.153425	-0.583413
H	1.537874	-0.131958	2.901326
H	4.337999	-0.342895	6.375417
H	2.797221	0.433878	6.855326
H	2.875982	-1.320283	6.697133

MeMIM – PhO^-

E(B3LYP/6-31+G*) = -612.301545

C	0.747482	-0.013156	-0.274214
C	0.306272	0.011848	1.015226
N	1.434613	0.034006	1.820150
C	2.539963	0.026063	1.055887
N	2.134328	-0.003652	-0.225431
C	1.474274	0.057467	3.285036
C	3.038654	-0.048391	-1.378544
O	4.879137	-0.154984	2.279556
C	5.903149	-0.067492	1.461406
H	2.521923	0.033549	3.591759
H	0.999559	0.970258	3.655486
H	0.953861	-0.818098	3.682296
H	4.058978	0.115718	-1.024194
H	2.971249	-1.024800	-1.866242
H	2.766238	0.739115	-2.086079
H	0.203305	-0.035715	-1.206295
H	-0.694620	0.017126	1.419719
H	3.621296	0.004301	1.510902
C	6.111849	1.076955	0.634702
C	7.178927	1.146225	-0.265999
C	8.087417	0.089105	-0.386984
C	7.910069	-1.041597	0.425861
C	6.849564	-1.124558	1.325205
H	5.439918	1.926300	0.755814
H	7.309716	2.043773	-0.870079
H	8.920223	0.148003	-1.083275
H	8.613183	-1.870689	0.354363
H	6.717734	-2.003938	1.952044

MeMIM – SH^-

E(B3LYP/6-31+G*) = -704.206564

C	0.092582	0.241130	-0.050348
N	-0.001201	-0.076754	1.294690
C	1.229944	-0.255708	1.796940
N	2.108635	-0.045238	0.803159
C	1.420583	0.262574	-0.361559
C	-1.225079	-0.198308	2.098580
C	3.561019	-0.140377	0.962974
S	1.302451	-0.235630	4.967972
H	-0.925289	-0.205416	3.153769
H	-1.871664	0.659451	1.898121
H	-1.745305	-1.126019	1.844985
H	3.775506	-0.303536	2.020649
H	3.948345	-0.977329	0.375383
H	4.029842	0.791120	0.635472
H	1.924805	0.469101	-1.293564
H	-0.778088	0.425541	-0.661309
H	1.435897	-0.367205	2.914542
H	1.556919	1.082602	5.160685

MeMIM – CN^-

E(B3LYP/6-31+G*) = -398.241483

C	0.078009	-0.010854	-0.049576
N	0.004752	-0.007900	1.333309
C	1.245089	0.006312	1.832688
N	2.112204	0.012166	0.811673
C	1.402146	0.001766	-0.379596
C	-1.207166	-0.018688	2.170118
C	3.569640	0.027089	0.969958
C	1.959252	-0.014940	5.052722
H	-0.881243	-0.019225	3.216929
H	-1.800580	0.873364	1.954218
H	-1.787493	-0.918119	1.949460
H	3.797290	0.025408	2.037411
H	4.000308	-0.861833	0.502250
H	3.981706	0.928157	0.508700
H	1.891842	0.003761	-1.341421
H	-0.804130	-0.022038	-0.671356
H	1.463395	0.009431	2.912626
N	0.814881	-0.013857	4.751028

1,3-dimesitylimidazolium 2,6-di-*tert*-butyl-4-methylphenolate

E(B3LYP/6-31+G*) = -1467.553968

C	-2.969865	-0.958091	-2.071914
C	-3.132675	-0.481964	-0.760632
C	-3.843667	-1.177596	0.231952
C	-4.409778	-2.406217	-0.127244
C	-4.264617	-2.911611	-1.419089
C	-3.551965	-2.194676	-2.379201
N	-2.574634	0.813220	-0.419264
C	-1.296720	1.075649	-0.080581
N	-1.209933	2.399088	0.155743
C	-2.453918	2.986374	-0.040201
C	-3.308651	1.993255	-0.400753
C	-0.017990	3.133603	0.538762
C	0.258631	3.292088	1.906709
C	1.393307	4.039291	2.246157
C	2.204381	4.600477	1.260185
C	1.896184	4.426541	-0.088519
C	0.774662	3.685762	-0.480705
C	-0.611498	2.677660	2.977563
C	0.453718	3.477593	-1.941363
C	-3.979148	-0.644947	1.638948
C	-2.190513	-0.191583	-3.112824
O	0.871430	-0.645301	-0.064640
C	1.822633	-1.535552	0.098383
C	2.964409	-1.568256	-0.792029
C	3.949397	-2.544193	-0.609389
C	3.880470	-3.490303	0.413331
C	2.794640	-3.455297	1.287240
C	1.768806	-2.511509	1.166848
C	3.107229	-0.526020	-1.922697
C	3.188579	0.893169	-1.310136
C	0.589164	-2.521619	2.162853
C	-0.730616	-2.805986	1.407305
C	4.381782	-0.723466	-2.771443
C	1.904270	-0.616493	-2.892474
C	0.723222	-3.606487	3.252613
C	0.505712	-1.161075	2.897071
H	-2.603412	4.046393	0.094671
H	-4.358649	2.007142	-0.648503
H	4.805598	-2.578126	-1.275931
H	4.662026	-4.237586	0.530172
H	2.758733	-4.193228	2.082810
H	-1.589651	-2.758880	2.093517
H	-0.875792	-2.088038	0.598015
H	-0.708011	-3.811483	0.968431
H	-0.138573	-3.547440	3.931111
H	0.739078	-4.618233	2.829771
H	1.628487	-3.474431	3.857338
H	-0.383102	-1.123387	3.546127

H	1.390096	-1.014379	3.530332
H	0.467020	-0.343740	2.173842
H	4.418833	0.047658	-3.552552
H	5.296350	-0.629465	-2.173448
H	4.399321	-1.699485	-3.271637
H	1.967599	0.166137	-3.663897
H	1.892810	-1.589645	-3.400348
H	0.970828	-0.507293	-2.336796
H	3.237242	1.655600	-2.102574
H	2.321572	1.087957	-0.675915
H	4.092410	0.990412	-0.695253
H	1.641073	4.174304	3.295697
H	3.083470	5.172630	1.544484
H	2.537024	4.857269	-0.853025
H	-0.562024	3.807509	-2.191933
H	1.151247	4.039066	-2.569021
H	0.538725	2.420335	-2.217821
H	-0.299575	3.023973	3.967061
H	-1.669198	2.938247	2.850621
H	-0.537154	1.584081	2.971924
H	-4.956903	-2.974036	0.620553
H	-4.704734	-3.871151	-1.677074
H	-3.437477	-2.595559	-3.382821
H	-2.486941	0.863199	-3.155347
H	-1.114661	-0.225828	-2.906272
H	-2.349646	-0.624628	-4.104548
H	-4.528352	-1.354639	2.263890
H	-2.997999	-0.486074	2.100489
H	-4.516482	0.311071	1.670538
H	-0.458138	0.338900	-0.013272

Hydrogen bridged carbene – acid pairs (type 3 structures)

MeMIM - $CH_3CH_2COO^-$

E(B3LYP/6-31+G*) = -573.244466

N	0.002908	-0.031109	0.028213
C	0.003512	0.024397	1.415539
C	1.307318	0.082133	1.798467
N	2.055481	0.059768	0.628299
C	1.264926	-0.010331	-0.480380
C	3.511733	0.105101	0.578705
C	-1.203719	-0.103036	-0.794892
O	2.219488	-0.081532	-3.066660
C	1.322027	-0.150942	-4.043301
C	1.966458	-0.184003	-5.421447
O	0.109136	-0.185006	-3.863416
H	3.817224	0.073049	-0.467796
H	3.881719	1.029451	1.034778
H	3.939644	-0.753872	1.106313
H	-0.902387	-0.136450	-1.843778
H	-1.772955	-1.004717	-0.545410
H	-1.829424	0.778283	-0.618553
H	-0.904716	0.018181	2.000329
H	1.754709	0.135858	2.780224
C	0.965796	-0.264060	-6.573481
H	2.600602	0.708658	-5.507943
H	2.659934	-1.035645	-5.438318
H	1.775318	-0.058427	-2.115298
H	1.491322	-0.284586	-7.535543
H	0.348227	-1.165131	-6.498831
H	0.288247	0.596060	-6.569182

MeMIM - CH_3COO^-

E(B3LYP/6-31+G*) = -533.929721

C	-0.018470	-0.000912	0.035855
C	-0.035619	-0.004704	1.395830
N	1.293494	-0.002347	1.799442
C	2.147993	0.002743	0.737051
N	1.317774	0.003528	-0.341025
C	1.733981	-0.004990	3.189083
C	1.785187	0.008518	-1.726832
O	4.892756	0.009440	0.957067
C	5.590523	0.016317	-0.172369
O	5.090907	0.020449	-1.292761
C	7.087057	0.018020	0.065412
H	2.824588	-0.002196	3.200119
H	1.365401	0.885471	3.709202
H	1.370029	-0.900172	3.704333
H	2.877022	0.010880	-1.721039
H	1.420695	-0.883471	-2.247228
H	1.416938	0.901931	-2.242111
H	-0.826882	-0.001036	-0.680627
H	-0.860699	-0.008756	2.093024
H	7.617958	0.028709	-0.888170
H	7.370189	0.894704	0.658787
H	7.374438	-0.869270	0.640798
H	3.854450	0.007518	0.786841

MeMIM - PhO-

E(B3LYP/6-31+G*) = -612.309603

C	-0.312830	-0.286000	0.169253
N	0.049430	-0.389493	1.480198
C	1.298161	0.168650	1.724726
C	1.743993	0.641560	0.530374
N	0.750251	0.353798	-0.397076
C	0.825829	0.688993	-1.814324
C	-0.781028	-1.023524	2.497388
H	-0.250145	-1.866498	2.951824
H	-1.050315	-0.303250	3.277108
H	-1.688141	-1.388996	2.014950
H	1.754733	0.180283	2.703740
H	2.663506	1.144767	0.268960
H	0.875766	1.774533	-1.950226
H	1.708648	0.226990	-2.268248
H	-0.070908	0.304779	-2.301702
O	-2.602585	-1.355966	-1.173608
C	-3.743092	-0.626232	-1.135662
C	-3.832035	0.631852	-0.511687
C	-5.043855	1.328741	-0.510123
C	-6.179871	0.794425	-1.124145
C	-6.087751	-0.456961	-1.746159
C	-4.885526	-1.163045	-1.754381
H	-4.806318	-2.134853	-2.233859
H	-6.961559	-0.888357	-2.229782
H	-7.118957	1.341271	-1.119602
H	-5.095572	2.300437	-0.023100
H	-2.953289	1.057030	-0.034843
H	-1.837656	-0.918488	-0.678978

MeMIM - SH-

E(B3LYP/6-31+G*) = -704.205227

C	0.078023	-0.071475	-0.091350
N	0.100641	-0.015726	1.297807
C	1.370476	0.059036	1.795797
N	2.138805	0.048446	0.666362
C	1.375964	-0.030612	-0.493466
C	-1.090275	-0.030222	2.137314
C	3.594188	0.117234	0.686023
S	2.398183	0.314344	5.141521
H	-0.769858	0.039117	3.177459
H	-1.736833	0.821780	1.900929
H	-1.652352	-0.959211	1.991892
H	3.913942	0.186810	1.726357
H	4.028066	-0.780523	0.232282
H	3.944032	1.000459	0.140731
H	1.808936	-0.049767	-1.483234
H	-0.836367	-0.133043	-0.663688
H	2.483352	-1.026527	5.279275
H	1.993043	0.229382	3.823728

MeMIM - CN-

E(B3LYP/6-31+G*) = -398.251772

C	-0.027479	0.005200	-0.000505
C	-0.045176	0.006060	1.358327
N	1.284536	0.001091	1.763293
C	2.152784	-0.002901	0.707427
N	1.312315	-0.000281	-0.370707
C	1.709068	0.000826	3.157192
C	1.772885	-0.002840	-1.753120
C	5.399897	-0.032454	0.744600
N	6.559540	-0.048717	0.757449
H	2.799170	-0.003465	3.180551
H	1.341670	0.895521	3.671130
H	1.334596	-0.889875	3.672946
H	2.863222	-0.007713	-1.748267
H	1.411433	-0.894131	-2.277074
H	1.419413	0.891256	-2.277756
H	-0.835960	0.007704	-0.717186
H	-0.872043	0.009464	2.053710
H	4.299060	-0.017771	0.732264

MeMIM - F-

E(B3LYP/6-31+G*) = -405.285646

C	0.023721	0.000040	0.139720
N	0.156163	0.016033	1.491628
N	1.303077	-0.013833	-0.316740
C	1.650571	-0.033495	-1.733996
C	2.219610	-0.006918	0.727023
C	-0.978170	0.032313	2.409695
C	1.491118	0.011915	1.875760
H	-1.892312	0.045014	1.814952
H	-0.968581	-0.860956	3.042502
H	-0.942955	0.925537	3.041554
H	0.723345	-0.033176	-2.308341
H	2.239219	0.852240	-1.993554
H	2.225305	-0.934247	-1.972209
H	3.287918	-0.015426	0.568269
H	1.803013	0.022740	2.909763
H	-1.296552	-0.002825	-0.693352
F	-2.172917	-0.004958	-1.243188

MeMIM - CH_3O-

E(B3LYP/6-31+G*) = -420.549990

C	0.022450	-0.128104	-0.039306
C	-0.183270	-0.227688	1.300878
N	1.381917	0.111703	-0.205600
N	1.057115	-0.045013	1.899761
C	2.048311	0.167877	0.984917
H	-0.667244	-0.204665	-0.867390
H	-1.087329	-0.407685	1.864440
C	1.285074	-0.069865	3.341306
C	2.028576	0.291293	-1.497929
H	0.688746	0.705925	3.833310
H	1.013031	-1.047990	3.752719
H	2.344449	0.119551	3.521412
H	1.911086	-0.605461	-2.116116
H	1.601344	1.150821	-2.025759
H	3.089427	0.470232	-1.319769
H	3.815263	0.532746	1.743391
O	4.604956	0.675476	2.330360
C	5.642214	-0.196771	1.927727
H	6.470178	-0.077012	2.634633
H	5.330144	-1.254250	1.940533
H	6.019084	0.038879	0.918502

