Supporting Information

Imidazolium based energetic ionic liquids for monopropellant applications: A theoretical study

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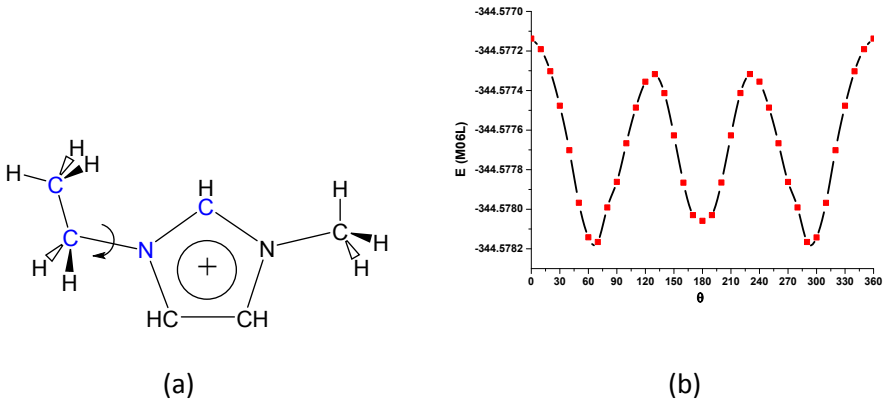
Captions

Part-I : Conformation Analysis

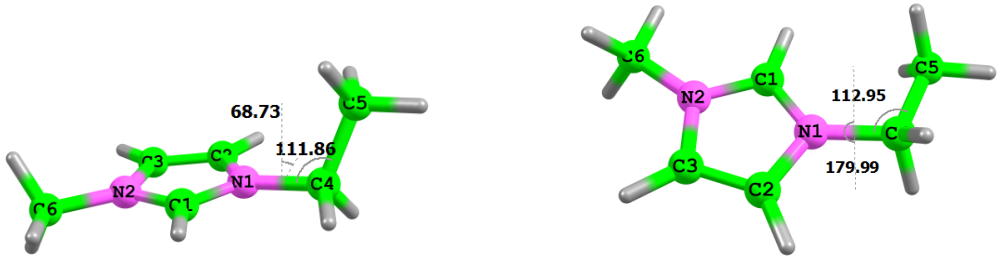
[1] 1-ethyl-3-methylimidazolium Cation $[EMIm]^+$

Imidazolium cation exists in two different conformations. We obtained these conformations by rotating the ethyl group around the C-N bond (Fig. S1). This is done by varying the dihedral angle (θ) defined by the four atoms colored in blue in the order CH_3-CH_2-N(ring)-CH(ring). The θ is varied from 0.0° to 360.0 ° in increments of 10°. Because of the planar symmetry of the molecule at θ = 0.0° and θ = 180.0°, the energy profile for the rotation values in the range 180.0° - 360.0° is same as that in the range 180° to 0.0°. The methyl group always showed a fixed orientation wherein a cis-arrangement of one of its CH bond with respect to the CH bond of the ring juxtaposed with the two nitrogen atoms.



(a) (b)

Fig. S1 (a) Structure of $[EMIm]^+$ cation and (b) the energy profile for the rotation of the C-N bond (energy values in au and angle in degrees).



(a) E(RM06L) = -344.578171173 au (b) E(RM06L) = -344.578058721

Fig. S2.The two different conformations obtained for 1-ethyl-3-methylimidazolium cation through the rotation of C-N bond. All distance parameters in Å and angle in degrees. The conformer in the left side is 0.295 kJ/mol more stable than the other.

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

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(a)E(RM06L) =  -344.578171173
7        0.618025000     -0.017179000     -0.312787000
6       -0.426176000     -0.836193000     -0.177711000
6        0.177681000      1.278916000     -0.169255000
6       -1.162428000      1.226227000      0.051483000
7       -1.521648000     -0.103641000      0.043416000
1       -1.886048000      2.008795000      0.206994000
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1         0.847374000      2.119653000     -0.242349000
6         2.019642000     -0.429008000     -0.533634000
1         1.993204000     -1.484895000     -0.807744000
1         2.376283000      0.123334000     -1.406057000
6         2.878472000     -0.180282000      0.685864000
1         2.521432000     -0.744332000      1.549367000
1         2.905834000      0.877905000      0.952533000
6        -2.873462000     -0.623472000      0.234704000
1        -2.848500000     -1.709291000      0.181162000
1        -3.247930000     -0.318229000      1.211212000
1        -3.527652000     -0.238633000     -0.546983000
1         3.902024000     -0.493729000      0.478436000
1        -0.393028000     -1.911968000     -0.239673000


(b) E(RM06L) =  -344.578058721
7         0.641358000      0.408058000     -0.000063000
6        -0.169257000     -0.652614000     -0.000032000
6        -0.133157000      1.547173000     -0.000009000
6        -1.433106000      1.151490000      0.000030000
7        -1.435469000     -0.224877000      0.000001000
1        -2.346346000      1.722809000      0.000160000
1         0.305425000      2.531438000      0.000013000
6         2.121197000      0.392547000     -0.000017000
1         2.437277000      0.956359000     -0.881202000
1         2.437195000      0.956427000      0.881157000
6         2.694042000     -1.000984000      0.000064000
1         2.405911000     -1.564540000     -0.890212000
1         2.405925000     -1.564431000      0.890408000
6        -2.622753000     -1.076021000      0.000010000
1        -2.313702000     -2.118528000     -0.000087000
1        -3.216877000     -0.875843000      0.890968000
1        -3.216989000     -0.875702000     -0.890840000
1         3.781762000     -0.934790000      0.000015000
1         0.137405000     -1.685014000     -0.000219000
```

The strategy used to locate various configurations of cation-anion complex .

The schematic shown in Fig.S3 (blue is cation and red is anion) is useful to explain the conformational space we scanned for the cation-anion complex. The illustration is based on $[EMIm]^+[dtrz]^-$ complex. To generate an initial structure of the cation-anion complex, we used the Chemcraft program to place the cation above the π-region of the anion to obtain a parallel orientation of its ring with respect to the ring of the anion while the distance between the centres of the two rings is selected close to 3.5 Å. While selecting this orientation, one of the ring atoms of the anion is oriented close to the C2 carbon of the cation. The initial geometry of another configuration is made in a similar manner but the nearest ring atom of the anion from C2 is changed. This way we can generate 5 initial structures (a -e). Also we used four different orientations for the in-plane configuration of the cation-anion complex as shown in (f - i). This exercise is done for all the tetrazolate and triazolate anions with both conformations obtained for the cation. For the open structures, viz. $[dc]^-$ and $[dn]^-$, the conformational space is scanned by

orienting the central nitrogen towards the π-region of the cation or that nitrogen orienting away from the π-region. Also the in plane configurations are considered.

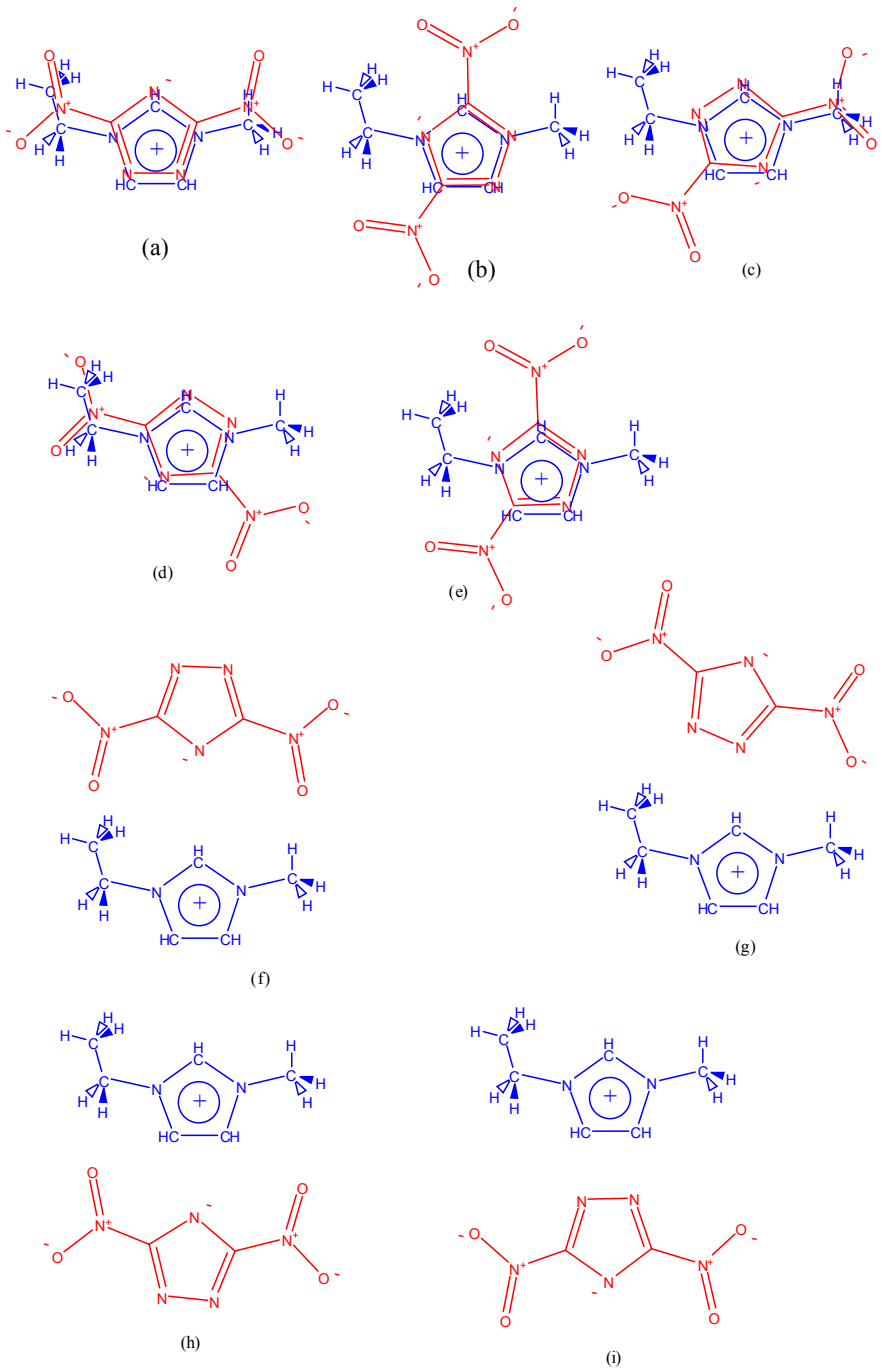
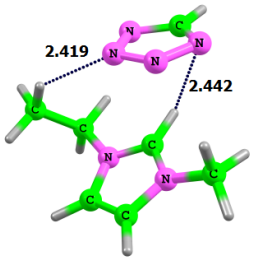
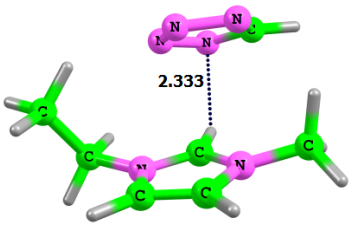


Fig. S3. The schematics showing the strategy used to search for the conformational space of the cation anion complex. The illustration is based on $[EMIm]^{+}[dtrz]^{-}$ complex.

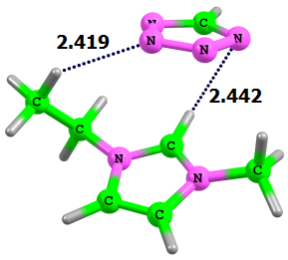
[2] 1-ethyl-3-methylimidazolium tetrazolate ($[EMIm]^{+}[tz]^{-}$



(a)E(RM06L) = -602.485001048



(b)E(RM06L) = -602.483193457



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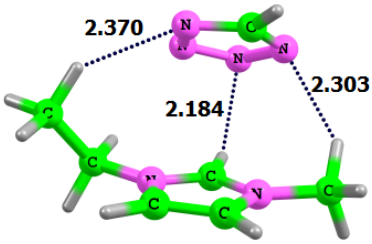

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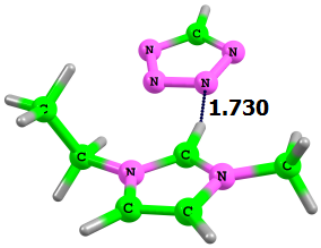

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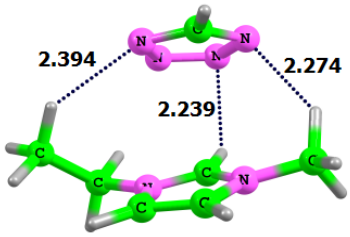

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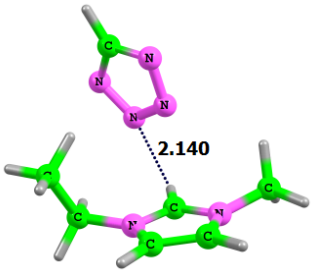

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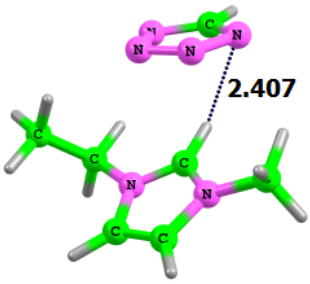

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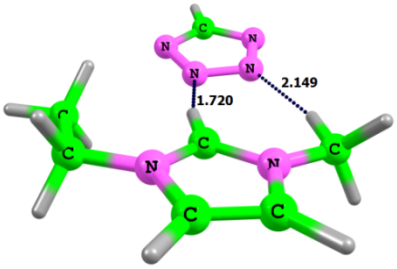
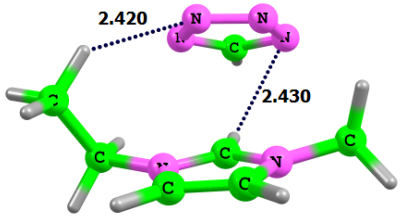


(i)E(RM06L) = -602.481131674



(j)E(RM06L) = -602.485040916

Fig. S4.Optimized conformers of 1-ethyl-3-methylimidazolium tetrazolate. All distance parameters in Å and energy in au.

Table S1. Relative energy of the a-j conformations.

Conformation	Rel. Energy (kJ/mol)
a	0.1046
b	4.8459
c	0.1035
d	5.5419

e	15.2928
f	5.4084
g	9.7594
h	0.3195
i	10.2539
j	0.0000

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

a) E(RM06L) = -602.485001048

7	-1.256492000	-0.874668000	0.981639000
7	-1.734818000	-1.578790000	-0.060882000
7	-1.790065000	0.339919000	0.982080000
7	-2.629754000	0.466561000	-0.060844000
6	-2.575045000	-0.727668000	-0.665202000
1	-3.160293000	-0.983158000	-1.538294000
7	1.450163000	-0.283593000	-0.470946000
6	0.419089000	0.522491000	-0.718125000
6	2.392064000	0.419849000	0.247290000
6	1.909983000	1.679748000	0.411364000
7	0.682018000	1.727812000	-0.211958000
1	-0.495217000	0.241422000	-1.224592000
1	2.326344000	2.538151000	0.910312000
1	3.314705000	-0.029863000	0.571823000
6	-0.295544000	2.805693000	-0.114288000
1	-0.953001000	2.771134000	-0.980628000
1	-0.904122000	2.640618000	0.777303000
1	0.230216000	3.759068000	-0.078713000
6	1.459723000	-1.730677000	-0.750326000
1	0.519162000	-1.940326000	-1.264046000
1	2.292252000	-1.931390000	-1.431844000
6	1.541954000	-2.536374000	0.526895000
1	0.702396000	-2.280441000	1.176560000
1	2.482203000	-2.365569000	1.058375000
1	1.484639000	-3.598700000	0.284463000

b) E(RM06L) = -602.483193457

7	-1.333086000	-1.666539000	-0.007275000
7	-2.316011000	-1.182476000	-0.787363000
7	-1.160447000	-0.872626000	1.042342000
7	-2.031042000	0.152507000	0.980609000
6	-2.718588000	-0.078728000	-0.144600000
1	-3.527404000	0.551486000	-0.492414000
7	1.489390000	-0.105194000	-0.461194000
6	0.370566000	0.558833000	-0.748505000
6	2.293080000	0.702572000	0.311146000
6	1.639000000	1.882197000	0.471662000
7	0.446759000	1.777585000	-0.210084000
1	-0.477153000	0.161629000	-1.294234000
1	1.911875000	2.777908000	1.002688000
1	3.250402000	0.372013000	0.675548000
6	-0.646454000	2.739609000	-0.171931000
1	-1.248884000	2.628848000	-1.072067000
1	-1.272042000	2.525221000	0.696663000
1	-0.232131000	3.746405000	-0.131088000
6	1.716526000	-1.532132000	-0.753678000
1	0.850750000	-1.859692000	-1.330732000
1	2.612107000	-1.601662000	-1.378856000
6	1.829567000	-2.335729000	0.522351000
1	0.931054000	-2.198046000	1.126554000
1	2.709072000	-2.052604000	1.107044000
1	1.921219000	-3.394031000	0.272972000

c) E(RM06L) = -602.485001453

```
7       -1.788725000      0.338389000      0.982904000
7       -2.629256000      0.466407000     -0.059321000
7       -1.255614000     -0.876301000      0.980772000
7       -1.735014000     -1.579279000     -0.062106000
6       -2.575449000     -0.727223000     -0.664844000
1       -3.161070000     -0.981475000     -1.538050000
7        1.449792000     -0.283146000     -0.471043000
6        0.418670000      0.522803000     -0.718271000
6        2.391631000      0.420383000      0.247202000
6        1.909389000      1.680223000      0.411286000
7        0.681452000      1.728185000     -0.212145000
1       -0.495532000      0.241671000     -1.224886000
1        2.325514000      2.538655000      0.910349000
1        3.314215000     -0.029257000      0.571985000
6       -0.296442000      2.805721000     -0.114194000
1       -0.953207000      2.771884000     -0.981072000
1       -0.905534000      2.639546000      0.776840000
1        0.229059000      3.759162000     -0.077165000
6        1.459557000     -1.730255000     -0.750385000
1        0.518510000     -1.940196000     -1.263119000
1        2.291494000     -1.930716000     -1.432694000
6        1.543264000     -2.535910000      0.526773000
1        0.704311000     -2.280337000      1.177366000
1        2.484032000     -2.364932000      1.057294000
1        1.486038000     -3.598239000      0.284320000

d)  E(RM06L) =  -602.482928108
7       -1.430977000     -1.734578000     -0.899684000
7       -2.222406000     -1.143741000      0.017312000
7       -0.291903000     -2.101740000     -0.331255000
7       -0.305079000     -1.763949000      0.971899000
6       -1.501164000     -1.190390000      1.143240000
1       -1.852891000     -0.814689000      2.095654000
7        1.253415000      0.684862000     -0.390134000
6        0.008630000      0.763262000     -0.858042000
6        1.405798000      1.613633000      0.613706000
6        0.217273000      2.260922000      0.742266000
7       -0.642588000      1.713936000     -0.183550000
1       -0.437109000      0.088607000     -1.577699000
1       -0.093721000      3.044238000      1.412226000
1        2.329419000      1.724125000      1.154787000
6       -2.058543000      2.024484000     -0.356221000
1       -2.601883000      1.079228000     -0.449218000
1       -2.403322000      2.556996000      0.528175000
1       -2.202864000      2.652542000     -1.236495000
6        2.250669000     -0.311222000     -0.828548000
1        1.708028000     -1.001658000     -1.476225000
1        3.005120000      0.218527000     -1.419395000
6        2.847438000     -1.055726000      0.342844000
1        2.052724000     -1.532467000      0.921361000
1        3.433344000     -0.400044000      0.992752000
1        3.519317000     -1.828715000     -0.033517000

e)E(RM06L) =  -602.479210613
7        2.079946000      0.511321000     -0.212088000
7        3.389976000      0.738908000     -0.117522000
7        1.848844000     -0.790688000     -0.069058000
7        2.993774000     -1.447745000      0.125656000
6        3.912812000     -0.477071000      0.087887000
1        4.971486000     -0.656418000      0.211542000
7       -1.495105000      0.775000000     -0.312804000
6       -0.967778000     -0.443500000     -0.164251000
6       -2.866457000      0.694366000     -0.194382000
6       -3.174289000     -0.611204000      0.021695000
7       -1.978272000     -1.299105000      0.039209000
1        0.122609000     -0.718970000     -0.164746000
1       -4.122150000     -1.104124000      0.157665000
1       -3.497800000      1.563120000     -0.279378000
6       -1.804157000     -2.729532000      0.242047000
1       -0.738406000     -2.950822000      0.245394000
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1       -2.237027000     -3.025362000      1.198119000
1       -2.286862000     -3.284818000     -0.562841000
6       -0.706925000      2.009829000     -0.492497000
1        0.296577000      1.688093000     -0.792654000
1       -1.179853000      2.573009000     -1.301311000
6       -0.630128000      2.802567000      0.792908000
1       -0.120204000      2.223243000      1.565418000
1       -1.615749000      3.098410000      1.163505000
1       -0.045221000      3.708074000      0.625080000