MeMIM - OH-

E(B3LYP/6-31+G*) = -381.247697

C	-0.074571	0.043367	0.017884
C	-0.145810	0.014112	1.375279
N	1.279127	0.022327	-0.299128
N	1.165438	-0.023024	1.833475
C	2.071734	-0.018927	0.812009
H	-0.853580	0.075391	-0.730012
H	-0.999880	0.014886	2.037017
C	1.541751	-0.072922	3.243234
C	1.801264	0.035797	-1.658300
H	1.170321	0.814483	3.767220
H	1.126087	-0.969668	3.715060
H	2.630693	-0.103604	3.304222
H	1.431643	-0.828445	-2.220737
H	1.506474	0.955018	-2.176454
H	2.889136	-0.013055	-1.599686
H	3.945655	-0.164613	1.383933
O	4.786851	-0.256120	1.907401
H	5.354348	0.474996	1.622285

1,3-dimesitylimidazol-2-ylidene - 2,6-di-*tert*-butyl-4-methylphenole

E(B3LYP/6-31+G*) = -1467.557107

C	3.742612	-0.228837	-0.405635
C	2.564879	-0.253041	0.397220
C	2.620628	-0.448786	1.804866
C	3.893051	-0.615058	2.376018
C	5.056798	-0.594710	1.617040
C	4.971497	-0.403488	0.240595
O	1.399380	-0.074424	-0.303133
C	-1.753226	0.167122	-0.236974
N	-2.439672	1.331595	-0.471794
C	-3.722800	1.109959	-0.974844
C	-3.866863	-0.235273	-1.063981
N	-2.666351	-0.786107	-0.611728
C	-1.903556	2.649427	-0.240887
C	-2.425620	-2.206170	-0.556109
H	-4.396861	1.917335	-1.220073
H	-4.692543	-0.843095	-1.403335
C	3.691489	-0.013274	-1.938570
H	5.889041	-0.391333	-0.335120
H	6.024419	-0.727511	2.094417
H	3.983875	-0.765999	3.444437
C	1.365751	-0.487480	2.711320
H	0.558979	-0.074266	0.195860
C	1.725119	-0.724344	4.196722
C	0.619795	0.870953	2.667264
C	0.438982	-1.662534	2.307001
C	5.099047	-0.035490	-2.575714
C	2.878931	-1.141844	-2.621556
C	3.077183	1.369880	-2.268955
H	-0.434569	-1.697301	2.970887
H	0.062762	-1.599755	1.284383
H	0.975295	-2.613914	2.405086
H	0.800231	-0.745118	4.785415
H	2.234450	-1.682171	4.353206
H	2.354723	0.074489	4.605302
H	-0.254467	0.839382	3.330426
H	1.280848	1.673091	3.016534
H	0.260547	1.148587	1.674411
H	5.001534	0.117800	-3.657114
H	5.743467	0.763084	-2.189303
H	5.609299	-0.994559	-2.426182
H	2.856290	-0.981882	-3.708075
H	3.345957	-2.117252	-2.435294
H	1.852680	-1.179175	-2.254922
H	3.046048	1.516478	-3.357228
H	2.064117	1.465789	-1.876846
H	3.689224	2.172828	-1.839123
C	-2.173184	3.286932	0.983008
C	-1.655894	4.574254	1.178555

C	-0.899881	5.200243	0.187405
C	-0.650280	4.546957	-1.019546
C	-1.148916	3.259587	-1.258099
C	-2.991683	2.611272	2.058193
H	-1.847017	5.084575	2.119615
H	-0.503201	6.198165	0.356593
H	-0.058929	5.036084	-1.789731
C	-0.877920	2.553539	-2.565100
H	-1.808148	2.269394	-3.072018
H	-0.307506	3.198209	-3.240574
H	-0.304177	1.634252	-2.406336
H	-3.017400	3.223934	2.964674
H	-4.027286	2.444865	1.736267
H	-2.576507	1.631622	2.318219
C	-2.871978	-2.925092	0.566820
C	-2.647174	-4.307762	0.591841
C	-1.998651	-4.946741	-0.464984
C	-1.564619	-4.209982	-1.566988
C	-1.771321	-2.825765	-1.635367
C	-3.562894	-2.234344	1.719364
H	-2.980002	-4.882974	1.452584
H	-1.828744	-6.019873	-0.428389
H	-1.056501	-4.709739	-2.388129
C	-1.299023	-2.031052	-2.829136
H	-2.123506	-1.486119	-3.304753
H	-0.548468	-1.288503	-2.537660
H	-0.852114	-2.690857	-3.578965
H	-3.771386	-2.945003	2.525093
H	-2.943566	-1.427205	2.126193
H	-4.515426	-1.783733	1.414559

Adducts of MeMIM and different anions (type 4 structures)

MeMIM - $CH_3CH_2COO^-$

E(B3LYP/6-31+G*) = -573.232042

C	0.052712	-0.019817	-0.142050
C	-0.099066	-0.043037	1.193265
N	1.169014	-0.014881	1.810690
C	2.157054	0.042319	0.774773
N	1.428357	0.036457	-0.463965
C	1.392616	0.710782	3.050295
O	3.005622	-1.185282	0.920886
C	4.236529	-1.168913	0.374912
C	4.970729	-2.471417	0.640946
C	1.877645	0.892658	-1.559365
O	4.695500	-0.228068	-0.250835
H	2.937160	0.714148	-1.750790
H	1.308680	0.637363	-2.458889
H	1.725102	1.963394	-1.343415
H	2.347244	0.405936	3.489775
H	1.395298	1.805252	2.909270
H	0.599569	0.455717	3.759747
H	-0.687362	-0.137247	-0.921858
H	-0.992859	-0.189168	1.784470
H	2.858602	0.879081	0.863688
H	4.972072	-2.637176	1.726295
H	4.357698	-3.281337	0.223529
C	6.388716	-2.500233	0.071149
H	6.863785	-3.463550	0.288366
H	6.382296	-2.356059	-1.013949
H	7.006194	-1.706351	0.503644

MeMIM - CH_3COO^-

E(B3LYP/6-31+G*) = -533.917153

C	0.059382	-0.476071	0.203253
N	0.047659	0.085275	1.497346
C	1.407592	0.242493	1.916725
N	2.212454	-0.248949	0.833510
C	1.330343	-0.679088	-0.184340
O	1.575976	-0.594488	3.153063
C	-0.939877	1.078769	1.885725
C	3.437667	0.461570	0.474143
H	4.052747	0.600562	1.364827
H	3.994232	-0.143907	-0.248106
H	3.232566	1.444990	0.019222
H	-0.939932	1.193635	2.973907
H	-0.760281	2.063124	1.420540
H	-1.932478	0.730214	1.584786
H	1.711306	-1.185224	-1.060824
H	-0.864453	-0.777763	-0.271298
H	1.671465	1.257895	2.231731
C	2.599377	-0.299553	3.975680
O	3.410485	0.588232	3.771370
C	2.620086	-1.213949	5.179584
H	1.641173	-1.225786	5.669625
H	2.835200	-2.238910	4.856264
H	3.389568	-0.882390	5.878990

MeMIM - PhO-

E(B3LYP/6-31+G*) = -612.299802

C	0.070474	-0.035807	0.041648
N	0.001194	-0.023893	1.486541
C	1.309017	0.167309	1.981506
C	2.181981	0.157641	0.959487
N	1.486844	-0.040378	-0.252743
C	1.923608	0.619597	-1.472019
C	-1.128580	0.653339	2.101334
O	-0.656655	-1.134242	-0.568990
H	-0.452328	0.824322	-0.413162
C	-0.284864	-2.429223	-0.238823
C	0.659338	-3.103149	-1.019702
C	0.973184	-4.434586	-0.734184
C	0.347978	-5.095389	0.327680
C	-0.597747	-4.417177	1.102735
C	-0.916010	-3.085679	0.822395
H	-1.654552	-2.551545	1.411254
H	-1.092852	-4.925655	1.926587
H	0.591865	-6.131914	0.546068
H	1.705425	-4.956677	-1.345458
H	1.131416	-2.582455	-1.846453
H	-1.124937	1.740829	1.909135
H	-2.062442	0.232033	1.716997
H	-1.101341	0.491645	3.183368
H	1.499393	0.161095	3.046335
H	3.263378	0.141400	0.981205
H	1.743417	1.708942	-1.450659
H	2.995276	0.447399	-1.611859
H	1.394897	0.193085	-2.329850

MeMIM - 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

MeMIM - F-

E(B3LYP/6-31+G*) = -405.281801

C	0.135772	0.148664	0.015268
N	0.077214	0.277500	1.418972
C	1.373216	0.075663	1.921732
N	2.212875	0.295123	0.817016
C	1.432001	0.159287	-0.349949
C	-1.093155	-0.063693	2.208122
C	3.628004	-0.024972	0.877980
F	1.524102	-1.366588	2.414236
H	-0.978451	0.341079	3.218434
H	-1.975671	0.396697	1.753148
H	-1.244639	-1.148446	2.280738
H	4.050783	0.381230	1.802080
H	3.811640	-1.106945	0.854953
H	4.136672	0.447940	0.032130
H	1.884851	0.158513	-1.330108
H	-0.762265	0.136804	-0.584022
H	1.628551	0.601724	2.842907

MeMIM - CH_3O-

E(B3LYP/6-31+G*) = -420.555094

C	-0.107411	0.181232	-0.011632
C	-0.113248	0.286172	1.329091
N	1.190727	0.080411	1.828970
C	2.095320	0.055164	0.682277
N	1.200634	-0.099003	-0.462161
C	1.643875	0.819744	2.996654
O	3.100028	-0.934347	0.764152
C	2.626893	-2.279749	0.867231
C	1.664391	0.449531	-1.726823
H	2.628167	0.001877	-1.986372
H	0.947560	0.199639	-2.515332
H	1.780950	1.547731	-1.692411
H	2.604952	0.418528	3.331278
H	1.761651	1.899179	2.792353
H	0.919943	0.695509	3.808147
H	-0.943596	0.150870	-0.697685
H	-0.955271	0.362859	2.004288
H	2.688294	0.989621	0.611602
H	3.521510	-2.904286	0.921372
H	2.021726	-2.415204	1.771244
H	2.031790	-2.555345	-0.011250

MeMIM - OH-

E(B3LYP/6-31+G*) = -381.252284

C	0.000127	-0.000672	-0.001566
N	-0.016386	-0.035956	1.410994
C	1.375538	-0.055552	1.850384
N	2.100620	-0.481802	0.657293
C	1.242772	-0.262375	-0.443975
O	1.600435	-0.880232	2.969911
C	-0.913964	0.841202	2.147336
C	3.499103	-0.088201	0.576188
H	4.031318	-0.462194	1.455289
H	3.950570	-0.536180	-0.314342
H	3.624879	1.007909	0.522484
H	-0.890670	0.574390	3.207624
H	-0.641407	1.906399	2.041375
H	-1.936081	0.703565	1.781434
H	1.582739	-0.451860	-1.453314
H	-0.922337	0.075714	-0.561452
H	1.710121	0.943646	2.199098
H	1.320271	-1.777566	2.713794

2. XYZ coordinates and total energies of the optimized structures at the B3LYP/aug-cc-pVTZ level

1,3-dimethylimidazol-2-ylidene

E(B3LYP/6-31+G*) = -304.910637

C	-0.011630	-0.094119	-0.010780
N	0.073399	-0.011468	1.346831
N	1.295010	-0.011442	-0.388991
C	1.723495	-0.054616	-1.774623
C	2.157178	0.117063	0.689207
C	-1.086281	-0.054600	2.217879
C	1.379366	0.116658	1.794493
H	0.836183	-0.159024	-2.390984
H	2.246014	0.863289	-2.047130
H	2.385675	-0.903726	-1.948889
H	-1.965987	-0.158883	1.590689
H	-1.026865	-0.903774	2.899942
H	-1.166347	0.863261	2.801794
H	3.224712	0.196088	0.585902
H	1.642485	0.195324	2.834264

1,3-dimethylimidazolium cation (MeMIM)

E(B3LYP/6-31+G*) = -305.339146

C	0.013974	-0.000109	0.013424
N	-0.014967	-0.000031	1.391894
C	1.240971	-0.000283	1.839045
N	2.071546	-0.000455	0.796067
C	1.319214	-0.000376	-0.359170
C	-1.224370	0.000294	2.223376
C	3.537484	-0.000667	0.863870
H	3.843039	-0.001011	1.905563
H	3.922240	-0.890851	0.372603
H	3.922495	0.889687	0.373106
H	-0.934029	-0.000007	3.269403
H	-1.810011	0.890840	2.009520
H	-1.810684	-0.889732	2.009205
H	1.768531	-0.000509	-1.335448
H	-0.883216	0.000033	-0.578181
H	1.535840	-0.000308	2.873294

Anions:

$(CF_3SO_2)_2N^-$

E(B3LYP/aug-cc-pVTZ) = -1827.779890

C	0.220304	-0.143864	0.155387
F	0.302497	0.556141	1.292423
S	1.745080	0.082536	-0.933629
O	1.834066	1.522637	-1.125728
N	2.799745	-0.496775	0.129683
O	1.486937	-0.749828	-2.100571
F	-0.855161	0.294168	-0.522532
F	0.014698	-1.429598	0.465393
S	4.280791	-0.957587	-0.228937
C	4.131745	-2.829950	-0.465506
F	5.353326	-3.353984	-0.674969
F	3.616245	-3.415898	0.625978
F	3.362861	-3.144670	-1.510761
O	4.800949	-0.479949	-1.501654
O	5.110841	-0.858693	0.960260

$CF_3SO_3^-$

E(B3LYP/aug-cc-pVTZ) = -961.823367

S	0.000000	0.000000	-0.168012
C	0.000000	0.000000	1.724006
F	1.252478	0.000000	2.227711
F	-0.626239	1.084678	2.227711
F	-0.626239	-1.084678	2.227711
O	-1.433025	0.000000	-0.483043
O	0.716512	1.241036	-0.483043
O	0.716513	-1.241036	-0.483043

Cl_3CCOO^-

E(B3LYP/aug-cc-pVTZ) = -1607.522261

C	-0.027522	-0.013685	-0.196944
C	0.004177	-0.040339	1.450834
Cl	1.681136	-0.009907	2.131153
Cl	-0.862520	1.448273	2.047681
Cl	-0.836133	-1.484080	2.148690
O	-1.041751	-0.537544	-0.658290
O	0.947613	0.559340	-0.683123

Cl_2CHCOO^-

E(B3LYP/aug-cc-pVTZ) = -1147.898605

C	-0.041737	-0.025663	-0.155986
C	-0.032149	0.013956	1.425610
H	0.964783	0.172754	1.810685
Cl	-1.034575	1.384287	2.091076
Cl	-0.593399	-1.557131	2.161984
O	-1.132977	-0.202324	-0.707182
O	1.111854	0.136194	-0.606521

Cl^-

E(B3LYP/aug-cc-pVTZ) = -460.310514

$ClCH_2COO^-$

E(B3LYP/aug-cc-pVTZ) = -688.265749

C	0.013560	-0.004836	-0.141269
C	-0.115508	-0.006262	1.414335
H	0.714048	-0.553722	1.850126
Cl	-0.115417	1.630787	2.276769
H	-1.049870	-0.476403	1.703749
O	-0.004232	-1.192348	-0.547672
O	0.110918	1.064542	-0.756696