f)E(RM06L) =  -602.482979005
7        0.024032000     -2.135796000     -0.370404000
7        0.026595000     -1.821148000      0.939061000
7       -1.174279000     -1.900617000     -0.883623000
7       -1.990915000     -1.423589000      0.077189000
6       -1.220222000     -1.396243000      1.169957000
1       -1.571535000     -1.076203000      2.142590000
7        1.108596000      0.851955000     -0.382307000
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6        1.108758000      1.753729000      0.656961000
6       -0.160901000      2.226256000      0.774889000
7       -0.915855000      1.606428000     -0.194432000
1       -0.454792000      0.080466000     -1.638596000
1       -0.592307000      2.929357000      1.466418000
1        1.993823000      1.967567000      1.229900000
6       -2.363102000      1.692870000     -0.368956000
1       -2.767017000      0.674898000     -0.327746000
1       -2.771167000      2.294312000      0.440816000
1       -2.598297000      2.165159000     -1.323529000
6        2.242686000      0.027521000     -0.846173000
1        1.794261000     -0.764159000     -1.449877000
1        2.870845000      0.659663000     -1.481980000
6        3.006439000     -0.575043000      0.308683000
1        2.328491000     -1.164000000      0.931081000
1        3.507485000      0.182693000      0.917500000
1        3.778835000     -1.236867000     -0.086111000

g)E(RM06L) =  -602.481320217
7        1.586234000     -0.532897000     -0.915542000
7        2.856193000     -0.201991000     -0.673987000
7        1.066779000     -1.135362000      0.156958000
7        1.987490000     -1.210025000      1.122274000
6        3.065521000     -0.633332000      0.576401000
1        4.010225000     -0.529287000      1.091871000
7       -1.149119000      1.106074000     -0.345635000
6       -1.134567000     -0.129950000     -0.842372000
6       -2.045972000      1.148692000      0.703261000
6       -2.587668000     -0.090862000      0.813615000
7       -2.021590000     -0.870820000     -0.174222000
1       -0.440645000     -0.471089000     -1.598728000
1       -3.322808000     -0.483940000      1.494619000
1       -2.224622000      2.049568000      1.264910000
6       -2.053951000     -2.323018000     -0.249397000
1       -1.126723000     -2.703128000      0.187853000
1       -2.921849000     -2.689415000      0.295468000
1       -2.122067000     -2.637714000     -1.289928000
6       -0.161598000      2.141159000     -0.692691000
1        0.393657000      1.750854000     -1.546976000
1       -0.708574000      3.035281000     -1.006574000
6        0.772412000      2.410867000      0.467371000
1        1.271041000      1.492419000      0.783504000
1        0.244573000      2.840570000      1.322866000
1        1.540817000      3.119679000      0.155070000

h)E(RM06L) =  -602.484919118
7       -1.791618000      0.386440000      0.988951000
7       -2.608310000      0.557607000     -0.067221000
7       -1.314460000     -0.850436000      0.985958000
7       -1.805892000     -1.524905000     -0.070941000
6       -2.596819000     -0.633051000     -0.681848000
1       -3.177358000     -0.854641000     -1.567340000
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7        1.441752000     -0.331569000     -0.469131000
6        0.431455000      0.506973000     -0.691219000
6        2.421380000      0.340596000      0.229651000
6        1.982644000      1.614432000      0.406656000
7        0.740057000      1.699569000     -0.182802000
1       -0.498134000      0.257492000     -1.186327000
1        2.435310000      2.456376000      0.901874000
1        3.332555000     -0.141546000      0.539939000
6       -0.175006000      2.833620000     -0.125177000
1       -1.160767000      2.495300000     -0.445572000
1       -0.257158000      3.164915000      0.909268000
1        0.193897000      3.644366000     -0.755519000
6        1.397151000     -1.777844000     -0.749607000
1        0.450205000     -1.951863000     -1.264774000
1        2.222055000     -2.007709000     -1.431095000
6        1.449295000     -2.587781000      0.526376000
1        0.616342000     -2.306515000      1.174269000
1        2.393034000     -2.447363000      1.060525000
1        1.358718000     -3.647421000      0.282061000

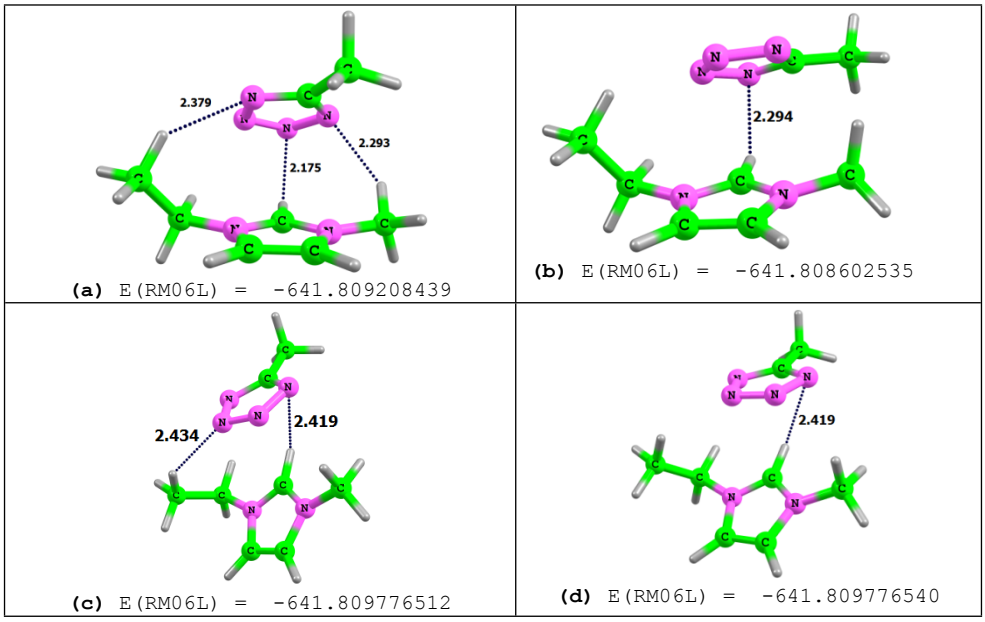
i)  E(RM06L) =  -602.481131674
7       -2.208910000     -0.936465000      0.038932000
7       -3.529785000     -0.948617000     -0.137048000
7       -1.791317000      0.320969000      0.134214000
7       -2.819635000      1.165303000      0.018801000
6       -3.865608000      0.348122000     -0.143640000
1       -4.880257000      0.699101000     -0.268332000
7        2.075077000      0.636269000     -0.034334000
6        0.999171000     -0.153635000      0.079306000
6        3.206032000     -0.146981000     -0.147268000
6        2.794424000     -1.440376000     -0.099320000
7        1.423622000     -1.421879000      0.040669000
1       -0.077412000      0.172599000      0.155253000
1        3.350704000     -2.361227000     -0.151402000
1        4.189261000      0.280182000     -0.251114000
6        0.543053000     -2.585933000      0.134918000
1       -0.497694000     -2.234076000      0.122925000
1        0.727964000     -3.241859000     -0.716171000
1        0.751802000     -3.123849000      1.060842000
6        2.048648000      2.108245000     -0.053772000
1        2.721543000      2.449277000      0.739187000
1        2.485332000      2.424179000     -1.006230000
6        0.656750000      2.664837000      0.124634000
1        0.209653000      2.358469000      1.072245000
1       -0.024953000      2.348323000     -0.666889000
1        0.705873000      3.754142000      0.111902000

j)  E(RM06L) =  -602.485040916

7       -1.259951000     -0.878590000      0.986703000
7       -1.724138000     -1.592705000     -0.056261000
7       -1.801259000      0.332097000      0.976173000
7       -2.633196000      0.446334000     -0.074688000
6       -2.565076000     -0.751175000     -0.672232000
1       -3.140895000     -1.015276000     -1.549066000
7        1.460061000     -0.271978000     -0.472347000
6        0.413838000      0.517122000     -0.710187000
6        2.396943000      0.447432000      0.237487000
6        1.896354000      1.699159000      0.405347000
7        0.660668000      1.725623000     -0.205079000
1       -0.498047000      0.222802000     -1.213568000
1        2.302711000      2.563930000      0.901648000
1        3.328352000      0.011892000      0.556527000
6       -0.326220000      2.794479000     -0.112838000
1       -1.157157000      2.561640000     -0.776292000
1       -0.722011000      2.819045000      0.902991000
1        0.137381000      3.743253000     -0.384390000
6        1.490062000     -1.719543000     -0.746241000
1        0.561332000     -1.942137000     -1.275544000
1        2.335417000     -1.912523000     -1.413976000
6        1.562626000     -2.519191000      0.535460000
```

1	0.710846000	-2.271486000	1.172216000
1	2.492482000	-2.333073000	1.079985000
1	1.523139000	-3.583230000	0.297187000

[3] 1-ethyl-3-methylimidazolium 5-methyl tetrazolate([EMIm]$^+$[mtz]$^-$)



(a) E(RM06L) = -641.809208439 **(b)** E(RM06L) = -641.808602535

(c) E(RM06L) = -641.809776512 **(d)** E(RM06L) = -641.809776540

Fig. S5.Optimized conformers of 1-ethyl-3-methylimidazolium 5-methyl tetrazolate. All distance parameters in Å and energy in au.

Table S2. Relative energy of the a-d conformations.

Conformation	Rel. Energy (kJ/mol)
a	1.4901
b	3.0794
c	0.0001
d	0.0000

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

(a)E(RM06L) = -641.809208439

7	-1.294161000	-1.496106000	-1.406341000
7	-2.117214000	-0.791230000	-0.604450000
7	-0.329545000	-2.036684000	-0.679355000
7	-0.495836000	-1.702236000	0.613991000
6	-1.602358000	-0.945646000	0.624314000
7	1.563246000	0.530332000	-0.282926000
6	0.443206000	0.785271000	-0.956746000
6	1.658849000	1.417251000	0.765353000
6	0.564748000	2.222589000	0.707240000
7	-0.183213000	1.810235000	-0.372300000
1	0.042649000	0.181902000	-1.762924000
1	0.248476000	3.034798000	1.339415000
1	2.478952000	1.393715000	1.461662000
6	-1.487408000	2.322784000	-0.780610000
1	-2.126799000	1.465568000	-1.012644000
1	-1.911788000	2.881950000	0.051411000
1	-1.381212000	2.981684000	-1.643574000
6	2.476368000	-0.590900000	-0.581118000
1	1.955478000	-1.199621000	-1.322794000

```
1        3.380315000     -0.166352000     -1.030210000
6        2.771711000     -1.416212000      0.649450000
1        1.837826000     -1.799322000      1.067868000
1        3.312216000     -0.845853000      1.409929000
1        3.401251000     -2.261090000      0.365830000
6       -2.190362000     -0.344918000      1.849576000
1       -2.911356000      0.433966000      1.589516000
1       -2.720498000     -1.090174000      2.450034000
1       -1.416960000      0.087330000      2.491387000

(b)E(RM06L) =  -641.808602535

7       -0.706058000     -1.899292000      0.002682000
7       -1.804123000     -1.535528000     -0.685054000
7       -0.588545000     -1.146078000      1.086308000
7       -1.612641000     -0.273151000      1.140628000
6       -2.340666000     -0.545610000      0.046573000
7        1.770111000      0.148714000     -0.497907000
6        0.537653000      0.597245000     -0.732084000
6        2.442438000      1.086225000      0.253615000
6        1.589771000      2.123778000      0.456775000
7        0.410131000      1.805088000     -0.180525000
1       -0.246234000      0.051821000     -1.244979000
1        1.713875000      3.050817000      0.989941000
1        3.458526000      0.936588000      0.576110000
6       -0.843795000      2.538937000     -0.083883000
1       -1.471294000      2.279663000     -0.935192000
1       -1.357744000      2.238703000      0.831852000
1       -0.635083000      3.608301000     -0.094319000
6        2.243683000     -1.209932000     -0.820058000
1        1.418711000     -1.696938000     -1.342437000
1        3.095904000     -1.109286000     -1.499487000
6        2.585092000     -1.976870000      0.437736000
1        1.710496000     -2.022897000      1.089330000
1        3.419547000     -1.523239000      0.979623000
1        2.875123000     -2.994168000      0.170540000
6       -3.612932000      0.141427000     -0.296913000
1       -3.687582000      0.333294000     -1.370767000
1       -4.478922000     -0.469578000     -0.025670000
1       -3.704899000      1.087438000      0.241969000

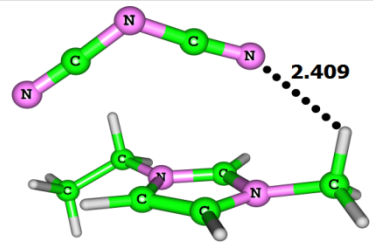
(c)E(RM06L) =  -641.809776512

7        0.941429000      0.532369000      1.318217000
7        1.726897000      1.130824000      0.403167000
7        1.187807000     -0.769316000      1.330752000
7        2.138051000     -1.057384000      0.423244000
6        2.456497000      0.130159000     -0.118402000
7       -1.566984000      0.576826000     -0.559780000
6       -0.699458000     -0.426548000     -0.681250000
6       -2.748809000      0.074211000     -0.060156000
6       -2.576942000     -1.264168000      0.099874000
7       -1.295267000     -1.559895000     -0.309831000
1        0.327740000     -0.338173000     -1.010535000
1       -3.245636000     -2.025706000      0.462926000
1       -3.600187000      0.703873000      0.133373000
6       -0.598457000     -2.827398000     -0.124746000
1       -0.115453000     -2.815676000      0.854577000
1       -1.315447000     -3.642109000     -0.216663000
1        0.177923000     -2.922439000     -0.881188000
6       -1.226666000      1.997618000     -0.747974000
1       -0.189472000      2.011985000     -1.088872000
1       -1.870505000      2.390215000     -1.541386000
6       -1.356427000      2.768795000      0.546266000
1       -0.705586000      2.324755000      1.302260000
1       -2.386877000      2.782325000      0.911871000
1       -1.047261000      3.802309000      0.381630000
6        3.520400000      0.320427000     -1.137732000
1        3.304927000      1.179333000     -1.776566000
1        4.490173000      0.505675000     -0.665726000
1        3.631299000     -0.568916000     -1.761366000
```

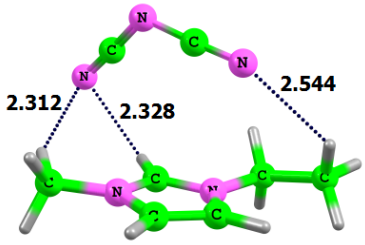
(d)E(RM06L) = -641.809776540

7	1.188122000	-0.769282000	1.330726000
7	2.138325000	-1.057282000	0.423212000
7	0.941671000	0.532429000	1.318180000
7	1.727004000	1.130895000	0.403065000
6	2.456635000	0.130278000	-0.118539000
7	-1.567248000	0.576796000	-0.559747000
6	-0.699534000	-0.426451000	-0.680980000
6	-2.749096000	0.074046000	-0.060327000
6	-2.577092000	-1.264318000	0.099725000
7	-1.295273000	-1.559863000	-0.309620000
1	0.327633000	-0.337968000	-1.010304000
1	-3.245663000	-2.025867000	0.462964000
1	-3.600663000	0.703542000	0.132941000
6	-0.598396000	-2.827341000	-0.124661000
1	0.177617000	-2.922506000	-0.881463000
1	-0.115006000	-2.815547000	0.854449000
1	-1.315417000	-3.642064000	-0.216262000
6	-1.227059000	1.997626000	-0.747938000
1	-0.189980000	2.012071000	-1.089194000
1	-1.871180000	2.390258000	-1.541104000
6	-1.356473000	2.768685000	0.546426000
1	-0.705597000	2.324442000	1.302274000
1	-2.386861000	2.782261000	0.912208000
1	-1.047193000	3.802177000	0.381903000
6	3.520551000	0.320402000	-1.137880000
1	3.631237000	-0.568971000	-1.761501000
1	3.305285000	1.179350000	-1.776724000
1	4.490364000	0.505417000	-0.665873000

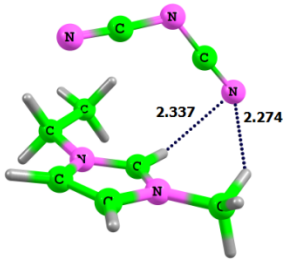
[4] 1-ethyl-3-methylimidazolium dicynamide([EMIm]⁺[dc]⁻)



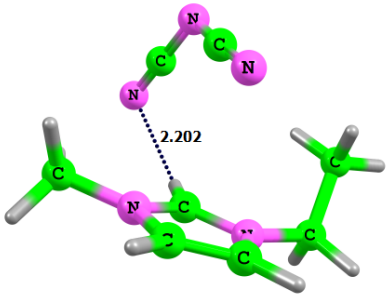
(a) E(RM06L) = -585.261586000



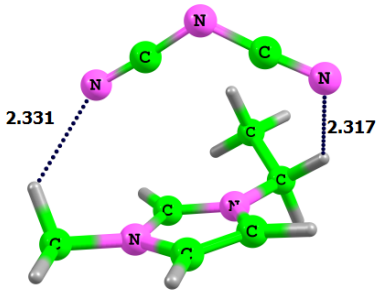
(b) E(RM06L) = -585.260586332



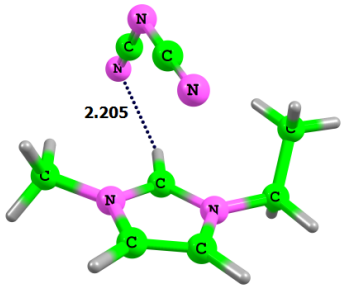
(c) E(RM06L) = -585.262732689



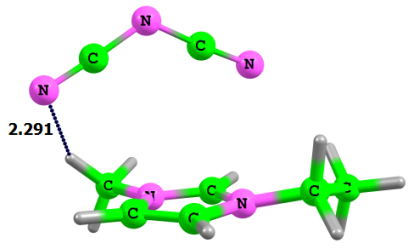
(d) E(RM06L) = -585.261118655



(e) E(RM06L) = -585.262576015



(f) E(RM06L) = -585.261225197



(g) E(RM06L) = -585.262072807

Fig. S6.Optimized conformers of 1-ethyl-3-methylimidazolium dicyanamide. All distance parameters in Å and energy in au.

Table S3. Relative energy of the a-g conformations.

Conformation	Rel. Energy (kJ/mol)
a	3.0078
b	5.6299
c	0.0000
d	4.2336
e	0.4110
f	3.9541
g	1.7309

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

a) E(RM06L) = -585.261586000

7	-0.169084000	-1.092132000	-0.229660000
6	1.068019000	-1.000840000	-0.717579000
6	-0.127319000	-0.824232000	1.121543000
6	1.174539000	-0.592578000	1.436365000
7	1.908731000	-0.730021000	0.279614000
1	1.340240000	-1.085435000	-1.755755000
1	1.639285000	-0.336944000	2.373113000
1	-1.023250000	-0.782184000	1.716266000
6	-1.379709000	-1.292269000	-1.047177000
1	-1.733300000	-0.300328000	-1.341382000
1	-1.055405000	-1.823753000	-1.945357000
6	-2.456304000	-2.038722000	-0.299170000
1	-2.839708000	-1.430485000	0.521936000
1	-2.097839000	-2.999102000	0.079372000
6	3.291177000	-0.316276000	0.095163000
1	3.827971000	-0.443198000	1.033508000
1	3.757515000	-0.933706000	-0.671449000
1	3.284571000	0.729873000	-0.220592000
7	-0.818200000	2.562411000	-0.035813000
6	-1.721679000	1.745850000	0.422359000
7	-2.569120000	1.048798000	0.851291000
6	0.271635000	2.105741000	-0.572187000
7	1.286137000	1.770273000	-1.072765000
1	-3.291487000	-2.230089000	-0.974230000

b) E(RM06L) = -585.260586332

7	1.179183000	0.571075000	0.489595000
6	-0.094885000	0.784012000	0.825600000
6	1.445721000	1.253841000	-0.672876000
6	0.306883000	1.904979000	-1.025712000
7	-0.644688000	1.594846000	-0.080911000
1	-0.639094000	0.321468000	1.636937000
1	0.083998000	2.531753000	-1.871752000
1	2.395511000	1.185221000	-1.171837000
6	2.052195000	-0.410586000	1.165350000