$CH_3CH_2COO^-$

E(B3LYP/aug-cc-pVTZ) = -267.950645

C	-0.000555	0.061628	0.042194
C	0.024092	-0.025458	1.604140
O	1.095052	-0.468395	2.084954
O	-1.012354	0.343690	2.206480
H	0.885208	0.625971	-0.264867
H	0.153130	-0.954546	-0.335592
C	-1.262395	0.668943	-0.564967
H	-1.220836	0.679881	-1.661013
H	-2.146232	0.109352	-0.256682
H	-1.406674	1.693080	-0.216980

CH_3COO^-

E(B3LYP/aug-cc-pVTZ) = -228.621934

C	-0.023163	-0.020899	-0.100828
C	-0.004291	-0.024220	1.458116
H	1.018062	0.007383	1.839140
H	-0.522788	0.871332	1.814693
H	-0.530277	-0.894356	1.855224
O	-1.018812	-0.569377	-0.632636
O	0.946270	0.552196	-0.654707

PhO-

E(B3LYP/aug-cc-pVTZ)= -307.023470

C	0.003475	0.000000	0.008882
C	0.015373	0.000000	1.392845
C	1.212436	0.000000	2.118187
C	2.409499	0.000000	1.392845
C	2.421397	0.000000	0.008882
C	1.212436	0.000000	-0.778649
O	1.212436	0.000000	-2.047240
H	3.361199	0.000000	-0.532924
H	3.355283	0.000000	1.929039
H	1.212436	0.000000	3.201016
H	-0.930411	0.000000	1.929039
H	-0.936327	0.000000	-0.532924

SH-

E(B3LYP/aug-cc-pVTZ) -398.867126

S	0.000000	0.000000	-0.199813
H	0.000000	0.000000	1.149813

CN-

E(B3LYP/aug-cc-pVTZ)= -92.895556

C	0.000000	0.000000	0.134306
N	0.000000	0.000000	1.305694

F-

E(B3LYP/aug-cc-pVTZ)= -99.8958522

CH_3O-

E(B3LYP/aug-cc-pVTZ)= -115.158389

O	0.000000	0.000000	0.015714
C	0.000000	0.000000	1.350927
H	1.025247	0.000000	1.840787
H	-0.512624	0.887890	1.840787
H	-0.512623	-0.887890	1.840787

OH-

E(B3LYP/aug-cc-pVTZ)= -75.836271

O	0.000000	0.000000	-0.007753
H	0.000000	0.000000	0.957753

Protonated anions:

$(CF_3SO_2)_2NH$

E(B3LYP/aug-cc-pVTZ)= -1828.258675

C	0.266020	-0.628863	0.104134
F	0.333232	-0.389996	1.412685
S	1.638297	0.330475	-0.780613
O	1.469786	1.704361	-0.383179
N	2.990853	-0.263447	0.051652
O	1.678312	-0.124526	-2.140856
F	-0.897214	-0.206084	-0.370027
F	0.396836	-1.930466	-0.116037
S	4.371316	-1.062628	-0.534697
H	3.188681	0.229870	0.916099
C	3.881953	-2.877920	-0.319772
F	4.942565	-3.615372	-0.619535
F	3.520786	-3.098917	0.939795
F	2.879052	-3.176301	-1.133389
O	4.544341	-0.838689	-1.940411
O	5.378343	-0.783620	0.458657

CF_3SO_3H

E(B3LYP/aug-cc-pVTZ)= -962.313044

C	0.052198	-0.019505	-0.008973
F	0.007039	0.038704	1.315276
S	1.840034	0.069336	-0.603541
O	2.450221	1.193305	0.044302
O	2.415916	-1.260023	0.100248
O	1.824176	-0.120896	-2.032606
F	-0.615160	1.004165	-0.527232
F	-0.493992	-1.163563	-0.422332
H	2.374370	-1.995025	-0.531463

Cl_3CCOOH

E(B3LYP/aug-cc-pVTZ)= -1608.043087

C	0.087267	-0.067419	-0.087260
C	0.015045	-0.021201	1.463200
Cl	1.631320	0.239592	2.140216
Cl	-1.067802	1.325619	1.944579
Cl	-0.643131	-1.582999	2.051209
O	-1.127046	-0.264063	-0.613598
O	1.097434	0.057553	-0.712302
H	-1.028227	-0.284709	-1.577102

$Cl_2CHCOOH$

E(B3LYP/aug-cc-pVTZ)= -1148.429581

C	0.058809	-0.061719	-0.069785
C	-0.028176	0.003894	1.450516
H	0.961520	0.194787	1.841091
Cl	-1.077395	1.360828	1.964340
Cl	-0.575226	-1.563723	2.120263
O	-1.120456	-0.296770	-0.654733
O	1.099130	0.087584	-0.650766
H	-0.976556	-0.322435	-1.612318

HCl

E(B3LYP/aug-cc-pVTZ)= -460.844264

H	0.000000	0.000000	-0.137742
Cl	0.000000	0.000000	1.145742

$ClCH_2COOH$

E(B3LYP/aug-cc-pVTZ)= -688.807447

C	0.080015	-0.032456	-0.067205
C	0.018643	-0.009844	1.443966
H	1.010351	0.179499	1.834895
Cl	-1.063028	1.310336	2.027662
H	-0.382281	-0.943945	1.826915
O	-1.092500	-0.402446	-0.616635
O	1.066107	0.223511	-0.705211
H	-0.983569	-0.382314	-1.579060

CH_3CH_2COOH

E(B3LYP/aug-cc-pVTZ)= -268.512752

C	-0.065401	-0.072931	0.041415
C	0.019199	0.089229	1.537339
O	0.845418	0.732496	2.132635
O	-0.983312	-0.567444	2.176307
H	0.904694	0.200671	-0.367631
H	-0.257902	-1.121793	-0.186971
C	-1.172219	0.802137	-0.565165
H	-0.878950	-0.391207	3.122967
H	-1.192554	0.680349	-1.647604
H	-2.150431	0.526580	-0.173733
H	-0.998949	1.856058	-0.347886

CH_3COOH

E(B3LYP/aug-cc-pVTZ)= -229.185824

C	0.073322	-0.024815	-0.051348
C	-0.003448	-0.006526	1.448135
H	0.982514	0.177128	1.861606
H	-0.696342	0.769223	1.773637
H	-0.389818	-0.959064	1.810391
O	-1.141089	-0.251933	-0.612546
O	1.066531	0.137229	-0.712051
H	-1.014347	-0.249856	-1.572829

PhOH

E(B3LYP/aug-cc-pVTZ)= -307.590315

C	0.013467	0.000000	-0.010162
O	-0.039546	0.000000	1.357796
H	0.852606	0.000000	1.718345
C	-1.196931	0.000000	-0.698607
C	-1.195498	0.000000	-2.086360
C	0.001502	0.000000	-2.796844
C	1.204526	0.000000	-2.101823
C	1.216296	0.000000	-0.711445
H	-2.120420	0.000000	-0.136959
H	-2.138454	0.000000	-2.616525
H	-0.004475	0.000000	-3.877626
H	2.142868	0.000000	-2.639981
H	2.156901	0.000000	-0.173143

H_2S

E(B3LYP/aug-cc-pVTZ)= -399.432264

S	-0.208384	0.000000	-0.145925
H	-0.010105	0.000000	1.184043
H	1.111328	0.000000	-0.403786

HCN

E(B3LYP/aug-cc-pVTZ)= -93.462750

C	0.000000	0.000000	0.090196
N	0.000000	0.000000	1.236214
H	0.000000	0.000000	-0.975410

HF

E(B3LYP/aug-cc-pVTZ)= -100.490070

H	0.000000	0.000000	0.041948
F	0.000000	0.000000	0.966052

CH_3OH

E(B3LYP/aug-cc-pVTZ)= -115.776759

O	0.018809	0.000000	0.013718
C	-0.018119	0.000000	1.436789
H	1.015233	0.000000	1.777273
H	-0.513788	0.890767	1.834030
H	-0.513788	-0.890767	1.834030
H	-0.881188	0.000000	-0.322506

H_2O

E(B3LYP/aug-cc-pVTZ)= -76.466197

O	-0.021085	0.000000	-0.013618
H	0.016613	0.000000	0.947537
H	0.897311	0.000000	-0.299605

Ion pairs (type 2 structures)

MeMIM – Cl^-

E(B3LYP/aug-cc-pVTZ) = -765.796591

N	-0.055877	0.000276	-1.562132
C	-0.090726	0.000037	-0.226543
N	1.167284	-0.000076	0.215715
C	2.028536	0.000082	-0.863112
C	1.261944	0.000300	-1.982139
C	1.525483	-0.000337	1.638341
C	-1.239880	0.000476	-2.416133
H	-0.971434	-0.000050	0.467860
H	3.096392	0.000028	-0.746651
H	1.536051	0.000473	-3.020783
H	0.594142	-0.000380	2.208592
H	2.107774	-0.891305	1.863992
H	2.107875	0.890488	1.864294
H	-1.245732	-0.889120	-3.042833
H	-2.119389	0.000388	-1.779242
H	-1.245671	0.890304	-3.042504
Cl	-1.994316	-0.000272	2.172045

MeMIM – $CH_3CH_2CO_2^-$

E(B3LYP/aug-cc-pVTZ) = -573.447652

C	-0.016912	-0.196115	-0.004061
C	-0.028241	-0.077073	1.347321
N	1.286066	0.084897	1.739904
C	2.077225	0.066563	0.662390
N	1.300641	-0.104043	-0.408966
C	1.787032	0.254075	3.102134
C	1.799989	-0.177823	-1.786649
O	4.787229	0.377165	1.144799
C	5.363670	0.337392	0.013327
O	4.778759	0.184066	-1.084991
C	6.890917	0.487556	-0.025890
H	2.868038	0.355419	3.050038
H	1.354491	1.148049	3.547439
H	1.527299	-0.615444	3.703022
H	2.887706	-0.066870	-1.747535
H	1.527064	-1.140517	-2.215283
H	1.352968	0.623212	-2.372730
H	-0.822380	-0.336175	-0.700932
H	-0.843263	-0.093997	2.046882
H	3.197813	0.180546	0.714214
H	7.107165	1.325254	-0.693941
C	7.575406	0.678606	1.322208
H	7.280257	-0.396362	-0.537698
H	8.656697	0.775937	1.199701
H	7.208061	1.572298	1.826739
H	7.382270	-0.165329	1.984489

MeMIM – $CH_3CO_2^-$

E(B3LYP/aug-cc-pVTZ) = -534.120279

C	-0.001412	0.095809	-0.002705
N	-0.005639	0.000917	1.375241
C	1.253638	-0.050812	1.822464
N	2.061913	0.009326	0.762256
C	1.299766	0.101058	-0.386397
C	3.526517	-0.020090	0.841736
C	-1.172595	-0.040033	2.253447
O	1.607067	-0.240882	4.542036
C	2.856379	-0.268450	4.786414
C	3.253276	-0.378560	6.257095
O	3.759011	-0.217732	3.920950
H	-0.817173	-0.115709	3.277739
H	-1.758752	0.869223	2.134180
H	-1.787683	-0.905151	2.013050
H	3.795580	-0.092486	1.899793
H	3.898676	-0.882477	0.291526
H	3.927925	0.893076	0.405956
H	1.740961	0.161418	-1.363990
H	-0.904518	0.150667	-0.581756
H	1.523910	-0.130539	2.921740
H	4.332864	-0.329365	6.377707
H	2.778420	0.420194	6.828149
H	2.884548	-1.323001	6.661062

MeMIM – PhO^-

E(B3LYP/aug-cc-pVTZ//B3LYP/6-31+G*) = -612.507484256

At the B3LYP/6-31+G* level geometry

MeMIM – SH^-

E(B3LYP/aug-cc-pVTZ) = -704.351105

C	0.100722	0.287720	-0.017419
N	0.001372	-0.101557	1.303471
C	1.224546	-0.320729	1.795269
N	2.103099	-0.063787	0.819449
C	1.422134	0.313221	-0.323463
C	-1.219477	-0.234770	2.101153
C	3.550512	-0.168560	0.978569
S	1.325975	-0.153527	4.938244
H	-0.922890	-0.232746	3.152474
H	-1.872753	0.610434	1.897210
H	-1.729585	-1.163578	1.852190
H	3.763580	-0.334756	2.031000
H	3.935010	-0.999648	0.389845
H	4.022766	0.757210	0.656809
H	1.924876	0.567207	-1.238295
H	-0.760686	0.516391	-0.617227
H	1.429603	-0.455212	2.906003
H	1.541098	1.176687	4.935859

MeMIM – CN^-

E(B3LYP/aug-cc-pVTZ) = -398.377060

C	0.081878	-0.010058	-0.045842
N	0.005115	-0.007919	1.332671
C	1.238365	0.005836	1.834020
N	2.104014	0.012185	0.819772
C	1.399905	0.002547	-0.369856
C	-1.205048	-0.019287	2.163786
C	3.556753	0.026322	0.984639
C	1.990717	-0.011049	4.991164
H	-0.884024	-0.020191	3.207044
H	-1.797588	0.867524	1.948935
H	-1.784173	-0.913568	1.943515
H	3.777545	0.026141	2.048642
H	3.988844	-0.858534	0.522099
H	3.971411	0.921366	0.525706
H	1.887190	0.005227	-1.327072
H	-0.792185	-0.020409	-0.670083
H	1.454479	0.008054	2.912990
N	0.846703	-0.014187	4.739010

Hydrogen bridged dimethylimidazol-2-ylidene – acid pairs (type 3 structures)

MeMIM - $CH_3CH_2COO^-$

E(B3LYP/aug-cc-pVTZ) = -573.447301

N	0.012186	-0.030545	0.030417
C	0.007196	0.024286	1.413115
C	1.301935	0.081908	1.799480
N	2.053304	0.060215	0.636811
C	1.270963	-0.009249	-0.470381
C	3.505578	0.105926	0.595147
C	-1.187729	-0.102574	-0.794880
O	2.217052	-0.082650	-3.083024
C	1.318255	-0.151305	-4.053443
C	1.958229	-0.185273	-5.428768
O	0.114836	-0.183814	-3.872590
H	3.816287	0.074776	-0.444377
H	3.872765	1.025017	1.051918
H	3.930609	-0.748247	1.122342
H	-0.885541	-0.134134	-1.838328
H	-1.755925	-1.000200	-0.550784
H	-1.813896	0.772588	-0.621199
H	-0.897062	0.017856	1.994367
H	1.739506	0.135152	2.779901
C	0.960190	-0.264200	-6.575560
H	2.590488	0.702099	-5.513352
H	2.647800	-1.032976	-5.443818
H	1.783391	-0.059222	-2.142730
H	1.480293	-0.285441	-7.533898
H	0.344831	-1.159861	-6.499753
H	0.286978	0.592174	-6.569986

MeMIM - CH_3COO^-

E(B3LYP/aug-cc-pVTZ) = -534.119238

C	-0.015473	-0.001040	0.039187
C	-0.038234	-0.005289	1.391316
N	1.284586	-0.002536	1.799888
C	2.139862	0.003214	0.745843
N	1.317880	0.004033	-0.331156
C	1.716329	-0.005468	3.187830
C	1.789075	0.009699	-1.711065
O	4.908643	0.010514	0.948739
C	5.599249	0.015126	-0.180980
O	5.100031	0.016681	-1.291430
C	7.091815	0.018074	0.052195
H	2.801624	-0.002280	3.205866
H	1.346515	0.879646	3.705535
H	1.351823	-0.895914	3.700129
H	2.875872	0.012478	-1.702870
H	1.428947	-0.877135	-2.232625
H	1.424385	0.898012	-2.226915
H	-0.819476	-0.001241	-0.674355
H	-0.864618	-0.009883	2.078748
H	7.617252	0.024357	-0.897872
H	7.372468	0.893188	0.638806
H	7.377025	-0.861872	0.629365
H	3.884132	0.008091	0.786504

MeMIM - PhO-

E(B3LYP/aug-cc-pVTZ) = -612.519473

C	-0.306692	-0.275937	0.174953
N	0.056277	-0.387059	1.478434
C	1.307303	0.156073	1.718854
C	1.751336	0.625498	0.531215
N	0.755394	0.351871	-0.391256
C	0.828685	0.691661	-1.803329
C	-0.774861	-1.013362	2.494004
H	-0.254473	-1.858569	2.944131
H	-1.033189	-0.296840	3.273710
H	-1.683370	-1.367012	2.017172
H	1.767689	0.162043	2.690290
H	2.671372	1.117977	0.273003
H	0.892913	1.771786	-1.935028
H	1.699074	0.223679	-2.262816
H	-0.070938	0.324292	-2.286763
O	-2.609836	-1.338213	-1.173443
C	-3.751179	-0.618889	-1.137731
C	-3.846832	0.633542	-0.518607
C	-5.055203	1.320884	-0.517343
C	-6.182722	0.783253	-1.127243
C	-6.085476	-0.461211	-1.744794
C	-4.886323	-1.158144	-1.752532
H	-4.804955	-2.125402	-2.229478
H	-6.953295	-0.894581	-2.225281
H	-7.119630	1.322743	-1.122913
H	-5.112165	2.288004	-0.033925
H	-2.973530	1.060727	-0.045399
H	-1.856488	-0.902368	-0.676871

MeMIM - SH-

E(B3LYP/aug-cc-pVTZ) = -704.350757

C	0.082078	-0.073693	-0.091372
N	0.103340	-0.011392	1.292753
C	1.367333	0.067587	1.786568
N	2.133468	0.052505	0.663812
C	1.372742	-0.033080	-0.491225
C	-1.083666	-0.025673	2.130828
C	3.584810	0.121273	0.684517
S	2.398613	0.311928	5.142163
H	-0.764621	0.039960	3.166164
H	-1.727563	0.822905	1.898556
H	-1.645833	-0.948404	1.984858
H	3.903194	0.186864	1.720059
H	4.018097	-0.770114	0.230135
H	3.934977	1.001154	0.144302
H	1.800538	-0.057055	-1.477373
H	-0.825723	-0.139697	-0.663748
H	2.493989	-1.017922	5.314789
H	1.996193	0.192354	3.829953

MeMIM - CN-

E(B3LYP/aug-cc-pVTZ) = -398.386915

C	-0.022828	0.005319	0.003381
C	-0.040119	0.006233	1.354572
N	1.284934	0.001251	1.758842
C	2.147094	-0.003149	0.706863
N	1.312133	-0.000360	-0.366848
C	1.709329	0.000594	3.148534
C	1.771908	-0.003056	-1.745239
C	5.398132	-0.032192	0.745831
N	6.546309	-0.047564	0.759202
H	2.794181	-0.004170	3.172520
H	1.344288	0.890323	3.661875
H	1.336458	-0.885000	3.663383
H	2.857017	-0.007994	-1.741528
H	1.412165	-0.889335	-2.268186
H	1.420246	0.885985	-2.269003
H	-0.830084	0.008135	-0.706710
H	-0.865280	0.010024	2.043768
H	4.303048	-0.018071	0.733019

MeMIM - F-

E(B3LYP/aug-cc-pVTZ) = -405.430381

C	0.028751	-0.000405	0.142872
N	0.162494	0.014907	1.489719
N	1.304191	-0.014094	-0.310151
C	1.654122	-0.033471	-1.722095
C	2.217646	-0.007500	0.730550
C	-0.965699	0.031592	2.408100
C	1.493224	0.012568	1.872558
H	-1.878314	0.041388	1.820443
H	-0.954102	-0.854935	3.041728
H	-0.931623	0.921060	3.036728
H	0.733470	-0.033499	-2.297157
H	2.241220	0.847310	-1.981044
H	2.228083	-0.928747	-1.959939
H	3.281440	-0.016360	0.576832
H	1.807511	0.023983	2.900400
H	-1.351505	-0.001558	-0.728638
F	-2.199338	-0.002382	-1.261418

MeMIM - CH_3O-

E(B3LYP/aug-cc-pVTZ) = -420.701655

C	0.029188	-0.122537	-0.034180
C	-0.188562	-0.219011	1.296556
N	1.387016	0.106589	-0.188547
N	1.043156	-0.045337	1.905405
C	2.038214	0.158664	1.002878
H	-0.652773	-0.195483	-0.862119
H	-1.096494	-0.391795	1.845867
C	1.258365	-0.071271	3.344442
C	2.046233	0.278881	-1.471082
H	0.667254	0.704775	3.830906
H	0.977030	-1.041767	3.753976
H	2.312646	0.108772	3.532701
H	1.924859	-0.611193	-2.089009
H	1.636325	1.138671	-2.001576
H	3.102497	0.444540	-1.284899
H	3.818465	0.518002	1.752976
O	4.611662	0.669722	2.319914
C	5.651325	-0.184593	1.894989
H	6.480737	-0.081688	2.595522
H	5.346845	-1.238451	1.882449
H	6.021534	0.074510	0.894853

MeMIM - OH-

E(B3LYP/aug-cc-pVTZ) = -381.391079

C	-0.068180	0.042628	0.024392
C	-0.153275	0.013363	1.373361
N	1.283817	0.021390	-0.278545
N	1.148781	-0.024191	1.843914
C	2.059947	-0.019987	0.836049
H	-0.838411	0.074673	-0.725015
H	-1.012098	0.014462	2.020170
C	1.511994	-0.072165	3.252090
C	1.820375	0.035422	-1.628050
H	1.148126	0.815497	3.770215
H	1.087334	-0.958287	3.724099
H	2.594927	-0.112921	3.320480
H	1.456646	-0.822181	-2.194441
H	1.535210	0.951036	-2.147064
H	2.902254	-0.015933	-1.558259
H	3.964987	-0.165071	1.343191
O	4.839565	-0.282917	1.787270
H	5.344684	0.505180	1.570845

Adducts of MeMIM and different anions (type 4 structures)

MeMIM - $CH_3CH_2COO^-$

E(B3LYP/aug-cc-pVTZ) = -573.429697

C	-0.022619	0.010437	0.057558
C	-0.010804	0.070869	1.392206
N	1.318882	0.075976	1.847976
C	2.174205	0.028425	0.706508
N	1.300440	-0.017483	-0.426408
C	1.723302	0.821806	3.022467
O	2.991135	-1.226501	0.825980
C	4.155966	-1.281609	0.161822
C	4.860950	-2.601649	0.382221
C	1.650072	0.713354	-1.636530
O	4.579557	-0.393887	-0.546414
H	2.663655	0.461804	-1.936030
H	0.967166	0.420837	-2.433131
H	1.578593	1.800362	-1.503410
H	2.696510	0.473801	3.366077
H	1.777793	1.903538	2.841580
H	1.005250	0.644374	3.821557
H	-0.855493	-0.107431	-0.613360
H	-0.830289	0.010499	2.086949
H	2.914281	0.828937	0.657607
H	4.791964	-2.868581	1.437120
C	4.248173	-3.717194	-0.475874
H	5.908602	-2.456485	0.124649
H	4.780037	-4.654164	-0.311686
H	3.199717	-3.871417	-0.224505
H	4.314651	-3.473815	-1.536479

MeMIM - CH_3COO^-

E(B3LYP/aug-cc-pVTZ) = -534.102722

C	0.063802	-0.457314	0.191387
N	0.058749	0.090584	1.485828
C	1.413672	0.246932	1.902324
N	2.207045	-0.236429	0.815137
C	1.325694	-0.654637	-0.201159
O	1.591413	-0.597451	3.136485
C	-0.943776	1.045332	1.912399
C	3.453713	0.434192	0.474697
H	4.068077	0.537618	1.364699
H	3.991239	-0.172373	-0.253004
H	3.287761	1.427942	0.039759
H	-0.947934	1.118205	2.999120
H	-0.783872	2.046542	1.490749
H	-1.925881	0.694980	1.598704
H	1.697852	-1.142841	-1.084767
H	-0.855400	-0.747246	-0.286905
H	1.678635	1.254712	2.226457
C	2.593576	-0.282020	3.969686
O	3.387295	0.612628	3.776853
C	2.609594	-1.186894	5.175542
H	1.643619	-1.160651	5.678925
H	2.780845	-2.215429	4.857054
H	3.396541	-0.875702	5.855752

MeMIM - PhO-

E(B3LYP/aug-cc-pVTZ) = -612.502772

C	-0.044612	-0.356710	-0.023440
N	-0.073979	0.042193	1.323250
C	1.281534	0.192431	1.777961
N	2.069962	-0.351140	0.706877
C	1.220420	-0.588882	-0.387237
O	1.488403	-0.544361	3.015278
C	-1.074856	0.958544	1.825821
C	3.429238	0.107617	0.528721
H	4.015669	-0.100951	1.423178
H	3.883265	-0.434511	-0.298898
H	3.488986	1.183234	0.308768
H	-1.107580	0.912061	2.913498
H	-0.885044	1.998416	1.524108
H	-2.053034	0.664406	1.448949
H	1.599901	-1.025443	-1.294372
H	-0.955403	-0.556680	-0.560142
H	1.529685	1.242400	2.007200
C	1.879863	0.109372	4.153172
C	1.306580	-0.320853	5.350942
C	1.688331	0.254213	6.554110
C	2.635072	1.274446	6.580828
C	3.206077	1.700403	5.388938
C	2.843268	1.119510	4.177161
H	0.568722	-1.110175	5.315847
H	1.239327	-0.092638	7.475400
H	2.927502	1.725521	7.518770
H	3.953395	2.482912	5.395787
H	3.326824	1.440807	3.266550

MeMIM - CN-

E(B3LYP/aug-cc-pVTZ) = -398.387291

C	0.045136	0.125763	0.074600
N	-0.029476	0.400994	1.461841
C	1.309050	0.139489	1.970193
N	2.146887	0.404962	0.810193
C	1.323319	0.128131	-0.308028
C	-1.165548	-0.052093	2.241287
C	3.526497	-0.041300	0.836659
H	1.560781	0.783256	2.814895
H	1.739797	0.072789	-1.297873
H	-0.846544	0.067779	-0.523586
H	4.047404	0.424745	1.673068
H	3.624900	-1.130214	0.926118
H	4.014855	0.280607	-0.081307
H	-1.193803	-1.141434	2.367415
H	-1.142838	0.411663	3.227440
H	-2.079482	0.267137	1.743728
C	1.461949	-1.293378	2.470537
N	1.590767	-2.358155	2.886855

MeMIM - F-

E(B3LYP/aug-cc-pVTZ) = -405.421577

C	0.019606	0.147776	0.015674
N	-0.015131	0.270114	1.415710
C	1.283131	0.063956	1.899043
N	2.101344	0.269868	0.781179
C	1.302082	0.147230	-0.368795
C	-1.176532	-0.031164	2.224853
C	3.516296	-0.031755	0.818031
H	1.555971	0.593900	2.808980
H	1.732363	0.137982	-1.353074
H	-0.881214	0.139027	-0.569549
H	3.954917	0.394875	1.719496
H	3.713415	-1.106562	0.813145
H	4.000711	0.425237	-0.043827
H	-1.343836	-1.105924	2.329796
H	-1.047132	0.396035	3.218747
H	-2.055113	0.425551	1.771203
F	1.431777	-1.367285	2.395422

MeMIM - CH_3O-

E(B3LYP/aug-cc-pVTZ) = -420.695048

C	0.018491	0.051742	0.006943
N	-0.069742	0.387468	1.371862
C	1.251653	0.277846	1.931443
N	2.089089	0.410760	0.761268
C	1.303942	0.063404	-0.356917
C	-1.216238	0.021760	2.175321
C	3.485104	0.040384	0.843723
H	1.459720	1.048271	2.683648
H	1.744766	-0.059778	-1.329713
H	-0.864670	-0.081287	-0.591477
H	3.972150	0.608508	1.637713
H	3.637217	-1.027579	1.034018
H	3.974233	0.299513	-0.094567
H	-1.262368	-1.048492	2.399094
H	-1.193398	0.569753	3.118248
H	-2.123263	0.311282	1.645466
O	1.417454	-1.002386	2.599906
C	2.062105	-0.961562	3.858965
H	1.959744	-1.950236	4.302829
H	3.128669	-0.727163	3.773785
H	1.598389	-0.228937	4.529199

MeMIM - OH-

E(B3LYP/aug-cc-pVTZ) = -381.389377

C	0.004912	-0.006103	0.002426
N	-0.010206	-0.027775	1.410202
C	1.376963	-0.050145	1.851188
N	2.098707	-0.471917	0.659383
C	1.239859	-0.266186	-0.437242
O	1.601034	-0.874642	2.968289
C	-0.913361	0.838268	2.143386
C	3.495219	-0.090191	0.573835
H	4.030533	-0.474668	1.440245
H	3.936987	-0.528362	-0.319888
H	3.630189	1.000042	0.531850
H	-0.903748	0.564504	3.196957
H	-0.642301	1.899839	2.052950
H	-1.927028	0.706615	1.767830
H	1.575030	-0.450749	-1.443245
H	-0.910359	0.072680	-0.558392
H	1.710805	0.945238	2.200076
H	1.324411	-1.766214	2.718709