```
1        2.305431000     -0.003619000      2.149097000
1        1.442996000     -1.306429000      1.305545000
6        3.279028000     -0.736256000      0.353488000
1        3.930017000      0.131899000      0.221015000
1        2.987488000     -1.141676000     -0.617615000
6       -2.037889000      2.027203000     -0.080765000
1       -2.439809000      1.907000000     -1.086470000
1       -2.594438000      1.381473000      0.600496000
1       -2.104544000      3.073394000      0.220940000
7       -1.753425000     -1.969759000     -0.672238000
6       -0.499052000     -1.824713000     -0.998741000
7        0.620496000     -1.721579000     -1.349323000
6       -2.200836000     -1.368206000      0.388481000
7       -2.648880000     -0.812394000      1.327953000
1        3.856656000     -1.497457000      0.879160000

c)   E(RM06L) =  -585.262732689
7        0.060099000     -1.431714000     -0.249715000
6        0.696670000     -0.388524000     -0.783630000
6        0.776629000     -1.875824000      0.836409000
6        1.879960000     -1.091834000      0.937665000
7        1.809828000     -0.164654000     -0.079076000
1        0.354669000      0.238448000     -1.592229000
1        2.684974000     -1.088855000      1.652333000
1        0.410765000     -2.667406000      1.466829000
6       -1.283823000     -1.916799000     -0.608910000
1       -1.176119000     -2.951863000     -0.947949000
1       -1.849543000     -1.899988000      0.326374000
6       -1.948098000     -1.048210000     -1.646021000
1       -1.407929000     -1.041266000     -2.596268000
1       -2.052476000     -0.019557000     -1.291406000
6        2.753417000      0.913289000     -0.352721000
1        3.556151000      0.557399000     -1.000736000
1        2.201034000      1.730330000     -0.822964000
1        3.172822000      1.257226000      0.591289000
7       -1.429144000      2.106306000      0.798255000
6       -1.489535000      0.931493000      1.361759000
7       -1.599288000     -0.106501000      1.907131000
6       -0.624635000      2.295671000     -0.201910000
7        0.085924000      2.511139000     -1.119448000
1       -2.949801000     -1.432075000     -1.841148000

d)   E(RM06L) =  -585.261118655

7       -1.575428000      0.022099000     -0.462845000
6       -0.398316000      0.476221000     -0.898965000
6       -2.073307000      0.906656000      0.464675000
6       -1.177270000      1.920936000      0.571063000
7       -0.142893000      1.634466000     -0.288263000
1        0.285400000     -0.018287000     -1.580326000
1       -1.165810000      2.790197000      1.204795000
1       -2.996282000      0.721413000      0.986259000
6       -2.126944000     -1.300631000     -0.791945000
1       -3.152874000     -1.304743000     -0.418207000
1       -2.179102000     -1.375004000     -1.881380000
6       -1.297166000     -2.411864000     -0.185502000
1       -1.213115000     -2.290859000      0.895777000
1       -0.284680000     -2.418140000     -0.597401000
6        1.107125000      2.374639000     -0.407869000
1        1.578545000      2.423711000      0.574909000
1        1.764427000      1.834075000     -1.089240000
1        0.910922000      3.381053000     -0.778734000
7        2.245557000     -1.148929000      0.809000000
6        1.209292000     -0.733872000      1.486638000
7        0.292022000     -0.393889000      2.142793000
6        2.335325000     -0.814674000     -0.443440000
7        2.428895000     -0.523896000     -1.583255000
1       -1.756955000     -3.376849000     -0.406383000
```

e) E(RM06L) = -585.262576015

7	0.009508000	-1.287949000	-0.039028000
6	1.001954000	-0.755102000	0.675839000
6	0.318931000	-1.171124000	-1.376163000
6	1.534591000	-0.570053000	-1.450905000
7	1.951332000	-0.329744000	-0.159267000
1	1.019459000	-0.632368000	1.744336000
1	2.126973000	-0.273808000	-2.299138000
1	-0.377690000	-1.474520000	-2.138614000
6	-1.240262000	-1.867024000	0.487295000
1	-1.985389000	-1.685948000	-0.290546000
1	-1.087121000	-2.945530000	0.596441000
6	-1.663431000	-1.219278000	1.783417000
1	-1.766595000	-0.138556000	1.664222000
1	-0.965893000	-1.414978000	2.602060000
6	3.100695000	0.469484000	0.244796000
1	2.726578000	1.415554000	0.643582000
1	3.672879000	-0.061783000	1.005235000
1	3.731039000	0.635872000	-0.626056000
7	-1.414167000	2.175584000	-0.258298000
6	-1.904237000	1.147865000	-0.889177000
7	-2.391172000	0.257029000	-1.486094000
6	-0.381524000	2.046742000	0.515745000
7	0.550037000	2.000233000	1.238642000
1	-2.633302000	-1.619078000	2.081715000

f) E(RM06L) = -585.261225197

7	-1.593331000	0.048548000	-0.414281000
6	-0.415436000	0.445975000	-0.899592000
6	-2.032680000	0.980300000	0.496112000
6	-1.098927000	1.964384000	0.543727000
7	-0.100827000	1.613158000	-0.334032000
1	0.230795000	-0.093287000	-1.582549000
1	-1.038161000	2.851162000	1.150015000
1	-2.943607000	0.842869000	1.052351000
6	-2.205930000	-1.258821000	-0.697039000
1	-3.157871000	-1.269002000	-0.163086000
1	-2.432991000	-1.297404000	-1.766317000
6	-1.305190000	-2.396002000	-0.265150000
1	-1.067228000	-2.318249000	0.797115000
1	-0.363811000	-2.391123000	-0.821078000
6	1.168534000	2.307118000	-0.513705000
1	1.667856000	2.376928000	0.453917000
1	1.790237000	1.719899000	-1.189771000
1	0.994099000	3.304931000	-0.917035000
7	2.284075000	-1.032643000	0.867567000
6	1.201776000	-0.703607000	1.519865000
7	0.252176000	-0.423711000	2.158122000
6	2.309906000	-0.850156000	-0.418365000
7	2.356326000	-0.678516000	-1.585017000
1	-1.800579000	-3.349718000	-0.455186000

g) E(RM06L) = -585.262072807

7	-1.380898000	-0.590982000	-0.472743000
6	-0.768543000	-0.735610000	0.700882000
6	-0.558715000	-1.102455000	-1.456550000
6	0.557884000	-1.575936000	-0.847217000
7	0.400923000	-1.347225000	0.503335000
1	-1.130851000	-0.375493000	1.646951000
1	1.467680000	-1.995490000	-1.240887000
1	-0.833251000	-1.062655000	-2.496590000
6	-2.579707000	0.226334000	-0.716306000
1	-2.222175000	1.179238000	-1.116851000
1	-3.157787000	-0.290755000	-1.487176000
6	-3.383837000	0.461434000	0.536874000
1	-2.817860000	1.075458000	1.240051000
1	-3.684629000	-0.475324000	1.013964000
6	1.390137000	-1.650425000	1.530105000

1	2.368777000	-1.356806000	1.144182000
1	1.160478000	-1.066534000	2.419902000
1	1.368830000	-2.714436000	1.770607000
7	1.835808000	2.024595000	-0.252656000
6	2.511518000	0.923039000	-0.398669000
7	3.165370000	-0.043983000	-0.556255000
6	0.637265000	2.007626000	0.241715000
7	-0.458971000	2.064519000	0.675373000
1	-4.290857000	1.010285000	0.281468000

[5] 1-ethyl-3-methylimidazolium 1,2,4-triazolate([EMIm]$^+$[trz]$^-$)

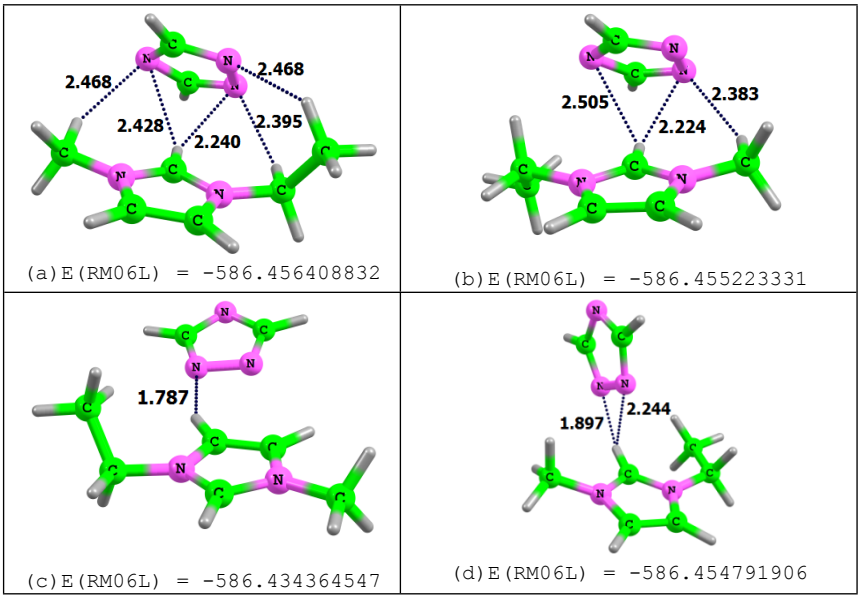


Fig. S7.Optimized conformers of 1-ethyl-3-methylimidazolium 1,2,4-triazolate. All distance parameters in Å and energy in au.

Table S4. Relative energy of the a-d conformations

Conformation	Rel. Energy (kJ/mol)
a	0.0000
b	3.1096
c	57.8220
d	4.2412

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

a)	E(RM06L) =	-586.456408832	
6	2.622351000	-0.303155000	-0.781490000
7	2.640952000	0.706196000	0.118058000
7	1.914733000	-1.377283000	-0.404553000
7	1.434677000	-1.071297000	0.841084000
6	1.897852000	0.157644000	1.101762000
1	1.691004000	0.664701000	2.039736000
7	-0.840599000	1.686132000	-0.144493000
6	-0.425335000	0.494801000	-0.583426000
6	-2.131382000	1.557132000	0.326974000
6	-2.489339000	0.258730000	0.148174000
7	-1.415825000	-0.383252000	-0.431428000
1	0.541862000	0.280146000	-1.026305000
6	0.004739000	2.871797000	-0.086968000
1	-0.287539000	3.585452000	-0.858920000

```
1       -0.096809000      3.334161000      0.894680000
1        1.041664000      2.554723000     -0.222487000
6       -1.290112000     -1.827415000     -0.704731000
1       -2.045393000     -2.082762000     -1.454621000
1       -0.291653000     -1.959673000     -1.130882000
6       -1.425697000     -2.642032000      0.562004000
1       -2.400534000     -2.506831000      1.039569000
1       -0.625569000     -2.366008000      1.252530000
1       -1.319289000     -3.700705000      0.318985000
1        3.149092000     -0.261614000     -1.728804000
1       -2.670173000      2.389655000      0.746675000
1       -3.402687000     -0.259730000      0.385372000

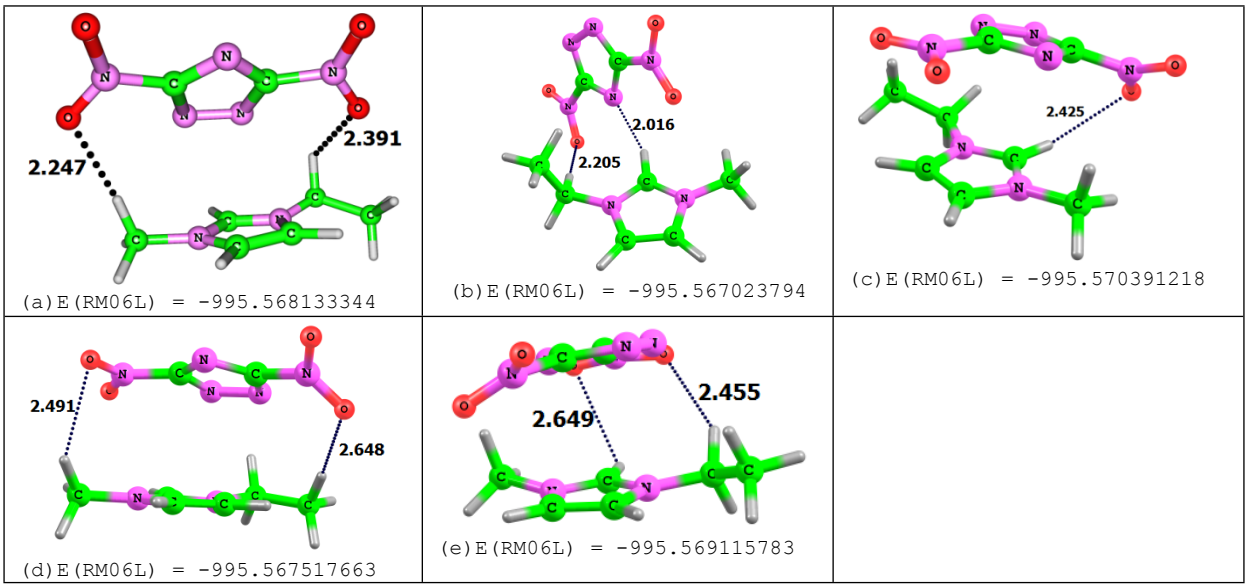
b)  E(RM06L) =  -586.455223331
6        2.514176000      0.315654000     -0.576206000
7        2.136683000      1.044424000      0.497135000
7        2.290285000     -1.002278000     -0.467679000
7        1.736142000     -1.171108000      0.772542000
6        1.674099000      0.059515000      1.296525000
1        1.290640000      0.240115000      2.296764000
7       -1.157008000     -1.377658000     -0.333440000
6       -0.586970000     -0.178433000     -0.454602000
6       -2.343529000     -1.236302000      0.351864000
6       -2.488023000      0.086645000      0.628227000
7       -1.389047000      0.732802000      0.102057000
1        0.365534000      0.007708000     -0.940083000
6       -0.516192000     -2.627072000     -0.731132000
1       -1.138890000     -3.142148000     -1.464391000
1        0.470075000     -2.389054000     -1.132700000
1       -0.371272000     -3.245587000      0.153862000
6       -1.031471000      2.149487000      0.285978000
1       -1.943145000      2.651456000      0.618246000
1       -0.290648000      2.192405000      1.090864000
6       -0.469756000      2.764766000     -0.973614000
1       -1.165208000      2.678993000     -1.812047000
1        0.483538000      2.300747000     -1.234766000
1       -0.271235000      3.823132000     -0.799536000
1        2.978583000      0.751544000     -1.454951000
1       -2.973010000     -2.079415000      0.579834000
1       -3.268344000      0.621262000      1.142353000

c)  E(RM06L) =  -586.434364547
6        3.293081000     -1.412989000      0.195232000
7        4.246095000     -0.460880000      0.159329000
7        2.051827000     -0.982533000     -0.027580000
7        2.188997000      0.373443000     -0.229906000
6        3.495927000      0.619610000     -0.108940000
1        3.907093000      1.616836000     -0.221838000
7       -2.383115000     -1.198066000      0.015355000
6       -2.783652000      0.080222000      0.015234000
6       -1.023443000     -1.233369000     -0.225246000
6       -0.601424000      0.049838000     -0.382443000
7       -1.714687000      0.845791000     -0.226080000
1       -3.790657000      0.423459000      0.186777000
6       -3.230744000     -2.350477000      0.266456000
1       -3.198383000     -3.028213000     -0.586867000
1       -2.884279000     -2.878532000      1.155347000
1       -4.256372000     -2.021255000      0.422929000
6       -1.684616000      2.313505000     -0.291961000
1       -1.519674000      2.590284000     -1.337384000
1       -2.679972000      2.668390000     -0.012120000
6       -0.601377000      2.876667000      0.602300000
1        0.381836000      2.478138000      0.336314000
1       -0.790509000      2.634845000      1.650115000
1       -0.571040000      3.962540000      0.501778000
1        3.511626000     -2.457236000      0.390850000
1       -0.441726000     -2.139977000     -0.236963000
1        0.425720000      0.448398000     -0.510555000
```

d) E(RM06L) = -586.454791906

6	-2.486277000	-0.101457000	1.297732000
7	-3.618937000	-0.014769000	0.578148000
7	-1.362251000	-0.006632000	0.583617000
7	-1.782060000	0.155005000	-0.718319000
6	-3.114860000	0.143694000	-0.657793000
1	-3.732384000	0.255618000	-1.541684000
7	1.263555000	-1.434600000	-0.372383000
6	0.952085000	-0.150820000	-0.575565000
6	2.340265000	-1.505494000	0.487925000
6	2.703683000	-0.229810000	0.771438000
7	1.835834000	0.599932000	0.086011000
1	0.067763000	0.174759000	-1.136687000
6	0.378861000	-2.526313000	-0.747506000
1	0.955328000	-3.446119000	-0.837235000
1	-0.401894000	-2.627032000	0.009609000
1	-0.096389000	-2.290568000	-1.697679000
6	1.729702000	2.054054000	0.263411000
1	1.421545000	2.221952000	1.300454000
1	2.734267000	2.470613000	0.141949000
6	0.738662000	2.673389000	-0.690880000
1	-0.260896000	2.253969000	-0.548651000
1	1.034526000	2.522606000	-1.732163000
1	0.689333000	3.747772000	-0.509994000
1	-2.474349000	-0.232945000	2.373834000
1	2.756571000	-2.446765000	0.804710000
1	3.500874000	0.160130000	1.381438000

[6] 1-ethyl-3-methylimidazolium 3,5-dinitro 1,2,4-triazolate([EMIm]$^+$[dtrz]$^-$)



(a)E(RM06L) = -995.568133344

(b)E(RM06L) = -995.567023794

(c)E(RM06L) = -995.570391218

(d)E(RM06L) = -995.567517663

(e)E(RM06L) = -995.569115783

Fig. S8.Optimized conformers of 1-ethyl-3-methylimidazolium 3,5-dinitro 1,2,4-triazolate. All distance parameters in Å and energy in au.

Table S5. Relative energy of the a-e conformations

Conformation	Rel. Energy (kJ/mol)
a	5.9224
b	8.8327
c	0.0000
d	7.5373
e	3.3455

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

a) E(RM06L) = -995.568133344

6	-2.029898000	0.501371000	-0.304719000
7	-1.588532000	1.648557000	0.207226000
7	-1.154922000	-0.213963000	-1.033732000
7	-0.025138000	0.508623000	-0.995905000
6	-0.339089000	1.580294000	-0.247019000
7	0.325115000	-2.336513000	0.342622000
6	1.246238000	-2.038825000	-0.572245000
6	0.585594000	-1.596317000	1.471568000
6	1.702858000	-0.860470000	1.220270000
7	2.112667000	-1.168346000	-0.054297000
1	1.256351000	-2.403215000	-1.585595000
6	-0.862977000	-3.151335000	0.113151000
1	-0.670686000	-3.829747000	-0.715926000
1	-1.074585000	-3.731768000	1.010271000
1	-1.703334000	-2.496890000	-0.136461000
6	3.130249000	-0.455949000	-0.846711000
1	3.483415000	-1.164837000	-1.599998000
1	2.595314000	0.357556000	-1.345495000
6	4.261115000	0.065441000	0.003085000
1	4.746180000	-0.727926000	0.577106000
1	3.919401000	0.847949000	0.682336000
1	5.012394000	0.518240000	-0.644999000
1	-0.041198000	-1.656589000	2.345145000
1	2.230503000	-0.148373000	1.830585000
7	-3.366234000	-0.004993000	-0.048613000
8	-3.543978000	-1.211954000	-0.233870000
8	-4.214058000	0.777751000	0.342415000
7	0.672245000	2.554653000	0.107169000
8	1.850975000	2.194952000	-0.008417000
8	0.313974000	3.646026000	0.510805000

b) E(RM06L) = -995.567023794

6	-1.340907000	1.500011000	0.166125000
7	-1.103038000	0.318235000	-0.411099000
7	-2.599125000	1.716350000	0.582120000
7	-3.259815000	0.599691000	0.254358000
6	-2.335073000	-0.185556000	-0.323273000
7	-0.281369000	2.463281000	0.350023000
8	-0.540144000	3.520109000	0.895843000
8	0.846572000	2.139134000	-0.056364000
7	-2.628721000	-1.521447000	-0.796793000
8	-3.793085000	-1.876536000	-0.838246000
8	-1.662224000	-2.223059000	-1.121079000
7	1.905746000	-1.389567000	0.390683000
6	1.717019000	-0.517549000	-0.600199000
6	3.232802000	-1.363354000	0.762656000
6	3.851620000	-0.456966000	-0.038169000
7	2.888358000	0.057885000	-0.879812000
1	0.736105000	-0.262341000	-0.997169000
1	4.879193000	-0.139008000	-0.086176000
1	3.616486000	-1.991951000	1.548618000
6	3.075875000	1.127788000	-1.848425000
1	3.384863000	2.036388000	-1.332222000
1	3.826520000	0.836668000	-2.583808000
1	2.125674000	1.319297000	-2.340527000
6	0.818626000	-2.135572000	1.047361000
1	0.012376000	-2.214851000	0.314029000
1	1.195855000	-3.141938000	1.245512000
6	0.358314000	-1.440445000	2.311001000
1	0.004517000	-0.430554000	2.091850000
1	1.155406000	-1.373885000	3.055736000
1	-0.469854000	-1.996143000	2.754107000

c) E(RM06L) = -995.570391218

6	1.541343000	0.393757000	-0.962142000
7	1.047273000	1.382310000	-0.219442000