3. XYZ coordinates and total energies of the optimized structures at the MP2/6-311+G** level

1,3-dimethylimidazol-2-ylidene

E(MP2/6-311+G**)= -303.9747495

C	-0.019890	-0.095017	-0.016593
N	0.075279	-0.011130	1.349869
N	1.298495	-0.011081	-0.388249
C	1.725719	-0.054614	-1.778439
C	2.163476	0.116974	0.681704
C	-1.089114	-0.054706	2.221268
C	1.374401	0.116949	1.802932
H	0.829043	-0.159270	-2.387784
H	2.246336	0.869022	-2.044975
H	2.386698	-0.909111	-1.946146
H	-1.965358	-0.159411	1.582898
H	-1.023830	-0.909191	2.900073
H	-1.164321	0.868934	2.801285
H	3.235504	0.195873	0.573038
H	1.633969	0.195808	2.848725

1,3-dimethylimidazolium cation

E(MP2/6-311+G**)= -304.4033914

C	0.004454	-0.000121	0.013500
N	-0.020682	-0.000037	1.388584
C	1.242694	-0.000270	1.845158
N	2.074610	-0.000464	0.790267
C	1.327289	-0.000391	-0.364153
C	-1.230562	0.000302	2.225319
C	3.543747	-0.000661	0.862256
H	3.838115	-0.001046	1.911237
H	3.923349	-0.897051	0.371817
H	3.923588	0.895944	0.372394
H	-0.926845	-0.000035	3.271621
H	-1.811355	0.897095	2.009522
H	-1.812077	-0.895935	2.009166
H	1.781026	-0.000535	-1.344020
H	-0.898417	0.000012	-0.578780
H	1.539122	-0.000290	2.883685

Anions

Cl-
E(MP2/6-311+G**)= -459.7035702

CH_3COO-
E(MP2/6-311+G**)= -228.0020101

C	-0.021727	-0.023358	-0.100405
C	-0.003991	-0.024703	1.458162
H	1.021456	0.006640	1.838959
H	-0.524515	0.874649	1.809468
H	-0.531734	-0.897433	1.854957
O	-1.025609	-0.571345	-0.629894
O	0.951120	0.557609	-0.652245

CN-
E(MP2/6-311+G**)= -92.3316498

C	0.000000	0.000000	0.122488
N	0.000000	0.000000	1.317512

F-
E(MP2/6-311+G**)= -99.6786867

OH-
E(MP2/6-311+G**)= -75.640014

O	0.000000	0.000000	-0.007545
H	0.000000	0.000000	0.957545

Protonated anions

HCl
E(MP2/6-311+G**)= -460.2447031
H 0.000000 0.000000 -0.132529
Cl 0.000000 0.000000 1.140529

CH_3COOH
E(MP2/6-311+G**)= -228.567971
C 0.074032 -0.024717 -0.053059
C -0.005383 -0.006864 1.448343
H 0.983862 0.177390 1.862757
H -0.699776 0.773099 1.768369
H -0.391675 -0.964099 1.805305
O -1.146809 -0.252785 -0.604996
O 1.071512 0.137968 -0.718789
H -1.008441 -0.248606 -1.562934

HCN
E(MP2/6-311+G**)= -92.8964497
C 0.000000 0.000000 0.082572
N 0.000000 0.000000 1.253915
H 0.000000 0.000000 -0.985487

HF
E(MP2/6-311+G**)= -100.2787946
H 0.000000 0.000000 0.045691
F 0.000000 0.000000 0.962309

H_2O
E(MP2/6-311+G**)= -76.2747201
O -0.026016 0.000000 -0.017100
H 0.024860 0.000000 0.941090
H 0.893994 0.000000 -0.289676

Ion pairs (type 2 structures)

Cl-

E(MP2/6-311+G**)= -764.2571897

N	-0.052516	0.000290	-1.565725
C	-0.093391	0.000134	-0.222245
N	1.175498	-0.000073	0.216364
C	2.037769	0.000124	-0.856868
C	1.258686	0.000375	-1.990769
C	1.528430	-0.000404	1.643669
C	-1.245556	0.000413	-2.413245
H	-0.978489	0.000063	0.475501
H	3.110492	0.000057	-0.738271
H	1.530010	0.000561	-3.035395
H	0.588809	-0.000461	2.203594
H	2.108269	-0.897413	1.865286
H	2.108382	0.896440	1.865654
H	-1.249789	-0.895109	-3.036228
H	-2.117597	0.000320	-1.759133
H	-1.249775	0.896128	-3.035951
Cl	-1.996776	-0.000134	2.132528

CH_3COO-

E(MP2/6-311+G**)= -532.5682926

C	0.017003	-0.214043	0.075592
N	0.049463	0.020179	1.431806
C	1.320997	0.187088	1.837081
N	2.104382	0.060195	0.754196
C	1.324433	-0.187500	-0.353759
C	3.568705	0.180061	0.792279
C	-1.084508	0.071069	2.358657
O	1.623177	0.370624	4.560584
C	2.775913	-0.148798	4.743555
C	3.100786	-0.601271	6.166074
O	3.633734	-0.343332	3.842986
H	-0.675014	0.180323	3.364934
H	-1.719973	0.923546	2.113575
H	-1.652005	-0.857676	2.283802
H	3.864412	0.100887	1.843918
H	3.996257	-0.637827	0.210798
H	3.861523	1.141122	0.365862
H	1.746845	-0.326891	-1.337076
H	-0.901621	-0.384533	-0.464576
H	1.602065	0.354011	2.916149
H	4.178907	-0.697173	6.304902
H	2.678887	0.096190	6.892956
H	2.638310	-1.579848	6.333400

CN-

E(MP2/6-311+G**)= -397.1819281

C	0.071100	-0.011204	-0.047821
N	-0.004630	-0.007632	1.327139
C	1.233492	0.007062	1.839021
N	2.103027	0.012583	0.818051
C	1.409259	0.001550	-0.372047
C	-1.214737	-0.018705	2.163844
C	3.557761	0.026750	1.004329
C	2.041721	-0.010698	4.852710
H	-0.886062	-0.021057	3.207965
H	-1.802083	0.874619	1.947803
H	-1.790182	-0.917873	1.940242
H	3.752339	0.024252	2.078203
H	3.988955	-0.863178	0.544187
H	3.971192	0.928663	0.551231
H	1.903391	0.003270	-1.331485
H	-0.806360	-0.022515	-0.676022
H	1.464107	0.009859	2.915702
N	0.847613	-0.015745	4.798089

Hydrogen bridged dimethylimidazol-2-ylidene – acid pairs (type 3 structures)

CH_3COO^-

E(MP2/6-311+G**)= -532.5688809

C	-0.020448	-0.001179	0.028865
C	-0.028911	-0.005362	1.401326
N	1.295228	-0.002406	1.787742
C	2.152665	0.003302	0.723373
N	1.306579	0.003957	-0.347055
C	1.751209	-0.005036	3.172102
C	1.772667	0.009516	-1.732234
O	4.900521	0.011229	0.981198
C	5.585226	0.015614	-0.157117
O	5.080367	0.017302	-1.271294
C	7.078419	0.017582	0.079181
H	2.840818	-0.001673	3.161477
H	1.386955	0.885879	3.689211
H	1.392419	-0.901161	3.684001
H	2.862785	0.012721	-1.715638
H	1.408566	-0.883376	-2.245964
H	1.403242	0.903294	-2.240597
H	-0.833281	-0.001499	-0.682407
H	-0.849427	-0.009973	2.103717
H	7.605148	0.025884	-0.874192
H	7.354016	0.895677	0.668460
H	7.357942	-0.868428	0.654691
H	3.887006	0.008593	0.791837

CN^-

E(MP2/6-311+G**)= -397.192754

C	-0.031969	0.004772	-0.006762
C	-0.049625	0.005790	1.364490
N	1.272589	0.001438	1.760389
C	2.149143	-0.002805	0.707075
N	1.300000	-0.000183	-0.368476
C	1.704779	0.001172	3.151594
C	1.767853	-0.002471	-1.748098
C	5.418602	-0.033158	0.745569
N	6.591686	-0.049272	0.758885
H	2.793881	-0.002963	3.159053
H	1.339330	0.896502	3.660480
H	1.332537	-0.890373	3.662188
H	2.856786	-0.006869	-1.727555
H	1.408636	-0.894639	-2.266868
H	1.415862	0.892235	-2.267458
H	-0.840472	0.007210	-0.723166
H	-0.876304	0.009269	2.059837
H	4.325617	-0.018683	0.733097

F-

E(MP2/6-311+G**)= -404.2821015

C	0.022338	-0.000590	0.140941
N	0.171124	0.014341	1.497022
N	1.310899	-0.013885	-0.306994
C	1.656298	-0.032336	-1.723719
C	2.228569	-0.007455	0.723350
C	-0.960013	0.032496	2.417292
C	1.495707	0.010765	1.883282
H	-1.870734	0.030891	1.819477
H	-0.937413	-0.853822	3.055468
H	-0.926275	0.933614	3.033867
H	0.725230	-0.035643	-2.289327
H	2.238401	0.856223	-1.978564
H	2.231578	-0.931252	-1.956787
H	3.296458	-0.016011	0.562470
H	1.809036	0.020814	2.916761
H	-1.396980	-0.003291	-0.756468
F	-2.222649	-0.004861	-1.278583

OH-

E(MP2/6-311+G**)= -380.265942

C	-0.074809	0.021125	0.009542
C	-0.140881	-0.005038	1.379367
N	1.269593	0.025142	-0.304381
N	1.165747	-0.014552	1.823381
C	2.076414	0.003847	0.801300
H	-0.856767	0.035240	-0.735549
H	-0.991664	-0.019796	2.044832
C	1.551325	-0.054454	3.230888
C	1.789682	0.051850	-1.663877
H	1.170575	0.830829	3.746263
H	1.147883	-0.954894	3.700342
H	2.639710	-0.071136	3.278327
H	1.412834	-0.805155	-2.227547
H	1.497411	0.978486	-2.164446
H	2.875490	-0.002943	-1.599052
H	3.958266	-0.150752	1.422493
O	4.758963	-0.250059	1.982572
H	5.376909	0.382259	1.610245

Adducts of MeMIM and different anions (type 4 structures)

CH_3COO^-

E(MP2/6-311+G**)= -532.5599818

C	0.101391	-0.276009	0.073490
N	-0.082430	0.356612	1.322769
C	1.206286	0.456526	1.909264
N	2.081152	0.492638	0.789099
C	1.412365	-0.194579	-0.249436
C	-1.207742	0.009028	2.175490
C	3.504479	0.284507	1.009467
H	1.335801	1.269683	2.622006
H	1.919731	-0.453406	-1.167482
H	-0.739834	-0.616821	-0.512504
H	3.855747	0.984502	1.769268
H	3.727122	-0.739608	1.338961
H	4.031970	0.480908	0.073225
H	-1.155122	-1.025499	2.535669
H	-1.223205	0.685167	3.034584
H	-2.131349	0.152369	1.609515
O	1.432981	-0.821163	2.726003
C	2.221742	-0.707820	3.810415
O	2.791264	0.315373	4.144102
C	2.311486	-2.024043	4.545438
H	1.309388	-2.368230	4.811806
H	2.758478	-2.775975	3.889841
H	2.919583	-1.901495	5.441315

CN^-

E(MP2/6-311+G**)= -397.2026728

C	0.038546	0.083571	0.091748
N	-0.032476	0.467983	1.456954
C	1.307019	0.192163	1.958215
N	2.144342	0.473370	0.800056
C	1.331679	0.086727	-0.298476
C	-1.137903	-0.041958	2.258344
C	3.510895	-0.030316	0.855390
H	1.563915	0.822577	2.814745
H	1.749675	-0.014390	-1.290390
H	-0.857966	-0.020858	-0.503417
H	4.023516	0.418114	1.710846
H	3.554562	-1.125944	0.944622
H	4.029511	0.278047	-0.054951
H	-1.119817	-1.137640	2.355363
H	-1.093775	0.405345	3.255169
H	-2.074970	0.262674	1.787305
C	1.442223	-1.257209	2.394107
N	1.554676	-2.371518	2.758406

F-

E(MP2/6-311+G**)= -404.2692481

C	0.015297	0.153736	0.025179
N	-0.023293	0.381294	1.417571
C	1.283722	0.150380	1.901007
N	2.109234	0.380943	0.778211
C	1.310884	0.153481	-0.363250
C	-1.150102	-0.068384	2.221246
C	3.492194	-0.069187	0.829442
H	1.554716	0.699899	2.804589
H	1.742293	0.120383	-1.352810
H	-0.889393	0.120897	-0.563802
H	3.957190	0.316788	1.740029
H	3.572381	-1.161860	0.825695
H	4.024424	0.341418	-0.031589
H	-1.219324	-1.161032	2.262590
H	-1.037480	0.317918	3.237348
H	-2.068136	0.342236	1.794814
F	1.418045	-1.250047	2.349769

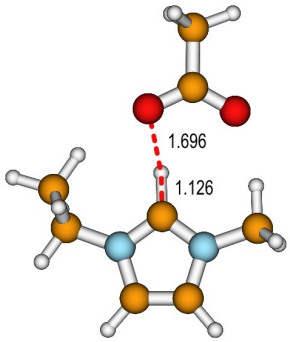
OH-

E(MP2/6-311+G**)= -380.2674792

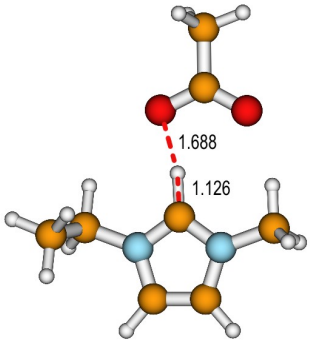
C	0.001900	0.027103	-0.001998
N	-0.026496	-0.093162	1.404980
C	1.366754	-0.057115	1.826637
N	2.083544	-0.537542	0.653759
C	1.251245	-0.236012	-0.446792
O	1.619579	-0.804775	2.979048
C	-0.900394	0.801776	2.151973
C	3.478137	-0.120354	0.593120
H	3.993449	-0.479964	1.486304
H	3.948893	-0.565170	-0.286659
H	3.574569	0.976101	0.538654
H	-0.851400	0.540374	3.211177
H	-0.607408	1.856836	2.027529
H	-1.928490	0.672622	1.805817
H	1.596306	-0.380306	-1.461885
H	-0.911415	0.147825	-0.569081
H	1.679193	0.976795	2.092618
H	1.349681	-1.704794	2.753355

4. XYZ coordinates and total energies of the EMIM-acetate H-shift isomers at different levels

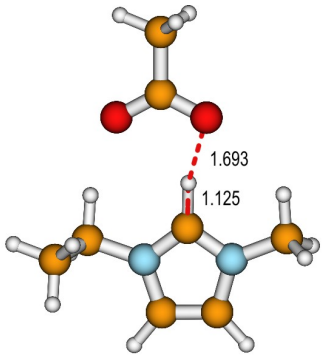
Investigated conformations of EMIM-acetate isomers at the B3LYP/6-31+G* level



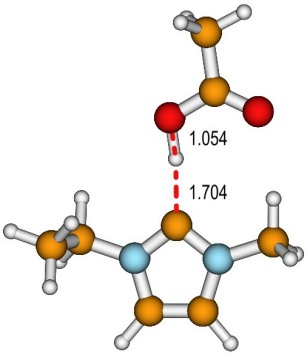
6a-1
0.0



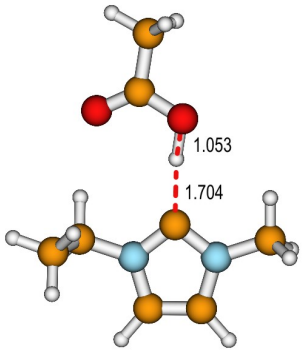
6a-2
0.0



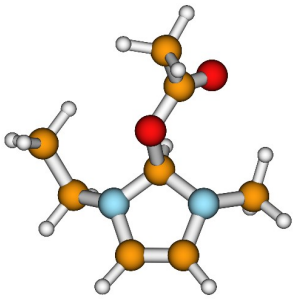
6a-3
0.1



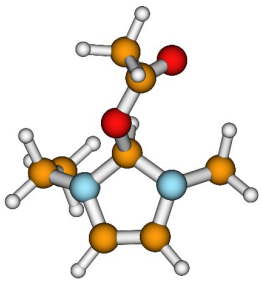
7a-1
3.0



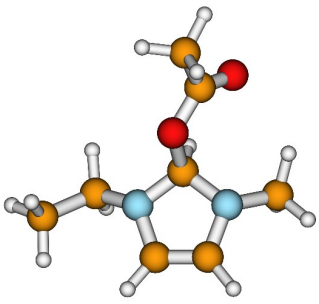
7a-2
3.1



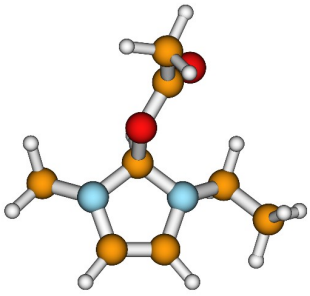
8a-1
11.4



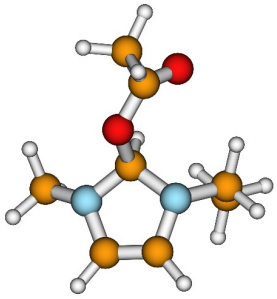
8a-2
11.4



8a-3
11.6



8a-4
11.6



8a-5
11.5

6a-1

E(B3LYP/6-31+G*) = -573.251920

E(MP2/6-311+G**//B3LYP/6-31+G*) = -571.7683114

C	1.312002	-0.010953	-0.342591
C	0.019169	0.131209	0.069309
N	0.040594	0.168507	1.453297
C	1.310838	0.054906	1.878753
N	2.096096	-0.055819	0.797827
C	-1.126252	0.333793	2.347397
C	3.559277	-0.203779	0.847382
O	1.793799	0.000739	4.647607
C	3.058069	-0.051525	4.831539
O	3.919752	-0.089588	3.913585
C	3.532589	-0.069321	6.287754
C	-1.232481	-0.783185	3.383913
H	-1.033349	1.308230	2.836817
H	-2.004324	0.364973	1.695906
H	3.858501	-0.182612	1.904244
H	3.838365	-1.155420	0.386509
H	4.019945	0.622822	0.299492
H	1.735261	-0.085199	-1.332641
H	-0.898327	0.208113	-0.493847
H	1.623692	0.044561	2.960409
H	4.623931	-0.091851	6.347743
H	3.152318	0.815397	6.812447
H	3.119495	-0.947243	6.799469
H	-2.129282	-0.617526	3.991562
H	-1.322343	-1.761949	2.898970
H	-0.362321	-0.783898	4.048744

6a-2

E(B3LYP/6-31+G*) = -573.251885

C	1.328447	0.174173	-0.432399
C	0.017621	0.196135	-0.054680
N	-0.000502	0.074063	1.325659
C	1.259452	-0.022785	1.778358
N	2.082213	0.036466	0.722495
C	-1.183589	0.024928	2.205416
C	3.548931	-0.030819	0.815167
O	1.541317	-0.252034	4.551903
C	2.795839	-0.307131	4.790906
O	3.699278	-0.273317	3.912246
C	3.204512	-0.425469	6.262291
H	-0.809209	0.171031	3.221780
H	-1.822201	0.875660	1.945549
C	-1.940739	-1.297203	2.087958
H	3.805272	-0.126286	1.878497
H	3.904774	-0.898467	0.252716
H	3.977218	0.884061	0.396478
H	1.783652	0.248243	-1.408353
H	-0.884165	0.292265	-0.639827
H	1.520430	-0.126174	2.868684
H	4.292268	-0.443121	6.370420
H	2.790704	0.416077	6.830814
H	2.778912	-1.341314	6.690416
H	-2.801953	-1.281687	2.764672
H	-2.312271	-1.467217	1.070822
H	-1.299300	-2.137194	2.373019

6a-3

E(B3LYP/6-31+G*) = -573.251732

N	-0.002560	-0.041527	0.039377
C	0.017469	-0.154438	1.420782
C	1.326181	-0.137644	1.806504
N	2.078346	-0.011908	0.649522
C	1.256294	0.044851	-0.410113
C	3.538655	0.046552	0.539666
C	-1.197710	-0.006108	-0.834411
O	2.536783	0.213475	-2.893075
C	1.618215	0.128287	-3.777833
C	2.073863	0.171112	-5.239624
O	0.387202	0.015391	-3.529760
H	3.791477	0.121404	-0.520036
H	3.915750	0.922742	1.074073
H	-0.816725	-0.118629	-1.857189
H	-1.811266	-0.875134	-0.573841
C	-1.978516	1.297342	-0.680247
H	-0.886620	-0.241620	2.003673
H	1.777345	-0.207437	2.784631
H	1.622715	0.129489	-1.469924
H	1.224249	0.079633	-5.921568
H	2.601175	1.112958	-5.434297
H	2.787151	-0.640149	-5.428978
H	3.977557	-0.861657	0.961363
H	-2.845111	1.273049	-1.349600
H	-2.343947	1.450651	0.342696
H	-1.359011	2.154123	-0.965061

7a-1

E(B3LYP/6-31+G*) = -573.247165

E(MP2/6-311+G**//B3LYP/6-31+G*) = -571.7678881

N	1.450679	-0.291291	-0.458742
C	0.167291	0.009970	-0.019884
C	0.294470	0.429601	1.267542
N	1.649317	0.373960	1.567118
C	2.383114	-0.069622	0.510917
C	2.223435	0.736188	2.862475
C	1.784493	-0.743534	-1.811961
O	5.082951	-0.495238	0.189368
C	5.864481	-0.238126	1.230932
C	7.327740	-0.509450	0.944569
O	5.460296	0.174842	2.313205
H	3.304901	0.595114	2.810757
H	1.997910	1.783193	3.091079
H	1.805398	0.098199	3.648381
C	1.807320	0.398368	-2.830018
H	2.764930	-1.221066	-1.747185
H	1.056667	-1.510201	-2.102520
H	-0.708281	-0.103567	-0.642246
H	-0.448778	0.748782	1.983492
H	7.930289	-0.284105	1.826327
H	7.464072	-1.558667	0.659174
H	7.662451	0.102338	0.099235
H	4.066556	-0.306984	0.392387
H	2.064167	0.008593	-3.821913
H	0.831715	0.893072	-2.901389
H	2.554742	1.148100	-2.550155

7a-2

E(B3LYP/6-31+G*) = -573.246991

N	1.279099	-0.060897	-0.329044
C	-0.048597	-0.160324	0.065880
C	-0.050376	-0.133996	1.425682
N	1.278907	-0.015605	1.811990
C	2.117768	0.030920	0.738477
C	1.733795	0.044054	3.195581
C	1.732893	-0.021834	-1.726685
O	4.860279	0.152018	0.926827
C	5.551793	-0.018339	-0.193481
C	7.049742	0.031229	0.031374
O	5.046588	-0.196749	-1.297036
H	2.821108	0.129602	3.192838
H	1.304185	0.914795	3.702117
H	1.444637	-0.865145	3.733246
H	2.806653	-0.221812	-1.711738
H	1.234528	-0.838284	-2.262826
C	1.445650	1.323029	-2.396365
H	-0.863560	-0.245795	-0.637876
H	-0.863867	-0.194745	2.133837
H	7.575516	-0.108386	-0.914898
H	7.329614	0.993819	0.474050
H	7.346758	-0.749919	0.740261
H	3.819926	0.107346	0.768070
H	1.809294	1.303606	-3.430063
H	0.373052	1.551363	-2.416939
H	1.961631	2.132657	-1.869221

8a-1

E(B3LYP/6-31+G*) = -573.233819

C	0.029771	-0.071241	0.004094
C	0.047607	-0.068771	1.347632
N	1.383097	-0.015063	1.807295
C	2.229706	-0.005699	0.648099
N	1.352055	-0.011649	-0.491513
C	1.733127	0.813361	2.962863
O	3.049244	-1.259442	0.698999
C	4.179185	-1.294694	-0.030435
C	4.891129	-2.619837	0.119741
C	1.653797	0.851800	-1.631837
O	4.576289	-0.374214	-0.725367
H	2.682220	0.681677	-1.955102
H	0.978913	0.593145	-2.453905
H	1.519584	1.920708	-1.395744
C	2.987313	0.328945	3.690212
H	1.853858	1.869052	2.660027
H	0.874425	0.776892	3.642019
H	-0.802969	-0.202513	-0.673561
H	-0.765725	-0.203739	2.047714
H	2.958269	0.811053	0.630987
H	5.037309	-2.858513	1.178201
H	4.275444	-3.417054	-0.312258
H	5.852587	-2.580264	-0.395233
H	3.177950	0.960261	4.566331
H	2.866775	-0.708009	4.021281
H	3.872418	0.377207	3.046338

8a-2

E(B3LYP/6-31+G*) = -573.233752

C	-0.001974	-0.024895	-0.058472
C	0.004428	0.021626	1.285997
N	1.335661	0.089375	1.738188
C	2.194910	0.053607	0.605194
N	1.329768	0.014911	-0.531642
C	1.730531	0.731491	2.985656
O	3.017146	-1.228651	0.725530
C	4.165588	-1.297582	0.034634
C	4.887304	-2.604355	0.282142
C	1.667751	0.772378	-1.732497
O	4.578296	-0.417322	-0.704806
H	2.700670	0.562047	-2.015640
H	1.007907	0.454073	-2.545838
H	1.544774	1.858823	-1.590463
C	1.687158	2.266056	2.961140
H	2.737504	0.379283	3.236976
H	1.065218	0.351265	3.770224
H	-0.824614	-0.181753	-0.742120
H	-0.811107	-0.091834	1.987191
H	2.952880	0.840428	0.561950
H	5.053589	-2.750260	1.354751
H	4.269639	-3.439144	-0.067709
H	5.840933	-2.604005	-0.248883
H	1.970368	2.670772	3.940738
H	2.381019	2.675385	2.217173
H	0.680287	2.625050	2.719236

8a-3

E(B3LYP/6-31+G*) = -573.233501

C	-0.015216	0.050478	-0.102225
C	-0.058042	0.076727	1.241280
N	1.258091	0.073616	1.752661
C	2.155142	0.049072	0.637164
N	1.328560	0.037302	-0.536257
C	1.626044	0.825668	2.952403
O	2.956950	-1.220123	0.756320
C	4.137266	-1.277851	0.113574
C	4.831699	-2.599879	0.351322
C	1.722752	0.826715	-1.700703
O	4.588375	-0.378886	-0.576970
H	2.759188	0.602590	-1.958877
H	1.081769	0.551177	-2.544127
H	1.620454	1.910586	-1.525332
C	0.924852	0.305132	4.207257
H	2.708838	0.718107	3.076153
H	1.414369	1.901815	2.820988
H	-0.822040	-0.056819	-0.814508
H	-0.910676	-0.015965	1.898401
H	2.904644	0.846975	0.635682
H	4.907714	-2.805013	1.424134
H	4.241908	-3.409078	-0.094205
H	5.824978	-2.579033	-0.100587
H	1.268334	0.863744	5.085682
H	-0.162578	0.426401	4.145854
H	1.144077	-0.757272	4.358825

8a-4

E(B3LYP/6-31+G*) = -573.233498

C	-0.051716	0.053988	0.096365
C	-0.007009	0.035392	1.439931
N	1.336399	0.019876	1.864364
C	2.162600	0.040541	0.697246
N	1.265225	0.069453	-0.421645
C	1.769617	0.710255	3.067319
O	2.972862	-1.231478	0.723738
C	4.120023	-1.260471	0.022882
C	4.827267	-2.588451	0.175772
C	1.595644	0.900634	-1.588412
O	4.537617	-0.333683	-0.652271
H	2.682174	0.875687	-1.698988
C	0.938258	0.385461	-2.868838
H	1.297919	1.948075	-1.407731
H	2.762269	0.354951	3.360277
H	1.803309	1.805964	2.942056
H	1.075926	0.476683	3.880626
H	-0.905653	-0.042220	-0.558397
H	-0.809901	-0.077546	2.155750
H	2.911064	0.839332	0.683150
H	4.996721	-2.809356	1.234929
H	4.198535	-3.390328	-0.227162
H	5.778293	-2.561397	-0.359019
H	1.237757	1.011289	-3.717647
H	1.245091	-0.646371	-3.072195
H	-0.156125	0.412555	-2.809960

8a-5

E(B3LYP/6-31+G*) = -573.233654

C	-0.025724	0.031390	0.043519
C	-0.019709	-0.016476	1.387867
N	1.316138	-0.011087	1.841177
C	2.172099	0.032945	0.702517
N	1.302942	0.079194	-0.428028
C	1.713664	0.635131	3.079272
O	2.993426	-1.253986	0.721882
C	4.173855	-1.249519	0.082920
C	4.900066	-2.566882	0.246194
C	1.663500	0.816731	-1.641830
O	4.609496	-0.301669	-0.552598
H	2.675711	0.516615	-1.924549
H	0.987761	0.470510	-2.433400
C	1.577401	2.342981	-1.509880
H	2.702483	0.277623	3.382429
H	1.739300	1.734999	2.997789
H	1.003122	0.364174	3.865997
H	-0.851926	-0.065705	-0.647491
H	-0.836070	-0.168193	2.080283
H	2.931379	0.819950	0.724137
H	5.047232	-2.788623	1.308702
H	4.295907	-3.378367	-0.174397
H	5.864277	-2.520892	-0.263237
H	1.822139	2.818972	-2.467438
H	0.569784	2.659446	-1.215936
H	2.286019	2.719426	-0.762489