```
7        0.705752000     -0.180646000     -1.846602000
7       -0.443379000      0.494973000     -1.698382000
6       -0.191597000      1.383533000     -0.722183000
7        0.215921000     -0.772921000      1.830296000
6        0.056423000     -1.553886000      0.757716000
6       -1.003818000     -0.226610000      2.161027000
6       -1.911383000     -0.708053000      1.269667000
7       -1.229758000     -1.531755000      0.401677000
1        0.853030000     -2.052822000      0.221812000
6        1.499846000     -0.391792000      2.409079000
1        2.259893000     -1.102412000      2.087507000
1        1.759406000      0.609011000      2.054695000
1        1.425896000     -0.406929000      3.495674000
6       -1.769502000     -2.204312000     -0.800343000
1       -0.975959000     -2.144294000     -1.549089000
1       -1.931522000     -3.256141000     -0.544740000
6       -3.028809000     -1.539533000     -1.297866000
1       -2.852711000     -0.478270000     -1.486874000
1       -3.863195000     -1.657732000     -0.601676000
1       -3.323569000     -2.006571000     -2.238336000
1       -1.110749000      0.477968000      2.968233000
1       -2.960584000     -0.498341000      1.155538000
7        2.847194000     -0.171127000     -0.676318000
8        2.951727000     -1.394596000     -0.800369000
8        3.727144000      0.572984000     -0.274130000
7       -1.263060000      2.145637000     -0.111052000
8       -2.394876000      1.984595000     -0.560788000
8       -0.983315000      2.841094000      0.858575000

d) E(RM06L) =  -995.567517663
6        0.364365000     -1.364699000     -0.757928000
7       -0.553796000     -1.906325000      0.049140000
7       -0.036019000     -0.329210000     -1.516798000
7       -1.320351000     -0.147468000     -1.181326000
6       -1.563575000     -1.102660000     -0.264505000
7        1.994072000      0.894228000      0.970684000
6        1.663101000      1.689248000     -0.049557000
6        0.875952000      0.704349000      1.753359000
6       -0.135014000      1.415242000      1.184132000
7        0.381235000      2.035097000      0.070095000
1        2.311537000      1.952981000     -0.868394000
6        3.310951000      0.312657000      1.209349000
1        3.949832000      0.524396000      0.355762000
1        3.741805000      0.738823000      2.116384000
1        3.217728000     -0.769089000      1.311059000
6       -0.381598000      2.760813000     -0.970054000
1        0.190552000      3.663021000     -1.204027000
1       -0.385909000      2.104359000     -1.844510000
6       -1.786745000      3.078958000     -0.529342000
1       -1.807494000      3.696177000      0.372702000
1       -2.362242000      2.164365000     -0.367193000
1       -2.282758000      3.638338000     -1.323242000
1        0.892967000      0.066302000      2.620533000
1       -1.174655000      1.500719000      1.453316000
7        1.759844000     -1.731292000     -0.694155000
8        2.550095000     -1.074099000     -1.376532000
8        2.090276000     -2.620526000      0.083217000
7       -2.838237000     -1.148084000      0.431987000
8       -3.451675000     -0.082947000      0.514226000
8       -3.199100000     -2.211488000      0.906276000

e) E(RM06L) =  -995.569115783
6       -1.635089000      0.214722000     -0.882667000
7       -0.844496000     -0.848463000     -1.002019000
7       -1.114230000      1.402451000     -1.247380000
7        0.128182000      1.109833000     -1.654841000
6        0.223032000     -0.224157000     -1.508924000
7        0.536347000     -1.311863000      1.666769000
6        1.570802000     -0.613611000      1.194443000
6       -0.424223000     -0.429671000      2.100041000
6        0.055364000      0.824241000      1.878013000
```

7	1.300401000	0.689936000	1.306979000
1	2.456776000	-1.033843000	0.744392000
6	0.327899000	-2.741884000	1.465541000
1	1.284051000	-3.214877000	1.251943000
1	-0.112339000	-3.173069000	2.363541000
1	-0.336651000	-2.863713000	0.607090000
6	2.162606000	1.771587000	0.772197000
1	3.060171000	1.811260000	1.396300000
1	2.449540000	1.455986000	-0.235511000
6	1.447632000	3.097815000	0.726965000
1	1.186849000	3.464290000	1.723244000
1	0.549784000	3.038327000	0.107634000
1	2.111650000	3.833930000	0.272882000
1	-1.379782000	-0.767290000	2.464133000
1	-0.396550000	1.786825000	2.041323000
7	-2.929651000	0.126204000	-0.232969000
8	-3.721962000	1.036719000	-0.415248000
8	-3.120101000	-0.848018000	0.496822000
7	1.471886000	-0.917528000	-1.704442000
8	2.459611000	-0.247966000	-2.003220000
8	1.497364000	-2.126495000	-1.470268000

[7] 1-ethyl-3-methylimidazolium dinitramine([EMIm]$^+$[dn]$^-$)

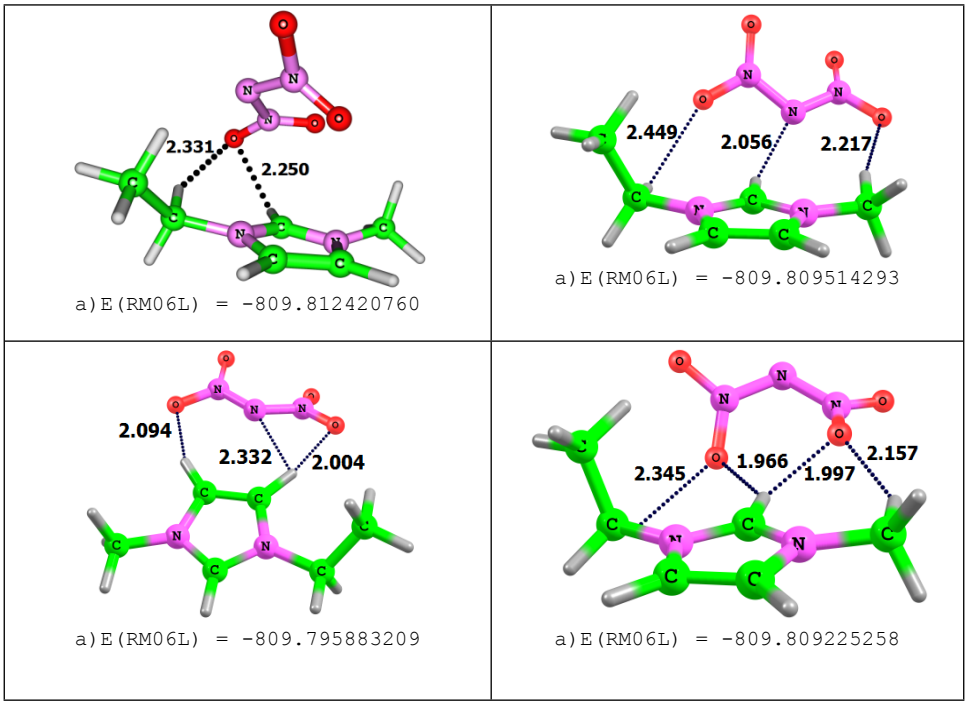


Fig. S9.Optimized conformers of 1-ethyl-3-methylimidazolium dinitramine. All distance parameters in Å and energy in au.

Table S6. Relative energy of the a-d conformations.

Conformation	Rel. Energy (kJ/mol)
a	0.0000
b	7.6236
c	43.3779
d	8.3818

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

a) E(RM06L) = -809.812420760

7	-0.919987000	1.301223000	-0.404370000
6	-1.239071000	0.101973000	-0.892329000
6	-1.583781000	1.475276000	0.789977000
6	-2.300533000	0.343741000	1.016347000
7	-2.078861000	-0.497202000	-0.047212000
1	-2.909497000	0.050260000	1.853746000
1	-1.472370000	2.365236000	1.383748000
6	0.041655000	2.227580000	-1.037657000
1	0.648590000	1.605994000	-1.702152000
1	-0.529800000	2.939595000	-1.641678000
6	0.907889000	2.925183000	-0.016446000
1	1.456157000	2.202124000	0.589909000
1	0.336196000	3.590235000	0.635681000
6	-2.394392000	-1.918376000	-0.083400000
1	-1.619954000	-2.451841000	0.470559000
1	-3.375939000	-2.080718000	0.359394000
1	-2.393124000	-2.261074000	-1.115922000
1	1.641752000	3.539408000	-0.540093000
1	-0.838142000	-0.325086000	-1.799929000
7	1.891405000	-0.320922000	-0.058494000
7	1.451456000	-0.606841000	1.244868000
8	0.292307000	-0.962580000	1.479062000
8	2.265261000	-0.311663000	2.108240000
7	1.280296000	-1.062762000	-1.022704000
8	0.710076000	-2.138827000	-0.815651000
8	1.369275000	-0.562039000	-2.163754000

b) E(RM06L) = -809.809514293

7	2.314106000	-0.058144000	-0.377015000
6	1.158488000	0.587179000	-0.546391000
6	3.169327000	0.744825000	0.346791000
6	2.501676000	1.898731000	0.611478000
7	1.248606000	1.778123000	0.050346000
1	2.801605000	2.783440000	1.147022000
1	4.164362000	0.428116000	0.609933000
6	2.570563000	-1.443720000	-0.804106000
1	1.724272000	-1.728723000	-1.429266000
1	3.472754000	-1.430162000	-1.422488000
6	2.700067000	-2.374643000	0.380314000
1	1.772385000	-2.386226000	0.953813000
1	3.528852000	-2.090609000	1.034008000
6	0.169698000	2.762654000	0.099025000
1	0.151633000	3.212923000	1.090754000
1	0.342046000	3.538352000	-0.648409000
1	-0.784871000	2.262018000	-0.086148000
1	2.888110000	-3.389326000	0.026209000
1	0.254696000	0.184918000	-0.989005000
7	-1.659479000	-0.099250000	-0.293455000
7	-1.494158000	-1.387841000	0.162057000
8	-2.257371000	-1.959666000	0.918127000
8	-0.397771000	-1.868700000	-0.213814000
7	-2.941146000	0.438607000	-0.147151000
8	-3.948777000	-0.241225000	-0.123650000
8	-2.922363000	1.677675000	-0.152234000

c) E(RM06L) = -809.795883209

7	-2.379656000	-0.460485000	-0.164996000
6	-3.001945000	0.720973000	-0.215438000
6	-1.027578000	-0.250034000	-0.002655000
6	-0.836433000	1.097289000	0.045240000
7	-2.078704000	1.682053000	-0.089875000
1	0.089897000	1.657416000	0.153201000
1	-0.299391000	-1.054616000	0.070199000
6	-3.012688000	-1.778022000	-0.325684000
1	-4.090494000	-1.625812000	-0.229530000
1	-2.819112000	-2.111897000	-1.349444000
6	-2.491972000	-2.777869000	0.681689000

1	-2.680404000	-2.446642000	1.704751000
1	-1.419200000	-2.944458000	0.566707000
6	-2.338145000	3.112606000	-0.059767000
1	-2.142014000	3.505599000	0.938165000
1	-1.685141000	3.614049000	-0.773099000
1	-3.376710000	3.299912000	-0.326230000
1	-2.993793000	-3.735166000	0.535077000
1	-4.061719000	0.874533000	-0.336258000
7	1.797095000	-0.053241000	0.268680000
7	2.713877000	0.987808000	0.196417000
8	3.921961000	0.848933000	0.209708000
8	2.137337000	2.095448000	0.207952000
7	2.236805000	-1.290163000	-0.153509000
8	3.288296000	-1.505653000	-0.728456000
8	1.365498000	-2.169276000	0.049437000

d) E(RM06L) = -809.809225258

7	2.105778000	0.572869000	0.343896000
6	1.245873000	-0.449692000	0.330154000
6	3.342233000	0.122354000	-0.063069000
6	3.219519000	-1.207075000	-0.316921000
7	1.905686000	-1.541802000	-0.069286000
1	3.941141000	-1.936097000	-0.644628000
1	4.191841000	0.780844000	-0.132087000
6	1.748941000	1.974392000	0.638705000
1	0.944117000	1.947940000	1.372754000
1	2.632221000	2.424036000	1.099453000
6	1.307713000	2.711270000	-0.605476000
1	0.396853000	2.268645000	-1.012854000
1	2.086432000	2.716266000	-1.372684000
6	1.313030000	-2.868431000	-0.208611000
1	1.514654000	-3.247577000	-1.210326000
1	1.745858000	-3.543364000	0.530725000
1	0.236965000	-2.784134000	-0.062292000
1	1.072147000	3.745430000	-0.350393000
1	0.178084000	-0.390820000	0.540096000
7	-3.020397000	0.242316000	-0.234380000
7	-2.060767000	1.191807000	-0.008336000
8	-1.145267000	1.033968000	0.828774000
8	-2.235697000	2.253748000	-0.599147000
7	-2.601776000	-1.047692000	-0.001830000
8	-1.407573000	-1.391289000	-0.148433000
8	-3.499443000	-1.846498000	0.216691000

[8] 1-ethyl-3-methylimidazolium 5-cyano tetrazolate([EMIm]⁺[CNtz]⁻)

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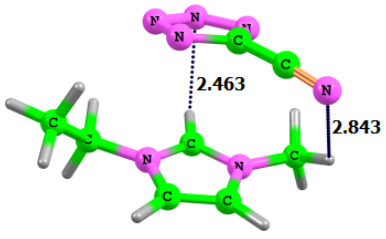
<td> 

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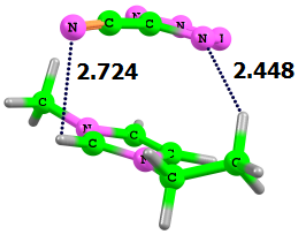
<td> 

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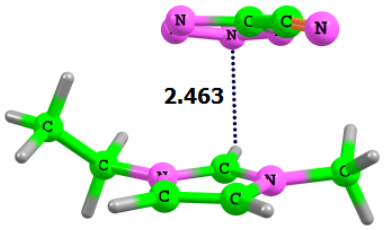
<td> 

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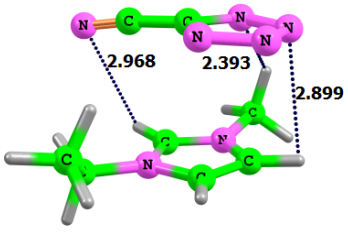
<td> 
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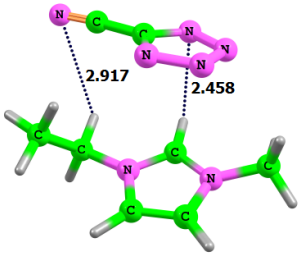
<td> 
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d)E(RM06L) = -694.748861957	e)E(RM06L) = -694.749384563	

Fig. S10.Optimized conformers of 1-ethyl-3-methylimidazolium 5-cyano tetrazolate. All distance parameters in Å and energy in au.

Table S7. Relative energy of the a-e conformations.

Conformation	Rel. Energy (kJ/mol)
a	10.0735
b	11.0458
c	0.0000
d	9.3461
e	7.9753

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

a) E(RM06L) = -694.748584643

7	0.646284000	-0.968398000	1.609885000
7	1.650041000	-1.195697000	0.757864000
7	0.427744000	0.337615000	1.717494000
7	1.281292000	1.008116000	0.939594000
6	2.022818000	0.038805000	0.370523000
7	-1.446096000	0.625788000	-0.652462000
6	-0.710485000	-0.420050000	-1.028910000
6	-2.502892000	0.165311000	0.097327000
6	-2.389808000	-1.187023000	0.160760000
7	-1.270704000	-1.534736000	-0.557710000
1	0.212103000	-0.371114000	-1.584510000
1	-2.984180000	-1.923962000	0.672656000
1	-3.220753000	0.831935000	0.540708000
6	-0.659337000	-2.857896000	-0.584400000
1	0.076183000	-2.894341000	-1.385044000
1	-0.150418000	-3.020479000	0.367648000
1	-1.432421000	-3.605777000	-0.757183000
6	-1.099022000	2.037152000	-0.909096000
1	-0.039002000	2.039280000	-1.169138000
1	-1.672706000	2.369571000	-1.780059000
6	-1.347452000	2.901380000	0.304556000
1	-0.815268000	2.501523000	1.169360000
1	-2.411781000	2.988980000	0.537289000
1	-0.975000000	3.907075000	0.105466000
6	3.009984000	0.288950000	-0.611780000
7	3.778638000	0.495530000	-1.459105000

b) E(RM06L) = -694.748213968

7	0.820862000	-2.246781000	-0.909405000
7	0.247204000	-1.946051000	0.256662000
7	1.940756000	-1.549233000	-1.059989000
7	2.139090000	-0.766585000	0.002561000
6	1.084974000	-1.040520000	0.796882000
7	-1.479341000	0.748557000	-0.281276000
6	-0.631285000	1.628435000	0.254291000
6	-0.956778000	0.310877000	-1.479462000
6	0.228947000	0.948299000	-1.654798000
7	0.412885000	1.769049000	-0.564305000
1	-0.729487000	2.082094000	1.226719000
1	0.982712000	0.836015000	-2.414714000
1	-1.431536000	-0.454746000	-2.066951000
6	1.657867000	2.453450000	-0.239296000
1	1.518013000	3.033090000	0.671054000
1	2.425715000	1.690572000	-0.082325000
1	1.937795000	3.115565000	-1.058269000
6	-2.710523000	0.269346000	0.375989000
1	-2.522452000	0.339459000	1.450368000
1	-3.516929000	0.968454000	0.132278000
6	-3.048602000	-1.147002000	-0.024347000

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1       -2.194513000     -1.808942000      0.140593000
1       -3.354942000     -1.211485000     -1.070966000
1       -3.887699000     -1.495102000      0.579374000
6        0.805572000     -0.334458000      1.986176000
7        0.517442000      0.330253000      2.898642000

c) E(RM06L) =  -694.752425116
7        0.306346000      2.127524000     -1.263152000
7        1.446030000      1.573200000     -0.846456000
7       -0.573619000      2.158024000     -0.265427000
7       -0.038819000      1.623348000      0.834593000
6        1.202663000      1.279602000      0.446943000
7       -1.436535000     -0.909623000     -0.277143000
6       -0.415918000     -0.792113000     -1.125530000
6       -1.061176000     -1.751992000      0.744994000
6        0.215377000     -2.144583000      0.492655000
7        0.599679000     -1.538402000     -0.680989000
1       -0.381686000     -0.127408000     -1.975275000
1        0.895632000     -2.756819000      1.059949000
1       -1.712124000     -1.973163000      1.572070000
6        1.925665000     -1.598908000     -1.289023000
1        2.147003000     -0.623571000     -1.724726000
1        2.652527000     -1.800133000     -0.503918000
1        1.960169000     -2.384765000     -2.044832000
6       -2.708838000     -0.168938000     -0.390333000
1       -2.513962000      0.645704000     -1.090258000
1       -3.447056000     -0.846189000     -0.831651000
6       -3.159629000      0.381389000      0.941574000
1       -2.375136000      1.001265000      1.379098000
1       -3.435553000     -0.408908000      1.644539000
1       -4.043886000      1.001052000      0.786617000
6        2.094969000      0.523210000      1.240892000
7        2.796261000     -0.190224000      1.835054000

d) E(RM06L) =  -694.748861957
7        1.467913000     -1.820387000     -1.290587000
7        0.364752000     -2.013272000     -0.570306000
7        2.362537000     -1.138202000     -0.581915000
7        1.873688000     -0.864415000      0.629762000
6        0.647143000     -1.420385000      0.607116000
7       -1.268548000      1.001296000     -0.331513000
6       -0.503010000      1.609458000      0.577310000
6       -0.525867000      0.823276000     -1.477272000
6        0.705117000      1.348213000     -1.243380000
7        0.696158000      1.843134000      0.040866000
1       -0.790792000      1.820760000      1.593916000
1        1.595779000      1.354194000     -1.847429000
1       -0.908700000      0.295494000     -2.332808000
6        1.875492000      2.298207000      0.765841000
1        2.485505000      1.420219000      0.993616000
1        2.427493000      3.005474000      0.148267000
1        1.561967000      2.786993000      1.686489000
6       -2.643856000      0.523070000     -0.089132000
1       -2.725985000      0.393770000      0.992109000
1       -3.334204000      1.314881000     -0.396985000
6       -2.915857000     -0.777362000     -0.808368000
1       -2.139223000     -1.516568000     -0.597673000
1       -2.976411000     -0.642905000     -1.890973000
1       -3.875646000     -1.174049000     -0.475533000
6       -0.301280000     -1.248626000      1.637720000
7       -1.117511000     -1.007207000      2.433406000

e) E(RM06L) =  -694.749384563
7       -0.079906000     -2.434447000      0.002858000
7        1.044639000     -2.110120000     -0.634914000
7       -0.194319000     -1.718073000      1.121381000
7        0.851903000     -0.902866000      1.249388000
6        1.598676000     -1.173909000      0.159552000
7       -0.624454000      1.448463000     -0.405028000
6       -1.030798000      0.269057000     -0.874839000
6       -1.572076000      1.918126000      0.475328000
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6	-2.567671000	0.994605000	0.519235000
7	-2.216821000	-0.021575000	-0.337225000
1	-0.461577000	-0.382804000	-1.522280000
1	-3.479882000	0.965148000	1.089910000
1	-1.455547000	2.854896000	0.991893000
6	-2.908891000	-1.299312000	-0.460473000
1	-2.699685000	-1.894621000	0.429369000
1	-3.977212000	-1.116176000	-0.575377000
1	-2.520257000	-1.832953000	-1.324060000
6	0.670719000	2.083576000	-0.712373000
1	1.237050000	1.355626000	-1.296702000
1	0.473920000	2.945218000	-1.357586000
6	1.414117000	2.469479000	0.546123000
1	1.489698000	1.616280000	1.223695000
1	0.926547000	3.295863000	1.069153000
1	2.423950000	2.786036000	0.282895000
6	2.795966000	-0.487897000	-0.151678000
7	3.739350000	0.133637000	-0.427339000

[9] 1-ethyl-3-methylimidazolium 5-amino tetrazolate([EMIm]$^+$[NH$_2$tz]$^-$)

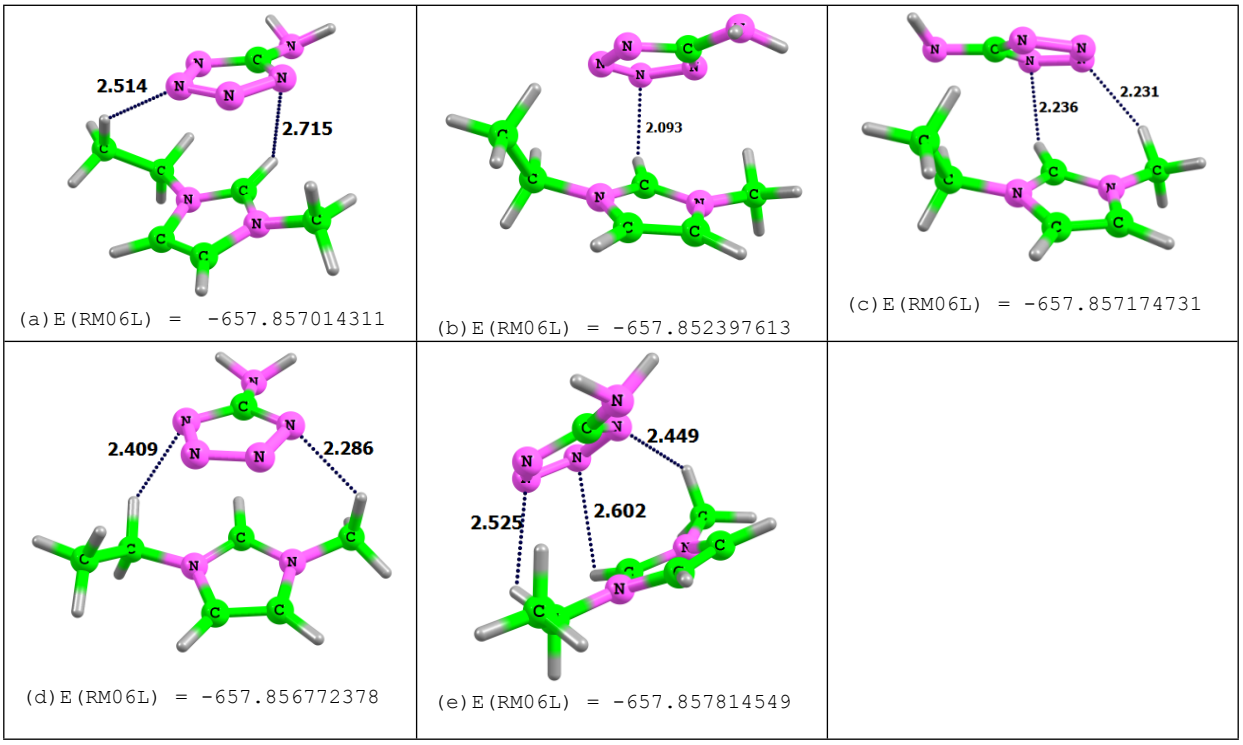

Fig. S11.Optimized conformers of 1-ethyl-3-methylimidazolium 5-amino tetrazolate. All distance parameters in Å and energy in au.

Table S8. Relative energy of the a-e conformations.

Conformation	Rel. Energy (kJ/mol)
a	2.0990
b	14.2086
c	1.6782
d	2.7336
e	0.0000

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

(a)E(RM06L) = -657.857014311

7	-1.226284000	0.632034000	1.460436000
7	-2.100576000	0.710169000	0.423083000
7	-0.746555000	-0.585918000	1.548139000
7	-1.285107000	-1.363938000	0.573104000
6	-2.101753000	-0.529447000	-0.073978000
7	1.481553000	-0.319175000	-0.557533000
6	0.552608000	0.550387000	-0.956267000
6	2.351077000	0.327802000	0.289460000
6	1.927126000	1.613517000	0.391069000
7	0.809004000	1.735376000	-0.400225000
1	-0.302235000	0.318229000	-1.572635000
1	2.299585000	2.438619000	0.973253000
1	3.169976000	-0.182502000	0.764396000
6	-0.084250000	2.885805000	-0.424697000
1	-0.772138000	2.783820000	-1.260781000
1	-0.665204000	2.885486000	0.499216000
1	0.507183000	3.795478000	-0.531770000
6	1.481318000	-1.757044000	-0.877946000
1	0.491152000	-1.967063000	-1.285274000
1	2.229535000	-1.927590000	-1.659305000
6	1.731309000	-2.595561000	0.353541000
1	1.009631000	-2.335853000	1.130279000
1	2.747306000	-2.470490000	0.737352000
1	1.606337000	-3.649329000	0.099613000
7	-2.767253000	-0.877337000	-1.256299000
1	-3.604502000	-0.320923000	-1.377908000
1	-3.014705000	-1.859123000	-1.258456000

(b)E(RM06L) = -657.852397613

7	-1.455448000	-1.353886000	-1.387706000
7	-2.239294000	-0.553476000	-0.620270000
7	-0.575272000	-1.970036000	-0.628024000
7	-0.744873000	-1.605799000	0.665291000
6	-1.777849000	-0.756614000	0.619106000
7	1.638491000	0.341150000	-0.301348000
6	0.512961000	0.715757000	-0.907678000
6	1.930837000	1.250883000	0.689047000
6	0.952363000	2.194551000	0.667065000
7	0.076476000	1.841409000	-0.336112000
1	-0.016708000	0.141478000	-1.662007000
1	0.797304000	3.070599000	1.273940000
1	2.792590000	1.146562000	1.325451000
6	-1.174007000	2.504405000	-0.689757000
1	-1.895068000	1.729136000	-0.967804000
1	-1.537945000	3.047626000	0.181121000
1	-1.014721000	3.204185000	-1.511588000
6	2.372033000	-0.907964000	-0.586458000
1	1.759177000	-1.448320000	-1.310165000
1	3.324049000	-0.628120000	-1.049212000
6	2.552592000	-1.739217000	0.662590000
1	1.575698000	-1.971615000	1.093473000
1	3.174927000	-1.235445000	1.407867000
1	3.049455000	-2.674291000	0.399106000
7	-2.359868000	-0.200259000	1.752737000
1	-2.888961000	0.638574000	1.563332000
1	-1.714864000	-0.084900000	2.521013000

(c)E(RM06L)= -657.857174731

7	0.989820000	-2.163397000	0.188967000
7	1.897509000	-1.581441000	-0.634010000
7	0.744548000	-1.378460000	1.216280000
7	1.488092000	-0.250766000	1.116142000
6	2.175151000	-0.428219000	-0.016981000
7	-1.027378000	1.164005000	-0.428497000
6	-0.893260000	-0.132457000	-0.704949000
6	-2.218931000	1.351503000	0.237197000