XYZ coordinates and total energy of 6a-1 at different levels of theory

E(B971/6-31+G*) = -573.075904

C	1.312142	-0.014941	-0.343276
C	0.017007	0.130489	0.070684
N	0.041658	0.172332	1.454866
C	1.313342	0.058344	1.881074
N	2.096962	-0.056849	0.797410
C	-1.122776	0.338062	2.351005
C	3.559583	-0.205500	0.844580
O	1.791635	0.013654	4.639522
C	3.055276	-0.048234	4.825181
O	3.919928	-0.094580	3.911694
C	3.525133	-0.069352	6.287362
C	-1.226717	-0.785479	3.385483
H	-1.025929	1.311898	2.844782
H	-2.003963	0.372153	1.700769
H	3.860792	-0.186781	1.903122
H	3.836944	-1.157743	0.380242
H	4.019765	0.623613	0.296907
H	1.735504	-0.093106	-1.334666
H	-0.902975	0.206390	-0.491593
H	1.626451	0.050909	2.968636
H	4.617967	-0.082759	6.350943
H	3.132884	0.809427	6.816004
H	3.117656	-0.956387	6.791063
H	-2.124930	-0.623429	3.994656
H	-1.314208	-1.763219	2.894762
H	-0.354117	-0.785530	4.050389

E(MPW1K/6-31+G*) = -573.069912

C	1.314731	-0.000351	-0.310821
C	0.035446	0.146700	0.102254
N	0.062082	0.170977	1.472261
C	1.318691	0.044827	1.887766
N	2.092432	-0.060597	0.816336
C	-1.086190	0.330426	2.361499
C	3.537013	-0.217607	0.859204
O	1.755436	0.003392	4.646157
C	3.005836	-0.049217	4.810056
O	3.843507	-0.094412	3.889939
C	3.497896	-0.055961	6.243855
C	-1.186087	-0.790026	3.373164
H	-0.989957	1.291907	2.860427
H	-1.963255	0.371861	1.720413
H	3.839008	-0.200067	1.908263
H	3.807780	-1.164387	0.400177
H	4.000647	0.601063	0.316104
H	1.732431	-0.068375	-1.297163
H	-0.877801	0.234672	-0.454795
H	1.628338	0.030222	2.961361
H	4.582328	-0.096009	6.287062
H	3.142273	0.837145	6.755905
H	3.078086	-0.912822	6.769302
H	-2.074279	-0.638570	3.984216
H	-1.273279	-1.755891	2.877922
H	-0.318099	-0.795516	4.030731

E(B3LYP/6-311+G**) = -573.451464

C	1.311757	-0.015668	-0.326851
C	0.025240	0.124240	0.080279
N	0.044815	0.167216	1.459348
C	1.309409	0.059315	1.887207
N	2.091712	-0.053621	0.811304
C	-1.122329	0.330718	2.346247
C	3.551202	-0.196795	0.859218
O	1.813406	0.010510	4.616084
C	3.069724	-0.053118	4.811925
O	3.936560	-0.099885	3.910916
C	3.523968	-0.073486	6.269703
C	-1.228985	-0.778626	3.382721
H	-1.036231	1.301838	2.832433
H	-1.995607	0.357776	1.696662
H	3.851683	-0.181192	1.911456
H	3.833272	-1.139601	0.393915
H	4.008542	0.629241	0.317639
H	1.731945	-0.092220	-1.312312
H	-0.885914	0.195556	-0.483853
H	1.620266	0.052042	2.973745
H	4.608237	-0.109631	6.343741
H	3.148484	0.813013	6.782811
H	3.093148	-0.940172	6.773610
H	-2.118363	-0.611501	3.990548
H	-1.321301	-1.753606	2.903249
H	-0.359625	-0.778961	4.039851

E(B971/6-311+G**) = -573.217127

C	1.312428	-0.016195	-0.337700
C	0.019219	0.122123	0.071628
N	0.040674	0.165607	1.454582
C	1.309644	0.059896	1.885360
N	2.093815	-0.052347	0.804308
C	-1.128012	0.330576	2.344177
C	3.556595	-0.193273	0.851662
O	1.817169	0.014001	4.597812
C	3.073842	-0.056088	4.806357
O	3.950288	-0.104309	3.914117
C	3.511312	-0.083731	6.275439
C	-1.216046	-0.768112	3.403172
H	-1.051855	1.315656	2.814100
H	-2.006845	0.334488	1.693518
H	3.859142	-0.178437	1.908226
H	3.839459	-1.139685	0.384117
H	4.012474	0.638842	0.309503
H	1.735075	-0.093272	-1.326467
H	-0.896288	0.191317	-0.493411
H	1.621948	0.054027	2.982601
H	4.599332	-0.114477	6.360475
H	3.122037	0.800527	6.791111
H	3.077940	-0.961121	6.767920
H	-2.112374	-0.603825	4.009571
H	-1.292714	-1.755261	2.936007
H	-0.343244	-0.743546	4.063414

E(MPW1K/6-311+G**) = -573.206850

C	1.317073	0.007900	-0.307061
C	0.037423	0.145760	0.096758
N	0.054354	0.159465	1.466337
C	1.307085	0.036758	1.891371
N	2.086457	-0.056983	0.824680
C	-1.102468	0.317516	2.343664
C	3.531149	-0.208567	0.874344
O	1.793483	-0.009424	4.597456
C	3.037435	-0.062209	4.788928
O	3.891563	-0.105514	3.893395
C	3.491725	-0.072132	6.232418
C	-1.175064	-0.761599	3.398578
H	-1.042246	1.301097	2.802087
H	-1.976428	0.305196	1.698673
H	3.829376	-0.192346	1.924575
H	3.808196	-1.152263	0.415002
H	3.994098	0.612358	0.336062
H	1.738972	-0.051508	-1.290368
H	-0.869793	0.232789	-0.467014
H	1.613243	0.017873	2.976709
H	4.573265	-0.105350	6.301762
H	3.115121	0.815127	6.736228
H	3.063056	-0.933896	6.739264
H	-2.063618	-0.604964	4.005046
H	-1.243096	-1.746264	2.941763
H	-0.305346	-0.725440	4.050939

E(B3LYP/def2-TZVPP) = -573.464113

C	1.309562	-0.037826	-0.326832
C	0.022377	0.099218	0.080453
N	0.044910	0.168344	1.458273
C	1.310848	0.077955	1.885657
N	2.091534	-0.048757	0.810304
C	-1.120272	0.334675	2.345407
C	3.551065	-0.179810	0.860505
O	1.821126	0.054091	4.601170
C	3.073411	-0.046374	4.803519
O	3.946108	-0.110604	3.912185
C	3.514044	-0.093618	6.265899
C	-1.221839	-0.767646	3.389909
H	-1.036483	1.309536	2.825084
H	-1.995741	0.355290	1.697987
H	3.849428	-0.165009	1.914229
H	3.842006	-1.119528	0.393878
H	4.004028	0.650647	0.321377
H	1.728227	-0.129233	-1.311970
H	-0.890615	0.152225	-0.483251
H	1.624605	0.088967	2.975346
H	4.597881	-0.130377	6.349308
H	3.130972	0.780736	6.794189
H	3.081241	-0.972543	6.747292
H	-2.110137	-0.598936	3.999279
H	-1.312871	-1.746406	2.917443
H	-0.350399	-0.761635	4.044958

E(B971/def2-TZVPP) = -573.281830

C	1.308164	-0.046847	-0.327287
C	0.018696	0.091905	0.083463
N	0.046474	0.172229	1.461141
C	1.315021	0.086800	1.888761
N	2.092537	-0.047559	0.809225
C	-1.115838	0.339116	2.350693
C	3.552006	-0.174597	0.855600
O	1.826962	0.082885	4.581322
C	3.076431	-0.045336	4.794133
O	3.955723	-0.134612	3.912761
C	3.501034	-0.096065	6.265408
C	-1.215683	-0.770931	3.392422
H	-1.027096	1.313154	2.836042
H	-1.994943	0.364180	1.704576
H	3.852954	-0.165500	1.911067
H	3.844186	-1.112671	0.381809
H	4.001846	0.661859	0.318967
H	1.726126	-0.145529	-1.314129
H	-0.898317	0.139051	-0.478013
H	1.632233	0.105470	2.989205
H	4.585580	-0.140530	6.359655
H	3.115776	0.781379	6.790625
H	3.056445	-0.975248	6.739933
H	-2.104442	-0.604635	4.005085
H	-1.306595	-1.748517	2.913199
H	-0.340267	-0.766068	4.045938

E(MPW1K/def2-TZVPP) = -573.274990

C	1.313569	-0.012986	-0.295974
C	0.037928	0.129028	0.109517
N	0.060649	0.168457	1.475133
C	1.312242	0.055804	1.897226
N	2.085237	-0.055858	0.831434
C	-1.089912	0.326958	2.352985
C	3.526086	-0.202267	0.880158
O	1.799535	0.030030	4.589495
C	3.040135	-0.048980	4.779904
O	3.895339	-0.107476	3.890225
C	3.490790	-0.071857	6.224042
C	-1.185217	-0.776682	3.376955
H	-1.009340	1.292992	2.840199
H	-1.963408	0.352015	1.710966
H	3.823414	-0.187919	1.929405
H	3.807047	-1.141650	0.418268
H	3.987732	0.618158	0.343178
H	1.731253	-0.088362	-1.278224
H	-0.870546	0.203708	-0.451010
H	1.622612	0.052538	2.984115
H	4.569670	-0.117473	6.297107
H	3.122357	0.814246	6.731877
H	3.052046	-0.930387	6.723853
H	-2.065445	-0.617764	3.991235
H	-1.275643	-1.745606	2.895891
H	-0.313115	-0.775282	4.023639

E(B3LYP/aug-cc-pVTZ) = -573.451464
E(B3LYP/def2-QZVPP//B3LYP/aug-cc-pVTZ) = -573.4992112
E(MP2/6-31+G*//B3LYP/aug-cc-pVTZ) = -571.4588778
E(MP2/6-311+G**//B3LYP/aug-cc-pVTZ) = -571.7680081

C	1.311757	-0.015668	-0.326851
C	0.025240	0.124240	0.080279
N	0.044815	0.167216	1.459348
C	1.309409	0.059315	1.887207
N	2.091712	-0.053621	0.811304
C	-1.122329	0.330718	2.346247
C	3.551202	-0.196795	0.859218
O	1.813406	0.010510	4.616084
C	3.069724	-0.053118	4.811925
O	3.936560	-0.099885	3.910916
C	3.523968	-0.073486	6.269703
C	-1.228985	-0.778626	3.382721
H	-1.036231	1.301838	2.832433
H	-1.995607	0.357776	1.696662
H	3.851683	-0.181192	1.911456
H	3.833272	-1.139601	0.393915
H	4.008542	0.629241	0.317639
H	1.731945	-0.092220	-1.312312
H	-0.885914	0.195556	-0.483853
H	1.620266	0.052042	2.973745
H	4.608237	-0.109631	6.343741
H	3.148484	0.813013	6.782811
H	3.093148	-0.940172	6.773610
H	-2.118363	-0.611501	3.990548
H	-1.321301	-1.753606	2.903249
H	-0.359625	-0.778961	4.039851

E(B971/aug-cc-pVTZ) = -573.266866
E(B971/def2-QZVPP//B971/aug-cc-pVTZ) = -573.3133282

C	1.311050	-0.017495	-0.327743
C	0.022186	0.125021	0.082247
N	0.045468	0.170586	1.461690
C	1.311751	0.060839	1.890424
N	2.091942	-0.054862	0.810629
C	-1.119310	0.334519	2.349826
C	3.550513	-0.199691	0.857210
O	1.819536	0.022775	4.596518
C	3.074903	-0.050209	4.801871
O	3.950010	-0.105365	3.910777
C	3.514579	-0.072304	6.269166
C	-1.224466	-0.781555	3.384904
H	-1.030007	1.305697	2.840792
H	-1.995974	0.364287	1.700767
H	3.852003	-0.183767	1.912136
H	3.830939	-1.145157	0.390979
H	4.008711	0.627383	0.313346
H	1.731145	-0.096088	-1.315440
H	-0.892151	0.196936	-0.480878
H	1.626163	0.055175	2.987338
H	4.600537	-0.095540	6.353614
H	3.119575	0.807267	6.783701
H	3.088719	-0.950615	6.761737
H	-2.115267	-0.616270	3.994843
H	-1.315847	-1.756005	2.899462
H	-0.351692	-0.782182	4.041686

E(MPW1K/aug-cc-pVTZ) = -573.260807
E(MPW1K/def2-QZVPP// MPW1K/aug-cc-pVTZ) = -573.3035877

C	1.312561	-0.012333	-0.298349
C	0.036895	0.131727	0.107325
N	0.059343	0.168891	1.473401
C	1.311170	0.054876	1.895208
N	2.084566	-0.056099	0.829378
C	-1.091734	0.327180	2.351135
C	3.525707	-0.202980	0.878188
O	1.799070	0.015952	4.595795
C	3.040852	-0.052169	4.785708
O	3.895871	-0.104791	3.893225
C	3.494415	-0.070242	6.229492
C	-1.186125	-0.776122	3.375799
H	-1.011295	1.293399	2.837971
H	-1.965168	0.351983	1.709028
H	3.823199	-0.187708	1.927027
H	3.806878	-1.142927	0.417526
H	3.987981	0.616957	0.340941
H	1.729881	-0.087540	-1.280752
H	-0.871264	0.208282	-0.453466
H	1.621485	0.048563	2.979083
H	4.573511	-0.112029	6.301388
H	3.123988	0.815911	6.735858
H	3.059114	-0.928684	6.732473
H	-2.065778	-0.617144	3.990828
H	-1.276588	-1.745528	2.895575
H	-0.313519	-0.774042	4.021810

XYZ coordinates and total energy of 7a-1 at different levels of theory

E(B971/6-31+G*) = -573.072285

N	1.282235	0.038643	-0.365076
C	-0.060372	0.073021	-0.010626
C	-0.097781	0.114233	1.351624
N	1.225738	0.108739	1.775248
C	2.097276	0.059124	0.726075
C	1.652920	0.098182	3.176847
C	1.771564	-0.003995	-1.742711
O	4.823529	0.006270	1.005112
C	5.536832	-0.041693	-0.111719
C	7.033051	-0.070528	0.152359
O	5.057472	-0.062555	-1.241129
H	2.694808	0.433375	3.187026
H	1.053976	0.840187	3.721254
C	1.524443	-1.287144	3.820911
H	2.865123	-0.026122	-1.717820
H	1.393729	-0.902773	-2.244764
H	1.431176	0.884772	-2.287664
H	-0.857808	0.073057	-0.741648
H	-0.934632	0.153551	2.036100
H	7.579692	-0.106690	-0.793422
H	7.328781	0.820131	0.720958
H	7.286721	-0.945928	0.763470
H	3.788557	0.026520	0.812688
H	1.858876	-1.245867	4.865587
H	0.485144	-1.640560	3.808504
H	2.145080	-2.016614	3.286737

E(MPW1K/6-31+G*) = -573.066267

N	1.299162	0.033948	-0.345942
C	-0.029958	0.067879	0.002584
C	-0.069080	0.105642	1.349587
N	1.239961	0.098438	1.770686
C	2.100840	0.051535	0.734390
C	1.658463	0.088393	3.156799
C	1.784890	-0.006188	-1.706634
O	4.826327	0.005605	0.998686
C	5.523042	-0.040076	-0.109156
C	7.003161	-0.060450	0.137685
O	5.038047	-0.064089	-1.220437
H	2.698902	0.399676	3.168354
H	1.081681	0.841039	3.693438
C	1.500813	-1.274077	3.800615
H	2.870094	-0.028895	-1.681372
H	1.412914	-0.896504	-2.209325
H	1.451224	0.876193	-2.248733
H	-0.821182	0.069018	-0.723930
H	-0.901629	0.143805	2.027351
H	7.537781	-0.100508	-0.804883
H	7.295944	0.828636	0.693064
H	7.262748	-0.922832	0.748848
H	3.807548	0.020214	0.819942
H	1.831219	-1.238275	4.837691
H	0.462796	-1.603920	3.789047
H	2.100420	-2.014872	3.275565

E(B3LYP/6-311+G**) = -573.396089

N	1.284136	0.038553	-0.357166
C	-0.058571	0.076462	-0.007981
C	-0.102524	0.115628	1.346678
N	1.217013	0.104856	1.778846
C	2.090038	0.054785	0.735898
C	1.634622	0.094090	3.183026
C	1.778065	-0.002108	-1.732804
O	4.840161	0.003637	0.994145
C	5.549128	-0.046371	-0.123823
C	7.039871	-0.068075	0.135021
O	5.067376	-0.072744	-1.243737
H	2.668460	0.438946	3.201300
H	1.029287	0.828107	3.722574
C	1.515978	-1.286553	3.826722
H	2.866758	-0.030894	-1.706176
H	1.399109	-0.892953	-2.239163
H	1.447634	0.886870	-2.275256
H	-0.852088	0.080006	-0.736491
H	-0.942037	0.156416	2.020406
H	7.581755	-0.108224	-0.808043
H	7.331220	0.823955	0.695099
H	7.296034	-0.934758	0.749479
H	3.813863	0.019890	0.814636
H	1.842779	-1.241434	4.869029
H	0.484731	-1.649111	3.810657
H	2.143332	-2.009641	3.301048

E(B971/6-311+G**) = -573.216537

N	1.282329	0.038711	-0.362068
C	-0.059120	0.074005	-0.008454
C	-0.097624	0.115115	1.349914
N	1.224085	0.108764	1.774985
C	2.094749	0.058067	0.728145
C	1.650211	0.096517	3.176111
C	1.773634	-0.003944	-1.738293
O	4.828777	0.006510	1.003081
C	5.537420	-0.044677	-0.113283
C	7.031747	-0.068067	0.148276
O	5.058388	-0.071102	-1.235133
H	2.689668	0.431623	3.186579
H	1.053557	0.836982	3.720332
C	1.522152	-1.287115	3.819102
H	2.864717	-0.030226	-1.711415
H	1.394960	-0.898573	-2.241892
H	1.439438	0.884806	-2.282280
H	-0.856321	0.074943	-0.735504
H	-0.934988	0.155144	2.029194
H	7.574738	-0.108871	-0.796042
H	7.322469	0.825329	0.709696
H	7.285130	-0.936742	0.763985
H	3.803690	0.023070	0.815383
H	1.856884	-1.247222	4.860758
H	0.485232	-1.638988	3.807819
H	2.140206	-2.014723	3.284926

E(MPW1K/6-311+G**) = -573.206489

N	1.299724	0.034286	-0.345414
C	-0.028432	0.065799	0.003738
C	-0.067622	0.102477	1.347528
N	1.240352	0.097047	1.769262
C	2.099796	0.052076	0.733932
C	1.659827	0.086523	3.154655
C	1.786997	-0.004031	-1.705278
O	4.826765	0.007657	0.997710
C	5.520662	-0.040302	-0.108388
C	6.998802	-0.060801	0.136733
O	5.037225	-0.066030	-1.213508
H	2.699588	0.396020	3.163832
H	1.087013	0.840875	3.690942
C	1.500785	-1.272655	3.800867
H	2.870956	-0.027964	-1.677893
H	1.415834	-0.892216	-2.209998
H	1.456066	0.878700	-2.246337
H	-0.820763	0.066427	-0.719050
H	-0.900959	0.138959	2.021710
H	7.530966	-0.102019	-0.805234
H	7.288745	0.828088	0.691024
H	7.255072	-0.921762	0.748676
H	3.815736	0.021648	0.820496
H	1.833029	-1.235545	4.835672
H	0.463201	-1.599286	3.792029
H	2.096765	-2.014633	3.276210

E(B3LYP/def2-TZVPP) = -573.463537

N	1.279374	0.038235	-0.351154
C	-0.059881	0.079503	-0.004836
C	-0.104905	0.119030	1.346411
N	1.210457	0.105005	1.778319
C	2.082177	0.053061	0.739423
C	1.625194	0.096110	3.178475
C	1.773320	-0.004826	-1.721540
O	4.845942	-0.007479	0.989099
C	5.555610	-0.046454	-0.126705
C	7.043776	-0.071142	0.135063
O	5.079497	-0.061490	-1.245940
H	2.653075	0.451281	3.200578
H	1.012060	0.819391	3.718966
C	1.521864	-1.283495	3.819011
H	2.859943	-0.027899	-1.695224
H	1.400145	-0.896442	-2.226085
H	1.439419	0.877532	-2.268150
H	-0.851221	0.084759	-0.732735
H	-0.943379	0.162548	2.018088
H	7.587074	-0.103921	-0.804621
H	7.334059	0.813995	0.702067
H	7.297962	-0.940502	0.742362
H	3.825697	0.012713	0.809297
H	1.840878	-1.236010	4.860898
H	0.497809	-1.658228	3.795787
H	2.160180	-1.995940	3.297070

E(B971/def2-TZVPP) = -573.282517

N	1.277983	0.038420	-0.356118
C	-0.060696	0.074428	-0.005525
C	-0.100647	0.115066	1.349525
N	1.217352	0.107736	1.774736
C	2.087478	0.057255	0.731954
C	1.640171	0.098593	3.172559
C	1.769153	-0.004343	-1.727804
O	4.836722	-0.001647	0.997624
C	5.545454	-0.044609	-0.117529
C	7.037613	-0.071638	0.146441
O	5.071186	-0.061767	-1.238578
H	2.674533	0.442590	3.186440
H	1.036372	0.830089	3.716799
C	1.525214	-1.283353	3.814110
H	2.858297	-0.027799	-1.701611
H	1.393498	-0.897609	-2.231753
H	1.433462	0.880207	-2.273675
H	-0.855636	0.075781	-0.732402
H	-0.937309	0.155618	2.026837
H	7.581822	-0.104647	-0.794852
H	7.327761	0.814340	0.715767
H	7.288687	-0.943841	0.754340
H	3.817404	0.018736	0.810304
H	1.851648	-1.239787	4.855774
H	0.494657	-1.646297	3.795507
H	2.153951	-2.002185	3.285051

E(MPW1K/def2-TZVPP) = -573.275811

N	1.292964	0.034568	-0.339367
C	-0.032489	0.070668	0.007174
C	-0.072389	0.108188	1.347814
N	1.232225	0.098623	1.769097
C	2.090680	0.050374	0.737525
C	1.647994	0.089294	3.151219
C	1.779474	-0.006290	-1.694663
O	4.832991	-0.000708	0.989700
C	5.530037	-0.043156	-0.112947
C	7.006431	-0.064172	0.138409
O	5.054572	-0.063943	-1.218928
H	2.681106	0.414488	3.166198
H	1.062737	0.829850	3.689700
C	1.509789	-1.271599	3.792821
H	2.861749	-0.028505	-1.669235
H	1.410518	-0.893661	-2.199009
H	1.447842	0.871865	-2.239478
H	-0.823000	0.073599	-0.715250
H	-0.904730	0.148071	2.020534
H	7.542212	-0.101763	-0.799378
H	7.293665	0.820887	0.696869
H	7.260330	-0.925312	0.748028
H	3.826884	0.015305	0.812109
H	1.831568	-1.230855	4.828631
H	0.480322	-1.616362	3.773631
H	2.122646	-2.000119	3.272714

E(B3LYP/aug-cc-pVTZ) = -573.449914
E(B3LYP/def2-QZVPP//B3LYP/aug-cc-pVTZ) = -573. 4980262
E(MP2/6-31+G*//B3LYP/aug-cc-pVTZ) = -571.4516402
E(MP2/6-311+G**//B3LYP/aug-cc-pVTZ) = -571.7676048

N	1.282801	0.037506	-0.350981
C	-0.056543	0.078834	-0.003894
C	-0.101169	0.116664	1.347154
N	1.214446	0.101428	1.779155
C	2.085911	0.050463	0.739688
C	1.628534	0.091609	3.180156
C	1.775976	-0.004316	-1.722498
O	4.848860	-0.000193	0.988371
C	5.557420	-0.044893	-0.128975
C	7.045917	-0.066067	0.129272
O	5.077029	-0.067068	-1.247580
H	2.660344	0.434351	3.201015
H	1.023873	0.823644	3.717871
C	1.508154	-1.284877	3.824633
H	2.862227	-0.028358	-1.696665
H	1.401588	-0.895073	-2.227157
H	1.442139	0.878978	-2.267173
H	-0.848096	0.085051	-0.731180
H	-0.939514	0.159541	2.018604
H	7.586746	-0.104796	-0.811359
H	7.336188	0.823328	0.689178
H	7.302279	-0.930637	0.742068
H	3.826033	0.015525	0.810138
H	1.827021	-1.237366	4.866381
H	0.479873	-1.647354	3.802080
H	2.138089	-2.006587	3.305617

E(B971/aug-cc-pVTZ) = -573.266682
E(B971/def2-QZVPP//B971/aug-cc-pVTZ) = -573.3135174

N	1.281784	0.037724	-0.356044
C	-0.056787	0.073508	-0.004727
C	-0.096392	0.112164	1.350084
N	1.221708	0.104191	1.775338
C	2.091414	0.055173	0.732074
C	1.644195	0.094322	3.173717
C	1.772032	-0.003260	-1.728752
O	4.837608	0.006636	0.995970
C	5.545972	-0.044279	-0.119635
C	7.038615	-0.066222	0.141890
O	5.068590	-0.071740	-1.240478
H	2.682493	0.425989	3.186254
H	1.048804	0.834429	3.715404
C	1.512627	-1.284530	3.819564
H	2.860994	-0.029651	-1.703206
H	1.393440	-0.894676	-2.233657
H	1.437845	0.883538	-2.271803
H	-0.852017	0.075592	-0.731200
H	-0.933037	0.151414	2.027377
H	7.581194	-0.104120	-0.800131
H	7.327433	0.823989	0.705182
H	7.292227	-0.934103	0.754880
H	3.815222	0.021644	0.809572
H	1.840748	-1.240991	4.860695
H	0.477588	-1.634604	3.803353
H	2.131827	-2.012799	3.292200

E(MPW1K/aug-cc-pVTZ) = -573.260925
E(MPW1K/def2-QZVPP//MPW1K/aug-cc-pVTZ) = -573.3040089

N	1.296307	0.034408	-0.339823
C	-0.029280	0.064173	0.007377
C	-0.069043	0.099078	1.348087
N	1.235798	0.094337	1.769374
C	2.094337	0.051881	0.737230
C	1.651837	0.086304	3.152156
C	1.782418	-0.001561	-1.696322
O	4.834968	0.008151	0.988642
C	5.531045	-0.040736	-0.115310
C	7.007628	-0.062643	0.133529
O	5.052099	-0.066312	-1.220814
H	2.688808	0.398517	3.164304
H	1.075873	0.836370	3.687245
C	1.497027	-1.269993	3.799959
H	2.864497	-0.024954	-1.670519
H	1.412107	-0.886819	-2.203107
H	1.451022	0.879167	-2.236913
H	-0.819909	0.064516	-0.714795
H	-0.901395	0.133802	2.020912
H	7.541820	-0.103474	-0.804971
H	7.296480	0.823495	0.689269
H	7.261080	-0.922505	0.745022
H	3.826808	0.022496	0.811818
H	1.820602	-1.228026	4.835124
H	0.463276	-1.601704	3.783863
H	2.099917	-2.008632	3.282583

5. XYZ coordinates and total energies of the examined radicals and radical cations related to the MS measurements of EMIM-acetate at the B3LYP/6-31+G* level

Acetic acid radical cation

E(B3LYP/6-31+G*) = -228.708986

C	-0.003161	-0.057680	-0.031638
C	0.009963	-0.005627	1.463051
H	0.991490	0.271640	1.858343
H	-0.741719	0.739207	1.762759
H	-0.271157	-1.007415	1.819452
O	-1.084755	-0.369671	-0.663454
O	1.076790	0.214226	-0.617373
H	-1.012116	-0.382044	-1.646144

1-ethyl-3-methylimidazol-2-ylidene radical cation

E(B3LYP/6-31+G*) = -343.830598

C	0.109961	-0.530703	0.395117
N	0.185076	0.254146	1.542277
C	1.451460	0.713932	1.787944
N	2.159353	0.184368	0.742420
C	1.368367	-0.572960	-0.116705
C	-0.944384	0.526160	2.429597
C	3.585010	0.405629	0.554659
H	3.932761	1.032508	1.376666
H	4.129638	-0.545396	0.567398
H	3.776944	0.915304	-0.396535
C	-1.285257	-0.656664	3.339196
H	-0.659872	1.397909	3.023298
H	-1.809615	0.803248	1.814361
H	1.753938	-1.058606	-1.001839
H	-0.808568	-0.977052	0.041481
H	-2.128572	-0.399539	3.991500
H	-1.564378	-1.543500	2.758112
H	-0.426336	-0.914488	3.967926

Acetate radical

E(B3LYP/6-31+G*) = -228.423666

C	-0.014549	0.000039	-0.020079
C	0.012916	0.000140	1.474344
O	1.067888	-0.000080	2.168454
O	-1.021209	0.000015	2.202039
H	1.004013	-0.000035	-0.417890
H	-0.551220	-0.886153	-0.376261
H	-0.551160	0.886190	-0.376466