```
6       -2.809183000      0.131887000      0.344093000
7       -1.969472000     -0.779515000     -0.254328000
1       -0.031926000     -0.591632000     -1.177894000
1       -3.738344000     -0.167324000      0.798435000
1       -2.536201000      2.320955000      0.580264000
6       -2.131538000     -2.229495000     -0.287341000
1       -2.688316000     -2.526066000     -1.177698000
1       -1.132059000     -2.675222000     -0.273646000
1       -2.673203000     -2.536372000      0.605638000
6        0.005008000      2.182567000     -0.682621000
1        0.848213000      1.659826000     -1.140915000
1       -0.402444000      2.890800000     -1.410950000
6        0.443606000      2.860891000      0.595951000
1        0.821952000      2.113167000      1.296854000
1       -0.368893000      3.422678000      1.064290000
1        1.244349000      3.567156000      0.368916000
7        3.022678000      0.550352000     -0.553907000
1        3.698120000      0.131056000     -1.181040000
1        3.513048000      1.045467000      0.181127000

(d)E(RM06L)= -657.856772378

7       -0.960978000     -0.209082000      1.662550000
7       -2.020310000      0.052731000      0.855129000
7       -0.340357000     -1.285724000      1.242421000
7       -0.959548000     -1.776796000      0.136584000
6       -1.972315000     -0.927128000     -0.052200000
7        1.481106000      0.140535000     -0.556037000
6        0.349720000      0.724636000     -0.952006000
6        2.088902000      0.951556000      0.372898000
6        1.296529000      2.043279000      0.530829000
7        0.222495000      1.890076000     -0.313539000
1       -0.373165000      0.302255000     -1.632423000
1        1.383553000      2.893081000      1.185234000
1        3.003497000      0.672111000      0.864293000
6       -0.980280000      2.712269000     -0.327140000
1       -1.397932000      2.719147000     -1.333590000
1       -1.702161000      2.262231000      0.361594000
1       -0.717243000      3.728126000     -0.037071000
6        1.923507000     -1.197804000     -0.992784000
1        1.005879000     -1.729894000     -1.254918000
1        2.543591000     -1.069792000     -1.886279000
6        2.646471000     -1.936074000      0.107706000
1        2.002087000     -1.996468000      0.987857000
1        3.599472000     -1.468271000      0.369869000
1        2.866290000     -2.949265000     -0.232123000
7       -2.806935000     -0.968328000     -1.175508000
1       -3.716307000     -0.573938000     -0.968543000
1       -2.921074000     -1.917606000     -1.508919000

(e)E(RM06L)= -657.857814549

7       -0.446588000      1.419292000     -1.596654000
7       -1.308128000      1.497433000     -0.558835000
7        0.785724000      1.603602000     -1.166283000
7        0.779333000      1.802377000      0.174205000
6       -0.516153000      1.730913000      0.493311000
7       -0.323670000     -1.413357000     -0.203729000
6        0.815715000     -1.098955000     -0.822084000
6       -0.077793000     -1.496638000      1.150642000
6        1.239018000     -1.221846000      1.332854000
7        1.785367000     -0.994784000      0.089138000
1        0.919198000     -0.896277000     -1.874075000
1        1.825598000     -1.136324000      2.231085000
1       -0.859058000     -1.695555000      1.861728000
6        3.078279000     -0.378784000     -0.168199000
1        3.407203000     -0.637163000     -1.173227000
1        2.952910000      0.704188000     -0.088612000
1        3.800443000     -0.748590000      0.558322000
6       -1.615469000     -1.577464000     -0.898333000
1       -1.624972000     -0.812425000     -1.679446000
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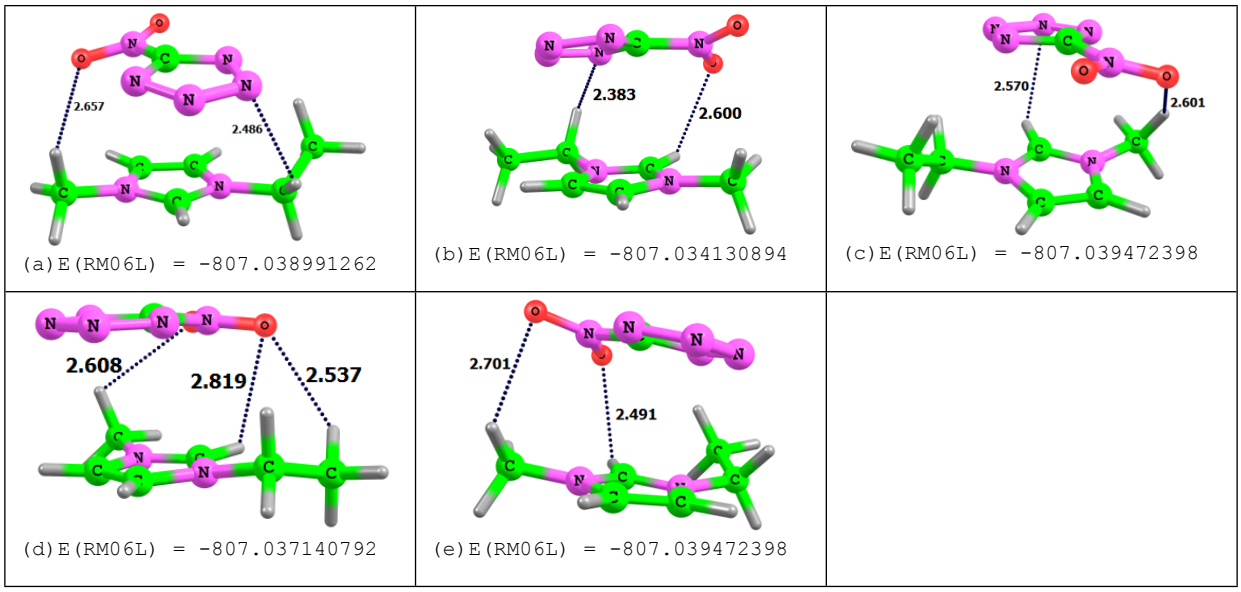
1	-1.618826000	-2.568443000	-1.364809000
6	-2.785455000	-1.395272000	0.034564000
1	-2.743005000	-0.409340000	0.501377000
1	-2.833665000	-2.171984000	0.802697000
1	-3.708943000	-1.451403000	-0.543037000
7	-0.993096000	1.789378000	1.805628000
1	-1.923553000	2.187770000	1.835896000
1	-0.374778000	2.336232000	2.391281000

[10] 1-ethyl-3-methylimidazolium 5-nitro tetrazolate ([EMIm]$^+$[NO_2tz]$^-$)



(a)E(RM06L) = -807.038991262 (b)E(RM06L) = -807.034130894 (c)E(RM06L) = -807.039472398

(d)E(RM06L) = -807.037140792 (e)E(RM06L) = -807.039472398

Fig. S12.Optimized conformers of 1-ethyl-3-methylimidazolium 5-nitro tetrazolate. All distance parameters in Å and energy in au.

Table S9. Relative energy of the a-e conformations

Conformation	Rel. Energy (kJ/mol)
a	1.2620
b	14.0107
c	0.0000
d	6.1158
e	0.0000

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

(a)E(RM06L) = -807.038991262

7	-0.277920000	-1.368406000	-2.085439000
7	-1.309830000	-0.972815000	-1.345676000
7	0.684644000	-1.864461000	-1.287954000
7	0.289880000	-1.816214000	-0.019430000
6	-0.924037000	-1.266742000	-0.100733000
7	1.507512000	0.959854000	-0.001568000
6	0.642629000	1.279592000	-0.965135000
6	0.958891000	1.312275000	1.210971000
6	-0.258035000	1.862882000	0.955317000
7	-0.436208000	1.837884000	-0.408288000
1	0.756068000	1.043044000	-2.011425000
1	-1.027813000	2.219489000	1.618495000
1	1.457835000	1.116392000	2.143419000
6	-1.670868000	2.159833000	-1.119667000
1	-2.165836000	1.222702000	-1.385579000

1	-2.306363000	2.744035000	-0.458403000
1	-1.435547000	2.739645000	-2.011520000
6	2.798150000	0.275645000	-0.229148000
1	2.648653000	-0.350345000	-1.111996000
1	3.542753000	1.044562000	-0.458227000
6	3.202828000	-0.572445000	0.951471000
1	2.415728000	-1.291779000	1.186835000
1	3.433763000	0.027040000	1.835596000
1	4.105753000	-1.126807000	0.692724000
7	-1.677921000	-0.874972000	1.062438000
8	-1.319225000	-1.297922000	2.153414000
8	-2.603705000	-0.077119000	0.889466000

(b)E(RM06L) = -807.034130894

7	0.738084000	-2.101977000	0.160091000
7	0.048138000	-1.434390000	-0.759029000
7	-0.006199000	-2.240273000	1.274755000
7	-1.194144000	-1.683169000	1.093426000
6	-1.121136000	-1.207991000	-0.154931000
7	1.601670000	0.908110000	-0.183772000
6	0.505662000	1.571803000	-0.551971000
6	1.526973000	0.657818000	1.167209000
6	0.369293000	1.208852000	1.615504000
7	-0.255055000	1.776459000	0.526512000
1	0.232297000	1.825632000	-1.562146000
1	-0.081538000	1.209285000	2.593200000
1	2.270232000	0.076116000	1.682408000
6	-1.561209000	2.423082000	0.542808000
1	-2.257251000	1.794377000	1.098707000
1	-1.490763000	3.404584000	1.013333000
1	-1.922273000	2.517380000	-0.479257000
6	2.555548000	0.308160000	-1.141251000
1	1.966258000	-0.404603000	-1.727415000
1	2.901512000	1.115086000	-1.793145000
6	3.697428000	-0.387376000	-0.446066000
1	3.332090000	-1.241573000	0.128354000
1	4.260083000	0.286260000	0.205856000
1	4.386653000	-0.770472000	-1.199203000
7	-2.154537000	-0.408470000	-0.749404000
8	-3.261292000	-0.398102000	-0.225049000
8	-1.848502000	0.276579000	-1.735770000

(c)E(RM06L) = -807.039472398

7	-0.908305000	-1.325666000	-2.044020000
7	-1.668206000	-0.957649000	-1.019359000
7	0.257425000	-1.825986000	-1.586588000
7	0.265242000	-1.802701000	-0.258946000
6	-0.920166000	-1.266803000	0.043826000
7	1.482246000	0.947897000	-0.210699000
6	0.501053000	1.191245000	-1.081429000
6	1.104164000	1.436073000	1.019863000
6	-0.130135000	1.985896000	0.872015000
7	-0.489093000	1.823031000	-0.446501000
1	0.468155000	0.844241000	-2.102553000
1	-0.802040000	2.423663000	1.590243000
1	1.718600000	1.323817000	1.895556000
6	-1.804938000	2.114290000	-1.005195000
1	-2.543171000	1.512120000	-0.473883000
1	-2.017159000	3.179220000	-0.904476000
1	-1.813233000	1.824387000	-2.053234000
6	2.699942000	0.168592000	-0.520114000
1	2.415396000	-0.510119000	-1.328200000
1	3.456092000	0.866637000	-0.892996000
6	3.185024000	-0.608200000	0.680012000
1	2.387891000	-1.250441000	1.060816000
1	3.551222000	0.043476000	1.477462000
1	4.017250000	-1.244018000	0.375482000
7	-1.271325000	-0.876258000	1.384425000
8	-0.546998000	-1.247364000	2.300953000

```
8       -2.243572000     -0.129912000      1.520762000

(d)E(RM06L) =  -807.037140792
7       -1.707637000     -1.644674000     -1.412138000
7       -0.809253000     -1.826159000     -0.453431000
7       -2.569478000     -0.672994000     -1.051756000
7       -2.245701000     -0.206794000      0.147113000
6       -1.177951000     -0.941542000      0.480483000
7        1.400937000      0.322286000     -0.889936000
6        1.136952000      1.154050000      0.120064000
6        0.474009000      0.537459000     -1.885712000
6       -0.358267000      1.519984000     -1.455950000
7        0.071769000      1.893591000     -0.202713000
1        1.648650000      1.180588000      1.068170000
1       -1.245001000      1.939414000     -1.899423000
1        0.451465000     -0.065724000     -2.776841000
6       -0.666934000      2.763985000      0.704528000
1       -0.889391000      3.706386000      0.204610000
1       -1.585640000      2.246980000      0.991709000
1       -0.064879000      2.947132000      1.591791000
6        2.336970000     -0.817547000     -0.860494000
1        1.714423000     -1.699231000     -0.669821000
1        2.751626000     -0.897935000     -1.868386000
6        3.415607000     -0.657494000      0.180269000
1        2.999865000     -0.668918000      1.189570000
1        3.996041000      0.257401000      0.033926000
1        4.103090000     -1.501036000      0.110120000
7       -0.402033000     -0.692876000      1.656593000
8       -0.761913000      0.216607000      2.406222000
8        0.635313000     -1.342242000      1.814943000

(e)E(RM06L) =  -807.039472398

7        0.161572000     -2.389235000     -0.545479000
7        0.002540000     -1.659379000      0.552557000
7       -0.862145000     -2.164284000     -1.393566000
7       -1.708716000     -1.299439000     -0.855961000
6       -1.149335000     -1.020519000      0.327514000
7        1.737726000      0.460180000     -0.400898000
6        0.913695000      1.381274000      0.094851000
6        1.344769000      0.165393000     -1.687576000
6        0.262294000      0.935335000     -1.963860000
7        0.007792000      1.690015000     -0.839155000
1        0.915406000      1.754758000      1.103973000
1       -0.378060000      0.969743000     -2.828220000
1        1.823093000     -0.611302000     -2.259000000
6       -1.133968000      2.577719000     -0.658286000
1       -1.007111000      3.483988000     -1.251910000
1       -2.038951000      2.051359000     -0.962898000
1       -1.222047000      2.831732000      0.396653000
6        2.754177000     -0.293318000      0.356670000
1        2.557179000     -1.344195000      0.128857000
1        3.734438000     -0.023984000     -0.048812000
6        2.652592000     -0.041077000      1.839360000
1        1.648597000     -0.287648000      2.194145000
1        2.894053000      0.992559000      2.103202000
1        3.364023000     -0.682796000      2.359828000
7       -1.672343000     -0.026156000      1.219047000
8       -2.807927000      0.393802000      1.025855000
8       -0.919691000      0.400578000      2.106187000
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[11] 1-ethyl-3-methylimidazolium 5-nitro tetrazolate-2N-oxide([EMIm]$^+$[NO_2Otz]$^-$)

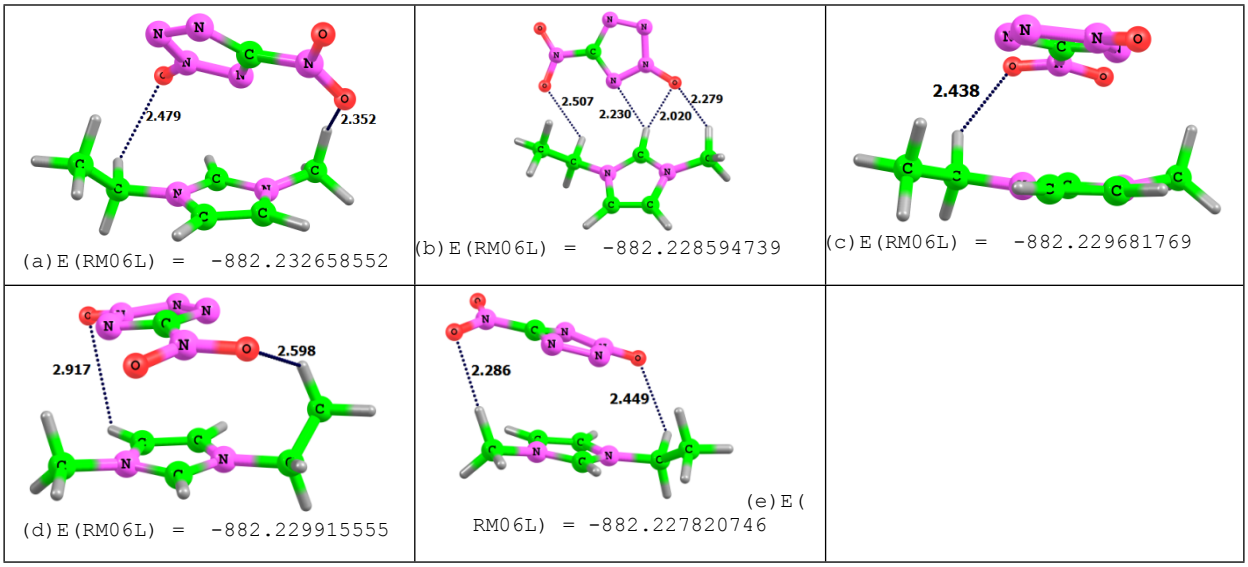


Fig. S13.Optimized conformers of 1-ethyl-3-methylimidazolium 5-nitro tetrazolate-2N-oxide. All distance parameters in Å and energy in au.

Table S10. Relative energy of the a-e conformations.

Conformation	Rel. Energy (kJ/mol)
a	0.0000
b	10.6593
c	7.8081
d	7.1949
e	12.6895

X, Y, Z Cartesian coordinates of conformers (coordinates in Å and energy in au.)

(a)E(RM06L) = -882.232658552

7	-0.169460000	-1.369059000	1.152990000
7	0.711672000	-0.374136000	1.018038000
7	0.156656000	-2.470816000	0.388034000
7	1.268453000	-2.157762000	-0.244457000
6	1.567731000	-0.921713000	0.142193000
7	-1.908291000	0.683585000	-0.441396000
6	-1.458722000	1.345876000	0.624537000
6	-1.140337000	1.038943000	-1.529362000
6	-0.217301000	1.936311000	-1.091551000
7	-0.447628000	2.131009000	0.250345000
1	-1.800666000	1.192349000	1.634693000
6	0.447333000	2.821583000	1.167662000
1	-0.095810000	3.064064000	2.079255000
1	1.287938000	2.159950000	1.383276000
1	0.801840000	3.738200000	0.698475000
6	-3.041746000	-0.260576000	-0.426711000
1	-3.217185000	-0.489962000	0.625266000
1	-3.913419000	0.268878000	-0.825270000
6	-2.746454000	-1.523645000	-1.200558000
1	-1.879172000	-2.046563000	-0.793032000
1	-2.581931000	-1.330428000	-2.263472000
1	-3.605337000	-2.192099000	-1.124074000
7	2.651583000	-0.169186000	-0.411519000

```
8        3.475431000     -0.749034000     -1.102502000
8        2.664378000      1.047519000     -0.165517000
8       -1.212127000     -1.293474000      1.842341000
1       -1.312585000      0.628520000     -2.509017000
1        0.590939000      2.430877000     -1.602187000

(b)E(RM06L) =  -882.228594739

7        0.988729000     -1.855472000     -0.118879000
7        1.133012000     -0.548284000     -0.362061000
7        2.121000000     -2.433087000      0.383135000
7        3.015872000     -1.466767000      0.458357000
6        2.406853000     -0.373255000      0.015108000
7       -1.980109000      1.152962000     -0.298977000
6       -1.899537000     -0.172320000     -0.421593000
6       -3.206636000      1.472247000      0.244189000
6       -3.872002000      0.304476000      0.448035000
7       -3.036100000     -0.708650000      0.031646000
1       -1.050825000     -0.757254000     -0.761111000
6       -3.291114000     -2.144366000      0.085966000
1       -2.338509000     -2.658667000     -0.040012000
1       -3.717266000     -2.395237000      1.056783000
1       -3.986299000     -2.432713000     -0.703501000
6       -0.887834000      2.099018000     -0.607209000
1       -0.082251000      1.510834000     -1.049050000
1       -1.269279000      2.799303000     -1.355347000
6       -0.403703000      2.803189000      0.638847000
1       -0.010670000      2.082596000      1.358783000
1       -1.193352000      3.387944000      1.118567000
1        0.412406000      3.475820000      0.375892000
7        3.033667000      0.914449000     -0.053473000
8        4.204185000      1.010336000      0.282088000
8        2.327803000      1.851997000     -0.447943000
8       -0.085279000     -2.478828000     -0.332919000
1       -3.495481000      2.491233000      0.439007000
1       -4.850794000      0.108102000      0.851899000

(c)E(RM06L) =  -882.229681769

7        0.727116000      2.081418000     -0.390895000
7        1.398939000      0.957197000     -0.662416000
7       -0.549160000      2.084880000     -0.961063000
7       -0.666632000      0.935604000     -1.584836000
6        0.490147000      0.297262000     -1.401401000
7       -1.169981000     -0.721340000      1.036678000
6       -0.080159000     -1.494703000      1.038127000
6       -0.875746000      0.441991000      1.711667000
6        0.417418000      0.353294000      2.122259000
7        0.895025000     -0.862900000      1.694005000
1        0.015038000     -2.445431000      0.537725000
6        2.298337000     -1.257351000      1.695025000
1        2.373369000     -2.313878000      1.447307000
1        2.811929000     -0.669774000      0.931356000
1        2.724065000     -1.073521000      2.680529000
6       -2.406088000     -1.026324000      0.277515000
1       -2.086558000     -1.238737000     -0.747721000
1       -2.832505000     -1.937838000      0.706341000
6       -3.384284000      0.119333000      0.303919000
1       -2.945127000      1.017819000     -0.134968000
1       -3.738258000      0.340107000      1.314223000
1       -4.253112000     -0.149441000     -0.297303000
7        0.662780000     -1.068448000     -1.756403000
8       -0.269037000     -1.652682000     -2.318323000
8        1.713731000     -1.618998000     -1.400063000
8        1.132575000      2.984005000      0.348832000
1       -1.581283000      1.248679000      1.803123000
1        1.049926000      1.077519000      2.607673000

(d)E(RM06L) =  -882.229915555

7        2.283594000     -0.922614000     -0.398114000
```

7	1.877123000	-0.189084000	0.644277000
7	1.404648000	-1.977408000	-0.676776000
7	0.433549000	-1.871104000	0.194670000
6	0.732717000	-0.820184000	0.961775000
7	-1.640425000	0.561292000	-0.833733000
6	-1.173186000	1.558347000	-0.079039000
6	-0.708546000	0.278632000	-1.807841000
6	0.337610000	1.125893000	-1.620340000
7	0.025821000	1.920557000	-0.539406000
1	-1.647836000	1.948582000	0.807167000
6	0.950590000	2.827638000	0.131862000
1	0.404457000	3.403081000	0.876251000
1	1.717609000	2.223199000	0.621042000
1	1.394803000	3.497187000	-0.603657000
6	-2.926197000	-0.132622000	-0.620845000
1	-3.229105000	0.107456000	0.399907000
1	-3.656468000	0.308969000	-1.306666000
6	-2.797369000	-1.625907000	-0.807704000
1	-2.016303000	-2.030328000	-0.161463000
1	-2.570796000	-1.890402000	-1.843328000
1	-3.747619000	-2.097504000	-0.552758000
7	-0.185149000	-0.286835000	1.901974000
8	-1.287146000	-0.836041000	2.027436000
8	0.136309000	0.757899000	2.485544000
8	3.277617000	-0.678945000	-1.088203000
1	-0.842678000	-0.521715000	-2.514090000
1	1.291838000	1.193749000	-2.118070000

(e)E(RM06L) = -882.227820746

7	0.088530000	-1.683073000	-0.064727000
7	-1.091144000	-1.572410000	0.553655000
7	0.130776000	-0.987794000	-1.259670000
7	-1.039712000	-0.390016000	-1.373521000
6	-1.732326000	-0.761626000	-0.299318000
7	2.109320000	0.568228000	0.549689000
6	1.541172000	1.380658000	-0.342996000
6	1.292244000	0.498141000	1.653296000
6	0.221609000	1.299680000	1.414544000
7	0.398594000	1.848817000	0.162536000
1	1.907653000	1.580766000	-1.334839000
6	-0.570876000	2.677274000	-0.548166000
1	-0.141006000	2.976449000	-1.501815000
1	-1.481261000	2.100709000	-0.734455000
1	-0.793593000	3.563733000	0.046093000
6	3.343416000	-0.217553000	0.356967000
1	4.168380000	0.343450000	0.808364000
1	3.185809000	-1.135130000	0.924518000
6	3.590381000	-0.533878000	-1.097415000
1	3.827079000	0.358001000	-1.684186000
1	2.718940000	-1.032762000	-1.526758000
1	4.446319000	-1.205130000	-1.175466000
7	-3.027860000	-0.215440000	-0.007976000
8	-3.358381000	0.799849000	-0.630388000
8	-3.700066000	-0.762309000	0.856378000
8	1.085280000	-2.278026000	0.393939000
1	1.515799000	-0.155829000	2.478744000
1	-0.662032000	1.495265000	1.999004000

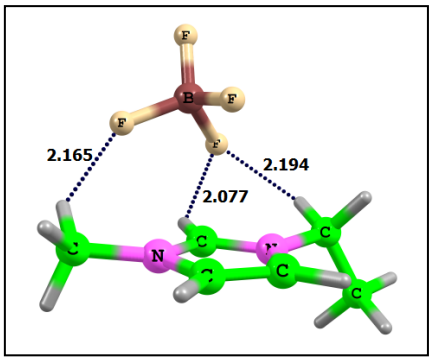
[12] 1-ethyl-3-methylimidazolium tetrafluoroborate

X, Y, Z Cartesian coordinates (coordinates in Å and energy in au.)

E(RM06L) = -769.323308133

7	-1.465430000	-0.338878000	0.103410000
6	-0.645816000	0.452365000	-0.585606000
6	-2.231178000	0.439875000	0.940500000
6	-1.860914000	1.730332000	0.734406000
7	-0.871268000	1.716363000	-0.224667000
1	0.130158000	0.108866000	-1.253208000
1	-2.199891000	2.646828000	1.186251000
1	-2.951282000	0.010446000	1.615889000

6	-1.413415000	-1.808344000	0.081375000
1	-0.449400000	-2.065847000	-0.361145000
1	-1.376430000	-2.131320000	1.124161000
6	-2.588120000	-2.406384000	-0.660542000
1	-2.600744000	-2.090540000	-1.705879000
1	-3.543709000	-2.126591000	-0.209116000
6	-0.120281000	2.864140000	-0.716484000
1	-0.627405000	3.312885000	-1.572164000
1	-0.039357000	3.596896000	0.084425000
1	0.877138000	2.521303000	-0.986492000
9	1.564274000	-1.334891000	-0.836924000
5	2.111459000	-0.439541000	0.140190000
9	2.152053000	0.849586000	-0.470039000
9	1.185368000	-0.376631000	1.211792000
9	3.349150000	-0.845230000	0.551363000
1	-2.518744000	-3.495032000	-0.642497000

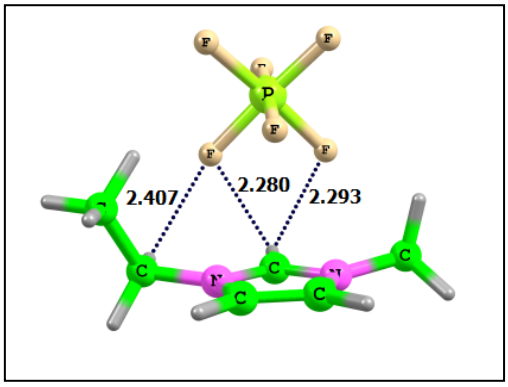


[13] 1-ethyl-3-methylimidazolium hexafluorophosphate

X, Y, Z Cartesian coordinates (coordinates in Å and energy in au.)

E(RM06L) = -1285.50299972

7	-2.152681000	0.612514000	-0.360375000
6	-1.522947000	-0.449846000	-0.857192000
6	-2.923348000	0.205909000	0.706546000
6	-2.750524000	-1.134454000	0.835034000
7	-1.880518000	-1.526850000	-0.158150000
1	-0.781008000	-0.429965000	-1.637491000
1	-3.161888000	-1.837477000	1.538620000
1	-3.521372000	0.898022000	1.274059000
6	-1.915693000	2.005370000	-0.772684000
1	-1.234776000	1.957400000	-1.621989000
1	-2.870291000	2.413576000	-1.118675000
6	-1.319076000	2.819176000	0.354409000
1	-0.386898000	2.373109000	0.701538000
1	-2.007489000	2.907727000	1.198625000
6	-1.258408000	-2.838714000	-0.270018000
1	-0.470938000	-2.923984000	0.479213000
1	-2.015739000	-3.608337000	-0.124883000
1	-0.807864000	-2.938298000	-1.253810000
15	1.732267000	0.004970000	0.073514000
9	0.354268000	-0.127185000	1.000072000
9	1.180370000	-1.288421000	-0.816259000
9	2.167597000	1.302236000	0.932539000
9	2.497463000	-1.001296000	1.072322000
9	0.866710000	0.990385000	-0.956089000
9	3.017140000	0.128952000	-0.885989000
1	-1.105319000	3.827357000	-0.004171000



Part-II : Thermochemical data from G3MP2 calculations

X, Y, Z Cartesian coordinates (coordinates in Å and energy values in au.)

Compound name is followed by charge and spin multiplicity.

[1]Hydrazine

0 1

7	0.700121000	-0.072981000	-0.097619000
1	1.043856000	0.826450000	-0.376492000
1	1.129779000	-0.315676000	0.771276000
7	-0.700117000	-0.072919000	0.097661000
1	-1.129800000	-0.316155000	-0.771073000
1	-1.043863000	0.826677000	0.375995000

RHF

Zero-point correction=	0.051849 (Hartree/Particle)
Thermal correction to Energy=	0.061242
Thermal correction to Enthalpy=	0.062186
Thermal correction to Gibbs Free Energy=	0.035542

```
 Sum of electronic and zero-point Energies=          -111.111303
 Sum of electronic and thermal Energies=             -111.108132
 Sum of electronic and thermal Enthalpies=           -111.107187
 Sum of electronic and thermal Free Energies=        -111.133831
```

G3MP2

```
Temperature=              298.150000 Pressure=                    1.000000
 E(ZPE)=                    0.058071 E(Thermal)=                  0.055121
 E(QCISD(T))=            -111.528791 E(Empiric)=                 -0.064953
 DE(MP2)=                  -0.157721
 G3MP2(0 K)=             -111.699616 G3MP2 Energy=             -111.696344
 G3MP2 Enthalpy=         -111.695400 G3MP2 Free Energy=        -111.722189
```

[2]Monomethyl Hydrazine

```
0 1
7       -1.153276000     -0.308383000     -0.046551000
1       -1.913828000      0.143776000     -0.511751000
1       -1.432826000     -0.507961000      0.897453000
7       -0.032813000      0.545686000     -0.095338000
6        1.192861000     -0.216071000     -0.006417000
1        2.033495000      0.469272000     -0.029369000
1        1.266589000     -0.822590000      0.898464000
1        1.257472000     -0.876632000     -0.860328000
1       -0.065445000      1.229440000      0.637260000
```

RHF

```
Zero-point correction=                           0.078876 (Hartree/Particle)
 Thermal correction to Energy=                   0.092420
 Thermal correction to Enthalpy=                 0.093364
 Thermal correction to Gibbs Free Energy=        0.063208
 Sum of electronic and zero-point Energies=          -150.111920
 Sum of electronic and thermal Energies=             -150.107841
 Sum of electronic and thermal Enthalpies=           -150.106897
 Sum of electronic and thermal Free Energies=        -150.137053
```

G3MP2

```
Temperature=              298.150000        Pressure=                    1.000000
 E(ZPE)=                    0.088342        E(Thermal)=                  0.083181
 E(QCISD(T))=            -150.705750        E(Empiric)=                 -0.092790
 DE(MP2)=                  -0.205923
 G3MP2(0 K)=             -150.925587        G3MP2 Energy=             -150.921282
 G3MP2 Enthalpy=         -150.920338        G3MP2 Free Energy=        -150.950874
```

[3]1,2,3-triazine

0 1

```
7       -1.204948000     -0.619599000      0.000000000
7       -0.130035000     -1.336591000      0.000000000
6        1.056998000     -0.755748000      0.000000000
6        1.191928000      0.612983000      0.000000000
6        0.000000000      1.299152000      0.000000000
7       -1.163283000      0.671612000      0.000000000
1        1.899717000     -1.421271000      0.000000000
1        2.146241000      1.103259000      0.000000000
1       -0.051648000      2.371736000      0.000000000
```

RHF

```
Zero-point correction=                           0.069282 (Hartree/Particle)
 Thermal correction to Energy=                   0.073173
 Thermal correction to Enthalpy=                 0.074117
 Thermal correction to Gibbs Free Energy=        0.042109
 Sum of electronic and zero-point Energies=          -278.542049
 Sum of electronic and thermal Energies=             -278.538158
 Sum of electronic and thermal Enthalpies=           -278.537214
 Sum of electronic and thermal Free Energies=        -278.569222
```

G3MP2

```
Temperature=              298.150000        Pressure=                    1.000000
 E(ZPE)=                    0.061859        E(Thermal)=                  0.066060
 E(QCISD(T))=            -279.531954        E(Empiric)=                 -0.139185
 DE(MP2)=                  -0.276400
 G3MP2(0 K)=             -279.885680        G3MP2 Energy=             -279.881479
```

G3MP2 Enthalpy= -279.880534 G3MP2 Free Energy= -279.912990

[4]1,2,4-triazine

0 1

7	-1.204901000	-0.629080000	0.000000000
6	-0.081423000	-1.294682000	0.000000000
6	1.144788000	-0.627731000	0.000000000
7	1.187161000	0.675028000	0.000000000
6	0.000000000	1.272596000	0.000000000
7	-1.166958000	0.680554000	0.000000000
1	2.075609000	-1.166126000	0.000000000
1	-0.149611000	-2.365787000	0.000000000
1	-0.013296000	2.345305000	0.000000000

RHF

Zero-point correction= 0.069998 (Hartree/Particle)
Thermal correction to Energy= 0.073848
Thermal correction to Enthalpy= 0.074793
Thermal correction to Gibbs Free Energy= 0.042853
Sum of electronic and zero-point Energies= -278.572025
Sum of electronic and thermal Energies= -278.568175
Sum of electronic and thermal Enthalpies= -278.567231
Sum of electronic and thermal Free Energies= -278.599170

G3MP2

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.062498 E(Thermal)= 0.066650
E(QCISD(T))= -279.557214 E(Empiric)= -0.139185
DE(MP2)= -0.276991
G3MP2(0 K)= -279.910892 G3MP2 Energy= -279.906740
G3MP2 Enthalpy= -279.905796 G3MP2 Free Energy= -279.938169

[5]1,2,5-triazine

0 1

6	1.108164000	-0.640290000	0.000000000
7	-0.000081000	-1.352932000	0.000000000
6	-1.107727000	-0.639180000	0.000000000
7	-1.172808000	0.677258000	0.000000000
6	0.000000000	1.278559000	0.000000000
7	1.172486000	0.676414000	0.000000000
1	-2.038928000	-1.175965000	0.000000000
1	-0.000017000	2.353200000	0.000000000
1	2.039149000	-1.176956000	0.000000000

RHF

Zero-point correction= 0.071190 (Hartree/Particle)
Thermal correction to Energy= 0.075026
Thermal correction to Enthalpy= 0.075970
Thermal correction to Gibbs Free Energy= 0.044051
Sum of electronic and zero-point Energies= -278.624651
Sum of electronic and thermal Energies= -278.620815
Sum of electronic and thermal Enthalpies= -278.619871
Sum of electronic and thermal Free Energies= -278.651791

G3MP2

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.063562 E(Thermal)= 0.067683
E(QCISD(T))= -279.600194 E(Empiric)= -0.139185
DE(MP2)= -0.277301
G3MP2(0 K)= -279.953117 G3MP2 Energy= -279.948996
G3MP2 Enthalpy= -279.948052 G3MP2 Free Energy= -279.980386

[6] $[BMIm]^+[dc]^-$

0 1

7	-0.212458000	-0.566928000	0.182860000
6	0.616846000	-1.236930000	-0.582762000
6	0.200548000	-0.713673000	1.491010000
6	1.275880000	-1.510465000	1.475123000
7	1.516166000	-1.844461000	0.156250000
1	0.589967000	-1.257880000	-1.648586000

1	1.902775000	-1.855532000	2.266981000
1	-0.282521000	-0.201588000	2.292154000
6	-1.337975000	0.260886000	-0.276214000
1	-1.260276000	1.201169000	0.248120000
1	-1.171580000	0.455407000	-1.327342000
6	-2.683189000	-0.421002000	-0.047303000
1	-2.800902000	-0.641491000	1.010643000
1	-2.701329000	-1.374585000	-0.570070000
6	2.707943000	-2.515070000	-0.353801000
1	2.989794000	-3.293754000	0.339285000
1	2.480149000	-2.956069000	-1.312018000
1	3.498434000	-1.790627000	-0.472913000
7	2.365306000	2.522423000	-0.259212000
6	1.373162000	2.522760000	0.598659000
7	0.510107000	2.546194000	1.358465000
6	2.477532000	1.450720000	-0.994634000
7	2.602359000	0.514585000	-1.655822000
6	-3.845265000	0.455273000	-0.520123000
1	-3.723045000	0.678107000	-1.577527000
1	-3.811347000	1.408408000	0.000659000
6	-5.205262000	-0.202995000	-0.293395000
1	-6.008656000	0.439196000	-0.637819000
1	-5.280965000	-1.144842000	-0.829051000
1	-5.372179000	-0.405631000	0.760330000

RHF

Zero-point correction=	0.267408 (Hartree/Particle)
Thermal correction to Energy=	0.283809
Thermal correction to Enthalpy=	0.284753
Thermal correction to Gibbs Free Energy=	0.219827
Sum of electronic and zero-point Energies=	-659.341885
Sum of electronic and thermal Energies=	-659.325484
Sum of electronic and thermal Enthalpies=	-659.324540
Sum of electronic and thermal Free Energies=	-659.389466

G3MP2

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.238758	E(Thermal)=	0.256314
E(QCISD(T))=	-661.869688	E(Empiric)=	-0.371160
DE(MP2)=	-0.731667		
G3MP2(0 K)=	-662.733758	G3MP2 Energy=	-662.716201
G3MP2 Enthalpy=	-662.715257	G3MP2 Free Energy=	-662.782940

[7] [EMIm]$^+$[dc]$^-$

0 1

7	1.155713000	-0.014794000	-0.074586000
6	0.620639000	1.031766000	-0.659298000
6	1.104473000	0.184817000	1.289621000
6	0.552315000	1.387580000	1.488786000
7	0.265483000	1.915352000	0.244565000
1	0.462041000	1.137103000	-1.708522000
1	0.317738000	1.909242000	2.389885000
1	1.422738000	-0.564539000	1.978581000
6	1.648924000	-1.225844000	-0.748761000
1	1.221885000	-2.065044000	-0.222253000
1	1.232650000	-1.216082000	-1.746419000
6	3.169862000	-1.276700000	-0.785066000
1	3.588532000	-1.286500000	0.215187000
1	3.582946000	-0.428981000	-1.321239000
6	-0.531284000	3.110335000	-0.015816000
1	-0.259178000	3.870867000	0.700989000
1	-0.317042000	3.464716000	-1.012095000
1	-1.578485000	2.861207000	0.054959000
7	-2.635907000	-1.449420000	-0.051798000
6	-1.637928000	-1.997961000	0.599011000
7	-0.778341000	-2.495984000	1.178483000
6	-2.339221000	-0.388876000	-0.751221000
7	-2.105021000	0.552210000	-1.374643000
1	3.485997000	-2.184250000	-1.286757000

RHF

Zero-point correction=	0.206372 (Hartree/Particle)

```
 Thermal correction to Energy=                  0.220154
 Thermal correction to Enthalpy=                0.221098
 Thermal correction to Gibbs Free Energy=       0.162960
 Sum of electronic and zero-point Energies=          -581.332883
 Sum of electronic and thermal Energies=             -581.319101
 Sum of electronic and thermal Enthalpies=           -581.318157
 Sum of electronic and thermal Free Energies=        -581.376295
```

G3MP2

```
Temperature=              298.150000        Pressure=                     1.000000
 E(ZPE)=                    0.184261        E(Thermal)=                   0.198991
 E(QCISD(T))=            -583.505289        E(Empiric)=                  -0.315486
 DE(MP2)=                  -0.627610
 G3MP2(0 K)=             -584.264124        G3MP2 Energy=              -584.249393
 G3MP2 Enthalpy=         -584.248449        G3MP2 Free Energy=         -584.308830
```

[8]Pyridine

0 1

```
6        0.000000000      0.000000000     -1.372256000
6        0.000000000      1.190250000     -0.666091000
6        0.000000000      1.131017000      0.717390000
7        0.000000000      0.000000000      1.400419000
6        0.000000000     -1.131017000      0.717390000
6        0.000000000     -1.190250000     -0.666091000
1        0.000000000      0.000000000     -2.447440000
1        0.000000000      2.139831000     -1.167910000
1        0.000000000      2.036082000      1.299140000
1        0.000000000     -2.036082000      1.299140000
1        0.000000000     -2.139831000     -1.167910000
```

RHF

```
Zero-point correction=                          0.095448 (Hartree/Particle)
 Thermal correction to Energy=                  0.099443
 Thermal correction to Enthalpy=                0.100387
 Thermal correction to Gibbs Free Energy=       0.068851
 Sum of electronic and zero-point Energies=          -246.600371
 Sum of electronic and thermal Energies=             -246.596376
 Sum of electronic and thermal Enthalpies=           -246.595432
 Sum of electronic and thermal Free Energies=        -246.626968
```

G3MP2

```
Temperature=              298.150000        Pressure=                     1.000000
 E(ZPE)=                    0.085222        E(Thermal)=                   0.089584
 E(QCISD(T))=            -247.551220        E(Empiric)=                  -0.139185
 DE(MP2)=                  -0.262421
 G3MP2(0 K)=             -247.867605        G3MP2 Energy=              -247.863242
 G3MP2 Enthalpy=         -247.862298        G3MP2 Free Energy=         -247.894354
```

[9]Pyridazine

0 1

```
7        0.000000000      0.654647000     -1.210650000
6        0.000000000      1.310141000     -0.075994000
6        0.000000000      0.683743000      1.169334000
6        0.000000000     -0.683743000      1.169334000
6        0.000000000     -1.310141000     -0.075994000
7        0.000000000     -0.654647000     -1.210650000
1        0.000000000      1.260314000      2.075767000
1        0.000000000      2.381131000     -0.161264000
1        0.000000000     -1.260314000      2.075767000
1        0.000000000     -2.381131000     -0.161264000
```

RHF

```
Zero-point correction=                          0.082398 (Hartree/Particle)
 Thermal correction to Energy=                  0.086330
 Thermal correction to Enthalpy=                0.087274
 Thermal correction to Gibbs Free Energy=       0.055845
 Sum of electronic and zero-point Energies=          -262.567630
 Sum of electronic and thermal Energies=             -262.563699
 Sum of electronic and thermal Enthalpies=           -262.562754
 Sum of electronic and thermal Free Energies=        -262.594184
```

G3MP2

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.073570	E(Thermal)=	0.077841
E(QCISD(T))=	-263.538386	E(Empiric)=	-0.139185
DE(MP2)=	-0.269196		
G3MP2(0 K)=	-263.873197	G3MP2 Energy=	-263.868926
G3MP2 Enthalpy=	-263.867982	G3MP2 Free Energy=	-263.899893

[10]Pyrazine

0 1

6	0.000000000	1.121676000	0.693093000
6	0.000000000	1.121676000	-0.693093000
7	0.000000000	0.000000000	-1.386548000
6	0.000000000	-1.121676000	-0.693093000
6	0.000000000	-1.121676000	0.693093000
7	0.000000000	0.000000000	1.386548000
1	0.000000000	2.043894000	1.245371000
1	0.000000000	2.043894000	-1.245371000
1	0.000000000	-2.043894000	-1.245371000
1	0.000000000	-2.043894000	1.245371000

RHF

Zero-point correction=	0.082940 (Hartree/Particle)
Thermal correction to Energy=	0.086830
Thermal correction to Enthalpy=	0.087774
Thermal correction to Gibbs Free Energy=	0.057073
Sum of electronic and zero-point Energies=	-262.600064
Sum of electronic and thermal Energies=	-262.596175
Sum of electronic and thermal Enthalpies=	-262.595231
Sum of electronic and thermal Free Energies=	-262.625932

G3MP2

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.074054	E(Thermal)=	0.078275
E(QCISD(T))=	-263.567114	E(Empiric)=	-0.139185
DE(MP2)=	-0.269710		
G3MP2(0 K)=	-263.901955	G3MP2 Energy=	-263.897734
G3MP2 Enthalpy=	-263.896790	G3MP2 Free Energy=	-263.927961

[11] HIm Cation

+1 1

7	1.062086000	-0.351834000	0.000011000
6	-0.000020000	-1.123816000	-0.000036000
6	0.669956000	0.972905000	-0.000008000
6	-0.669920000	0.972930000	0.000088000
7	-1.062099000	-0.351796000	-0.000048000
1	-0.000040000	-2.193081000	-0.000072000
1	-1.374685000	1.774775000	0.000154000
1	1.374750000	1.774725000	-0.000010000
1	-2.005829000	-0.681526000	-0.000085000
1	2.005804000	-0.681598000	0.000005000

RHF

Zero-point correction=	0.091931 (Hartree/Particle)
Thermal correction to Energy=	0.095479
Thermal correction to Enthalpy=	0.096423
Thermal correction to Gibbs Free Energy=	0.065698
Sum of electronic and zero-point Energies=	-225.104421
Sum of electronic and thermal Energies=	-225.100873
Sum of electronic and thermal Enthalpies=	-225.099929
Sum of electronic and thermal Free Energies=	-225.130654

G3MP2

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.082081	E(Thermal)=	0.085925
E(QCISD(T))=	-225.948012	E(Empiric)=	-0.120627
DE(MP2)=	-0.238751		
G3MP2(0 K)=	-226.225309	G3MP2 Energy=	-226.221465
G3MP2 Enthalpy=	-226.220521	G3MP2 Free Energy=	-226.251639

[12] tetrazolate anion

-1 1

```
7        0.641597000     -0.922106000      0.000000000
7        1.094555000      0.319671000      0.000000000
7       -0.641597000     -0.922108000      0.000000000
7       -1.094554000      0.319670000      0.000000000
6        0.000000000      1.051511000      0.000000000
1        0.000000000      2.125049000      0.000000000
```

RHF

```
Zero-point correction=                           0.037898 (Hartree/Particle)
 Thermal correction to Energy=                    0.041014
 Thermal correction to Enthalpy=                  0.041958
 Thermal correction to Gibbs Free Energy=         0.012046
 Sum of electronic and zero-point Energies=           -256.163326
 Sum of electronic and thermal Energies=              -256.160210
 Sum of electronic and thermal Enthalpies=            -256.159266
 Sum of electronic and thermal Free Energies=         -256.189178
```

G3MP2

```
Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                    0.033837 E(Thermal)=                   0.037097
 E(QCISD(T))=            -257.030510 E(Empiric)=                  -0.120627
 DE(MP2)=                  -0.268490
 G3MP2(0 K)=             -257.385789 G3MP2 Energy=               -257.382530
 G3MP2 Enthalpy=         -257.381586 G3MP2 Free Energy=          -257.411681
```

[13]1,2,4-triazolium cation

```
+1 1
7       -1.138984000      0.368478000      0.000000000
6       -0.751883000     -0.847773000      0.000000000
7        0.000000000      1.087534000      0.000000000
6        1.057221000      0.332475000      0.000000000
7        0.616739000     -0.913944000      0.000000000
1       -1.391576000     -1.703954000      0.000000000
1        2.077863000      0.654066000      0.000000000
1        1.181377000     -1.740390000      0.000000000
1       -0.043979000      2.087587000      0.000000000
```

RHF

```
Zero-point correction=                           0.079534 (Hartree/Particle)
 Thermal correction to Energy=                    0.082956
 Thermal correction to Enthalpy=                  0.083900
 Thermal correction to Gibbs Free Energy=         0.053390
 Sum of electronic and zero-point Energies=           -241.082426
 Sum of electronic and thermal Energies=              -241.079005
 Sum of electronic and thermal Enthalpies=            -241.078061
 Sum of electronic and thermal Free Energies=         -241.108571
```

G3MP2

```
Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                    0.071013 E(Thermal)=                   0.074685
 E(QCISD(T))=            -241.943081 E(Empiric)=                  -0.120627
 DE(MP2)=                  -0.246668
 G3MP2(0 K)=             -242.239363 G3MP2 Energy=               -242.235691
 G3MP2 Enthalpy=         -242.234747 G3MP2 Free Energy=          -242.265588
```

[14]EMImdc

```
0 1
7        1.155713000     -0.014794000     -0.074586000
6        0.620639000      1.031766000     -0.659298000
6        1.104473000      0.184817000      1.289621000
6        0.552315000      1.387580000      1.488786000
7        0.265483000      1.915352000      0.244565000
1        0.462041000      1.137103000     -1.708522000
1        0.317738000      1.909242000      2.389885000
1        1.422738000     -0.564539000      1.978581000
6        1.648924000     -1.225844000     -0.748761000
1        1.221885000     -2.065044000     -0.222253000
1        1.232650000     -1.216082000     -1.746419000
6        3.169862000     -1.276700000     -0.785066000
1        3.588532000     -1.286500000      0.215187000
```

1	3.582946000	-0.428981000	-1.321239000
6	-0.531284000	3.110335000	-0.015816000
1	-0.259178000	3.870867000	0.700989000
1	-0.317042000	3.464716000	-1.012095000
1	-1.578485000	2.861207000	0.054959000
7	-2.635907000	-1.449420000	-0.051798000
6	-1.637928000	-1.997961000	0.599011000
7	-0.778341000	-2.495984000	1.178483000
6	-2.339221000	-0.388876000	-0.751221000
7	-2.105021000	0.552210000	-1.374643000
1	3.485997000	-2.184250000	-1.286757000

RHF

Zero-point correction=	0.206860 (Hartree/Particle)
Thermal correction to Energy=	0.220425
Thermal correction to Enthalpy=	0.221369
Thermal correction to Gibbs Free Energy=	0.163710
Sum of electronic and zero-point Energies=	-581.333480
Sum of electronic and thermal Energies=	-581.319915
Sum of electronic and thermal Enthalpies=	-581.318971
Sum of electronic and thermal Free Energies=	-581.376630

G3MP2

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.184696	E(Thermal)=	0.199219
E(QCISD(T))=	-583.506440	E(Empiric)=	-0.315486
DE(MP2)=	-0.627599		
G3MP2(0 K)=	-584.264828	G3MP2 Energy=	-584.250306
G3MP2 Enthalpy=	-584.249362	G3MP2 Free Energy=	-584.309248

[15]EMIm-trz

0 1

6	2.705726000	-0.024344000	-0.842461000
7	2.746469000	0.788371000	0.217891000
7	2.096881000	-1.168794000	-0.624866000
7	1.721718000	-1.135238000	0.674136000
6	2.131558000	0.025314000	1.127042000
1	1.981449000	0.331053000	2.145765000
7	-0.973613000	1.636384000	-0.078945000
6	-0.526397000	0.460093000	-0.466858000
6	-2.299916000	1.496196000	0.278462000
6	-2.621773000	0.209862000	0.088851000
7	-1.493194000	-0.426181000	-0.385973000
1	0.462029000	0.247243000	-0.817182000
6	-0.172545000	2.857278000	-0.005167000
1	-0.446388000	3.525917000	-0.809793000
1	-0.354555000	3.336271000	0.946026000
1	0.870255000	2.585562000	-0.071846000
6	-1.340585000	-1.866233000	-0.667434000
1	-2.118709000	-2.136092000	-1.370345000
1	-0.377740000	-1.983216000	-1.139725000
6	-1.404837000	-2.700302000	0.603580000
1	-2.345988000	-2.565829000	1.128494000
1	-0.579170000	-2.440044000	1.251220000
1	-1.316990000	-3.748419000	0.339501000
1	3.132403000	0.228580000	-1.795015000
1	-2.880629000	2.318812000	0.633544000
1	-3.541168000	-0.308814000	0.247560000

RHF

Zero-point correction=	0.234876 (Hartree/Particle)
Thermal correction to Energy=	0.247220
Thermal correction to Enthalpy=	0.248164
Thermal correction to Gibbs Free Energy=	0.194677
Sum of electronic and zero-point Energies=	-582.448750
Sum of electronic and thermal Energies=	-582.436405
Sum of electronic and thermal Enthalpies=	-582.435461
Sum of electronic and thermal Free Energies=	-582.488948

G3MP2

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.209711	E(Thermal)=	0.223020
E(QCISD(T))=	-584.686217	E(Empiric)=	-0.324765
DE(MP2)=	-0.647033		
G3MP2(0 K)=	-585.448305	G3MP2 Energy=	-585.434995
G3MP2 Enthalpy=	-585.434051	G3MP2 Free Energy=	-585.489635

[16]EMIM-dtrz

0 1

6	2.382504000	-0.737001000	0.052467000
7	2.978064000	0.433469000	-0.018038000
7	1.070383000	-0.708146000	0.047567000
7	0.760696000	0.572423000	-0.032009000
6	1.912623000	1.200491000	-0.068311000
7	-2.509010000	-1.783592000	-0.084740000
6	-2.068027000	-0.544673000	-0.084736000
6	-3.880505000	-1.750569000	-0.227970000
6	-4.237293000	-0.460542000	-0.311687000
7	-3.080011000	0.284571000	-0.220480000
1	-1.046747000	-0.239275000	0.001544000
6	-1.669089000	-2.980026000	0.036513000
1	-1.944087000	-3.518158000	0.932270000
1	-1.819763000	-3.606583000	-0.830679000
1	-0.636357000	-2.671604000	0.091512000
6	-2.955430000	1.752979000	-0.254055000
1	-1.906083000	1.970913000	-0.390142000
1	-3.490840000	2.100274000	-1.127388000
6	-3.484514000	2.399182000	1.018334000
1	-2.932464000	2.053349000	1.884094000
1	-4.537599000	2.187199000	1.170167000
1	-3.363561000	3.473689000	0.947690000
1	-4.467946000	-2.641699000	-0.260609000
1	-5.197319000	-0.009176000	-0.432197000
7	3.095266000	-1.989359000	0.129325000
8	2.433788000	-2.987734000	0.176168000
8	4.282361000	-1.952153000	0.140875000
7	1.966736000	2.639359000	-0.159796000
8	3.035977000	3.155301000	-0.170247000
8	0.918659000	3.219704000	-0.219596000

RHF

Zero-point correction=	0.241216 (Hartree/Particle)
Thermal correction to Energy=	0.258925
Thermal correction to Enthalpy=	0.259869
Thermal correction to Gibbs Free Energy=	0.188713
Sum of electronic and zero-point Energies=	-989.399758
Sum of electronic and thermal Energies=	-989.382049
Sum of electronic and thermal Enthalpies=	-989.381105
Sum of electronic and thermal Free Energies=	-989.452262

G3MP2

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.215372	E(Thermal)=	0.234334
E(QCISD(T))=	-992.731454	E(Empiric)=	-0.473229
DE(MP2)=	-1.049864		
G3MP2(0 K)=	-994.039176	G3MP2 Energy=	-994.020214
G3MP2 Enthalpy=	-994.019270	G3MP2 Free Energy=	-994.093435

[17]EMIM-dn

0 1

7	-2.039106000	-0.283199000	0.020226000
6	-1.286091000	0.460064000	0.801004000
6	-2.461880000	0.499348000	-1.034007000
6	-1.942071000	1.720095000	-0.849879000
7	-1.213031000	1.678911000	0.316874000
1	-2.015082000	2.607490000	-1.438604000
1	-3.085255000	0.115860000	-1.810752000
6	-2.299057000	-1.722251000	0.195230000
1	-1.941989000	-1.983063000	1.178881000

```
1       -3.372520000     -1.858379000      0.169934000
6       -1.595490000     -2.560338000     -0.863179000
1       -0.524362000     -2.424544000     -0.804401000
1       -1.934692000     -2.308003000     -1.862330000
6       -0.350569000      2.746726000      0.824284000
1        0.528580000      2.808991000      0.203401000
1       -0.905653000      3.673626000      0.815279000
1       -0.055536000      2.502797000      1.830904000
1       -1.820905000     -3.606508000     -0.688412000
1       -0.781538000      0.113683000      1.675894000
7        1.913938000     -1.086717000     -0.197303000
7        2.345746000      0.049187000     -0.870440000
8        1.538125000      0.897773000     -1.145143000
8        3.465152000      0.037943000     -1.255366000
7        1.407040000     -0.789811000      0.954896000
8        1.549264000      0.303648000      1.480998000
8        0.774682000     -1.674666000      1.509475000

RHF
Zero-point correction=                           0.216093 (Hartree/Particle)
 Thermal correction to Energy=                    0.231004
 Thermal correction to Enthalpy=                  0.231949
 Thermal correction to Gibbs Free Energy=         0.170762
 Sum of electronic and zero-point Energies=           -804.772118
 Sum of electronic and thermal Energies=              -804.757207
 Sum of electronic and thermal Enthalpies=            -804.756263
 Sum of electronic and thermal Free Energies=         -804.817449

G3MP2
Temperature=              298.150000        Pressure=                     1.000000
 E(ZPE)=                    0.192940        E(Thermal)=                   0.208903
 E(QCISD(T))=            -807.478986        E(Empiric)=                  -0.389718
 DE(MP2)=                  -0.888131
 G3MP2(0 K)=             -808.563895        G3MP2 Energy=              -808.547932
 G3MP2 Enthalpy=         -808.546988        G3MP2 Free Energy=         -808.610653

[18]EMIM-tz

0 1
7        2.485704000     -0.225208000     -0.964270000
7        2.553136000     -0.982838000      0.115850000
7        2.171539000      0.978404000     -0.633565000
7        2.021188000      1.061554000      0.673799000
6        2.271995000     -0.158634000      1.105339000
1        2.253791000     -0.444242000      2.137330000
7       -1.461395000      0.529647000     -0.362232000
6       -0.590484000     -0.446353000     -0.490232000
6       -2.614212000      0.007604000      0.186624000
6       -2.404064000     -1.302574000      0.374029000
7       -1.121688000     -1.570420000     -0.057947000
1        0.395283000     -0.345389000     -0.896709000
1       -3.038123000     -2.063388000      0.772971000
1       -3.469430000      0.612540000      0.392006000
6       -0.438353000     -2.864110000     -0.028807000
1        0.620714000     -2.692474000     -0.147839000
1       -0.619535000     -3.330550000      0.928626000
1       -0.814749000     -3.495209000     -0.821789000
6       -1.201349000      1.945764000     -0.684149000
1       -0.273373000      1.969319000     -1.233788000
1       -2.003628000      2.275417000     -1.331636000
6       -1.092221000      2.801710000      0.569460000
1       -0.245964000      2.483281000      1.162970000
1       -1.997902000      2.758712000      1.166705000
1       -0.934347000      3.833560000      0.276131000

RHF
 Zero-point correction=                           0.222023 (Hartree/Particle)
 Thermal correction to Energy=                    0.234397
 Thermal correction to Enthalpy=                  0.235341
 Thermal correction to Gibbs Free Energy=         0.181418
 Sum of electronic and zero-point Energies=           -598.433170
```

```
 Sum of electronic and thermal Energies=             -598.420797
 Sum of electronic and thermal Enthalpies=           -598.419853
 Sum of electronic and thermal Free Energies=        -598.473775
```

G3MP2

```
 Temperature=              298.150000       Pressure=                    1.000000
 E(ZPE)=                     0.198235       E(Thermal)=                  0.211531
 E(QCISD(T))=             -600.692961       E(Empiric)=                 -0.324765
 DE(MP2)=                   -0.653225
 G3MP2(0 K)=              -601.472715       G3MP2 Energy=             -601.459419
 G3MP2 Enthalpy=          -601.458475       G3MP2 Free Energy=        -601.514453
```

[19]EMIm-mtz

```
0 1
7       -2.077280000     -0.086565000     -1.537175000
7       -2.396192000      0.703180000     -0.524827000
7       -1.724044000     -1.238186000     -1.092934000
7       -1.797182000     -1.253594000      0.224760000
6       -2.226163000     -0.046949000      0.547768000
7        1.753933000     -0.444721000     -0.267394000
6        0.837392000      0.438172000     -0.596156000
6        2.749305000      0.208073000      0.429640000
6        2.400276000      1.500066000      0.499244000
7        1.190951000      1.625968000     -0.152389000
1       -0.054097000      0.225985000     -1.151403000
1        2.891231000      2.334707000      0.949094000
1        3.605812000     -0.303728000      0.809121000
6        0.406211000      2.849951000     -0.317901000
1       -0.599902000      2.573948000     -0.595472000
1        0.385415000      3.378614000      0.624008000
1        0.855340000      3.473109000     -1.078690000
6        1.672960000     -1.892013000     -0.541856000
1        0.856383000     -2.026689000     -1.233839000
1        2.598194000     -2.174000000     -1.027682000
6        1.425894000     -2.697362000      0.725590000
1        0.465497000     -2.435752000      1.148690000
1        2.208393000     -2.540460000      1.461767000
1        1.411657000     -3.751761000      0.473041000
6       -2.514450000      0.400584000      1.946182000
1       -2.498771000      1.482566000      2.009767000
1       -3.496427000      0.064497000      2.264540000
1       -1.788584000     -0.006734000      2.641701000
```

RHF

```
Zero-point correction=                           0.251394 (Hartree/Particle)
 Thermal correction to Energy=                    0.265487
 Thermal correction to Enthalpy=                  0.266432
 Thermal correction to Gibbs Free Energy=         0.208222
 Sum of electronic and zero-point Energies=           -637.445249
 Sum of electronic and thermal Energies=              -637.431156
 Sum of electronic and thermal Enthalpies=            -637.430212
 Sum of electronic and thermal Free Energies=         -637.488422
```

G3MP2

```
 Temperature=              298.150000       Pressure=                    1.000000
 E(ZPE)=                     0.224459       E(Thermal)=                  0.239600
 E(QCISD(T))=             -639.881516       E(Empiric)=                 -0.352602
 DE(MP2)=                   -0.704724
 G3MP2(0 K)=              -640.714383       G3MP2 Energy=             -640.699242
 G3MP2 Enthalpy=          -640.698298       G3MP2 Free Energy=        -640.758890
```

[20]EMIM-CNtz

```
0 1
7       -1.753565000     -1.237344000     -1.591624000
7       -2.318517000     -0.216123000     -0.997621000
7       -1.187417000     -2.000836000     -0.714110000
7       -1.359605000     -1.511211000      0.486534000
6       -2.066551000     -0.415678000      0.282461000
7        1.925580000     -0.127649000     -0.202395000
```

```
6        0.874630000      0.416218000     -0.774046000
6        2.602297000      0.862800000      0.478099000
6        1.925819000      2.004096000      0.290341000
7        0.839796000      1.703570000     -0.504132000
1        0.155773000     -0.109726000     -1.366453000
1        2.108279000      2.993519000      0.647640000
1        3.493513000      0.664335000      1.030815000
6       -0.208623000      2.636369000     -0.923057000
1       -0.974769000      2.082814000     -1.441830000
1       -0.640902000      3.095146000     -0.046264000
1        0.217850000      3.389138000     -1.570542000
6        2.259880000     -1.564577000     -0.221508000
1        1.580962000     -2.028422000     -0.919690000
1        3.268724000     -1.652328000     -0.603227000
6        2.114451000     -2.198868000      1.154515000
1        1.092723000     -2.117627000      1.500089000
1        2.779481000     -1.741924000      1.880225000
1        2.371103000     -3.249744000      1.083231000
6       -2.440820000      0.507631000      1.318376000
7       -2.691878000      1.273432000      2.119765000

RHF
Zero-point correction=                           0.220398 (Hartree/Particle)
 Thermal correction to Energy=                    0.234526
 Thermal correction to Enthalpy=                  0.235470
 Thermal correction to Gibbs Free Energy=         0.176628
 Sum of electronic and zero-point Energies=           -690.175513
 Sum of electronic and thermal Energies=              -690.161384
 Sum of electronic and thermal Enthalpies=            -690.160440
 Sum of electronic and thermal Free Energies=         -690.219283

G3MP2
Temperature=              298.150000 Pressure=                     1.000000
 E(ZPE)=                     0.196784 E(Thermal)=                   0.211959
 E(QCISD(T))=             -692.720567 E(Empiric)=                  -0.361881
 DE(MP2)=                   -0.724819
 G3MP2(0 K)=              -693.610484 G3MP2 Energy=              -693.595308
 G3MP2 Enthalpy=          -693.594364 G3MP2 Free Energy=         -693.655592
```

[21]EMIM-NO_2tz

```
0 1
7       -1.427740000     -0.992339000     -1.995803000
7       -1.962857000     -0.031161000     -1.286475000
7       -0.998752000     -1.933293000     -1.214179000
7       -1.253378000     -1.632001000      0.032267000
6       -1.844270000     -0.466060000     -0.056246000
7        2.121544000     -0.164699000     -0.112691000
6        1.170467000      0.447821000     -0.782879000
6        2.717450000      0.757666000      0.721107000
6        2.094300000      1.927938000      0.523718000
7        1.121410000      1.713493000     -0.428189000
1        0.529038000     -0.016085000     -1.502141000
1        2.244309000      2.885234000      0.972024000
1        3.519374000      0.497149000      1.375415000
6        0.168448000      2.709244000     -0.930213000
1       -0.289319000      3.205190000     -0.089139000
1        0.690423000      3.420084000     -1.554918000
1       -0.601105000      2.200132000     -1.486876000
6        2.432192000     -1.604756000     -0.194240000
1        1.832689000     -2.002750000     -0.998274000
1        3.476806000     -1.691362000     -0.463277000
6        2.119487000     -2.330022000      1.107131000
1        1.065801000     -2.254892000      1.339836000
1        2.701461000     -1.938799000      1.935185000
1        2.370410000     -3.378199000      0.990593000
7       -2.245913000      0.298858000      1.092903000
8       -2.437850000     -0.285659000      2.110957000
8       -2.333216000      1.487072000      0.956101000
```

RHF

Zero-point correction= 0.225238 (Hartree/Particle)
Thermal correction to Energy= 0.240138
Thermal correction to Enthalpy= 0.241082
Thermal correction to Gibbs Free Energy= 0.179746
Sum of electronic and zero-point Energies= -801.902142
Sum of electronic and thermal Energies= -801.887242
Sum of electronic and thermal Enthalpies= -801.886297
Sum of electronic and thermal Free Energies= -801.947633

G3MP2

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.201105	E(Thermal)=	0.217088
E(QCISD(T))=	-804.713356	E(Empiric)=	-0.398997
DE(MP2)=	-0.857593		
G3MP2(0 K)=	-805.768842	G3MP2 Energy=	-805.752858
G3MP2 Enthalpy=	-805.751914	G3MP2 Free Energy=	-805.815761

[22]EMIm-NO_2Otz

0 1

7	-1.125290000	-1.515497000	-0.265665000
7	-1.406221000	-0.253130000	-0.194686000
7	-2.148135000	-2.284270000	-0.113041000
7	-3.184747000	-1.506447000	0.071660000
6	-2.706993000	-0.300096000	0.016826000
7	2.969691000	-0.057289000	-0.220929000
6	1.761049000	0.452554000	-0.330078000
6	3.841776000	0.960237000	0.101406000
6	3.120225000	2.087725000	0.173343000
7	1.811393000	1.747699000	-0.099697000
1	0.890270000	-0.136491000	-0.545681000
6	0.667779000	2.663035000	-0.127617000
1	-0.238547000	2.088248000	-0.226171000
1	0.640968000	3.219451000	0.797992000
1	0.771415000	3.342763000	-0.961607000
6	3.289493000	-1.490526000	-0.353019000
1	2.574002000	-1.908728000	-1.042832000
1	4.275058000	-1.547367000	-0.795288000
6	3.223366000	-2.213689000	0.984130000
1	2.209742000	-2.200759000	1.362512000
1	3.890367000	-1.765901000	1.713726000
1	3.517357000	-3.247853000	0.844526000
7	-3.490352000	0.892442000	0.172521000
8	-4.657765000	0.770831000	0.346497000
8	-2.900993000	1.936023000	0.116431000
8	0.059764000	-1.937469000	-0.465580000
1	4.886122000	0.789234000	0.243744000
1	3.410660000	3.092317000	0.389201000

RHF

Zero-point correction= 0.229823 (Hartree/Particle)
Thermal correction to Energy= 0.245562
Thermal correction to Enthalpy= 0.246506
Thermal correction to Gibbs Free Energy= 0.182023
Sum of electronic and zero-point Energies= -876.697989
Sum of electronic and thermal Energies= -876.682251
Sum of electronic and thermal Enthalpies= -876.681307
Sum of electronic and thermal Free Energies= -876.745790

G3MP2

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.205199	E(Thermal)=	0.222100
E(QCISD(T))=	-879.700011	E(Empiric)=	-0.426834
DE(MP2)=	-0.942222		
G3MP2(0 K)=	-880.863867	G3MP2 Energy=	-880.846967
G3MP2 Enthalpy=	-880.846023	G3MP2 Free Energy=	-880.913195

[23]EMIM-NH_2tz

0 1

7	-2.052952000	0.010465000	-1.506430000

```
7       -2.398738000      0.771624000     -0.466833000
7       -1.732367000     -1.155121000     -1.104667000
7       -1.850851000     -1.233302000      0.218162000
6       -2.282591000     -0.038221000      0.564649000
7        1.755429000     -0.466079000     -0.268977000
6        0.855265000      0.440159000     -0.578781000
6        2.768425000      0.155375000      0.431214000
6        2.446644000      1.453274000      0.522578000
7        1.235625000      1.613486000     -0.118563000
1       -0.044212000      0.253895000     -1.131923000
1        2.958301000      2.270858000      0.980684000
1        3.616956000     -0.379483000      0.796701000
6        0.476559000      2.855486000     -0.268317000
1       -0.539676000      2.602560000     -0.531763000
1        0.483423000      3.382200000      0.675052000
1        0.927350000      3.471185000     -1.034127000
6        1.643165000     -1.906488000     -0.568915000
1        0.828131000     -2.010172000     -1.268100000
1        2.564960000     -2.200717000     -1.053888000
6        1.369211000     -2.727967000      0.682456000
1        0.408962000     -2.456287000      1.099593000
1        2.147103000     -2.597364000      1.428681000
1        1.338145000     -3.777629000      0.412472000
7       -2.619602000      0.312024000      1.865804000
1       -2.577450000      1.293550000      2.032931000
1       -2.127870000     -0.213974000      2.554916000
```

RHF

```
 Zero-point correction=                           0.240668 (Hartree/Particle)
 Thermal correction to Energy=                    0.254298
 Thermal correction to Enthalpy=                  0.255243
 Thermal correction to Gibbs Free Energy=         0.198442
 Sum of electronic and zero-point Energies=           -653.449526
 Sum of electronic and thermal Energies=              -653.435896
 Sum of electronic and thermal Enthalpies=            -653.434952
 Sum of electronic and thermal Free Energies=         -653.491752
```

G3MP2

```
 Temperature=              298.150000       Pressure=                     1.000000
 E(ZPE)=                     0.214882       E(Thermal)=                   0.229575
 E(QCISD(T))=             -655.899107       E(Empiric)=                  -0.352602
 DE(MP2)=                   -0.721987
 G3MP2(0 K)=              -656.758814       G3MP2 Energy=              -656.744121
 G3MP2 Enthalpy=          -656.743177       G3MP2 Free Energy=         -656.802322
```

Part-III : Theoretical density specific impulse of EILs

Table S11: Theoretical density specific impulse of EILs

IL	Theoretical density (g/cc)	Isp (s)	Density Isp (s)
$[EMIm]^+[BF_4]^-$	1.730	-	-
$[EMIm]^+[PF_6]^-$	1.907	105	200
$[EMIm]^+[dc]^-$	1.684	209	350
$[EMIm]^+[trz]^-$	1.592	207	330
$[EMIm]^+[dtrz]^-$	1.469	241	354
$[EMIm]^+[dn]^-$	1.485	252	374
$[EMIm]^+[tz]^-$	1.545	201	341
$[EMIm]^+[Mtz]^-$	1.282	213	273
$[EMIm]\ ]^+[CN\text{-}tz]^-$	1.427	221	315
$[EMIm]\ ]^+[NH_2\text{-}tz]^-$	1.172	220	257
$[EMIm]\ ]^+[NO_2\text{-}tz]^-$	1.603	239	383
$[EMIm]^+[NO_2\text{-}O\text{-}tz]^-$	1.542	246	379
Hydrazine	0.947	263	249

Part-IV : Thermochemical calculation exemplified for $[EMIm]^+[dn]^-$

MF : $C_6N_5O_4H_{11}$

G3MP2 (all energy values in au)

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.192940	E(Thermal)=	0.208903
E(QCISD(T))=	-807.478986	E(Empiric)=	-0.389718
DE(MP2)=	-0.888131		
G3MP2(0 K)=	-808.563895	G3MP2 Energy=	-808.547932
G3MP2 Enthalpy=	-808.546988	G3MP2 Free Energy=	-808.610653

Table S12: Energy parameters for $[EMIm]^+[dn]^-$ (Experimetnal values in kcal/mol and G3MP2 values in au).

		Experimental			Computaional values-G3MP2			
Element	n	ΔH^0_f(0K)	H^0(298K)-H^0(0K)	S^O(298K)	ε_0	ε_{ZPE}	Hcorr	Gcorr
H	11	51.63	1.01	27.418	-0.500423	0.000000	0.002360	-0.010654
C	6	169.98	0.25	37.787	-37.787922	0.000000	0.002360	-0.014545
N	5	112.53	1.04	36.64	-54.523780	0.000000	0.002360	-0.015036
O	4	58.99	1.04	38.494	-74.988358	0.000000	0.002360	-0.014952

(a) Atomization energy of the molecule, $\sum D_o$(M)

$\sum D_o$(M) $= \sum$n.X(ε_o)- M(ε_{o+ZPE})

= [(11 * -0.500423) + (6 * -37.787922) + (5 * -54.523780) + (4 * - 74.988358)] - [-808.547932]

= 3.743415 H * 627.51

= 2349.03 kcal/mol

(b) Heat of formation of the molecule at 0K, $\Delta_f H^o$(M,0K)

$\Delta_f H^o$(M,0K) = $\sum$n.$\Delta_f H^o$(X,0K)- $\sum D_o$(M)

= [(11*51.63) + (6*169.98) + (5*112.53) + (4* 58.99)] - 2349.03

= 2386.42 - 2349.03

= 37.39 kcal/mol

(c) Enthalpy correction for the molecule, H^o_M(298 K)- H^o_M(0 K)

(i) H^o_M(298 K)- H^o_M(0 K) = [H_{corr}- M(ε_{ZPE})]

= (0.231949 - 0.192940)

= 0.039009 H * 627.51

= 24.48 kcal/mol

(ii) $\sum$[n.(H^o(298K)-H^o(0K))] = [(11*1.01) + (6*0.25) +(5*1.04) + (4*1.04)]

= 21.97 kcal/mol

(d) Heat of formation of the molecule at 298K, $\Delta_f H^o$(M,298K).

$\Delta_f H^o$(M,298K) = $\Delta_f H^o$(M,0K) + [H^o_M(298 K)- H^o_M(0 K)]-[$\sum$n.(H^o(298K)-H^o(0K))]

= 37.39 + 24.48 - 21.97

= 39.90 kcal/mol

= 166.86 kJ/mol

Part-V : Energetics for conformers of $[EMIm]^+[dn]^-$

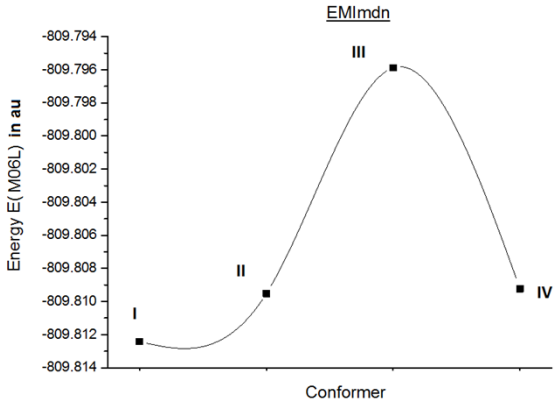


Table S13: Energy parameters for $[EMIm]^+[dn]^-$ at M06L/6-311+g(d,p) level.

Conformer	E (au)	$\Delta_f H°$(M,298K) (kJ/mol)	BE (kJ/mol)	ΔE^* (eV)	MK charge
I	-809.812420760	196.25	356.1	3.32	-0.850
II	-809.809514293	202.90	364.3	3.48	-0.809
III	-809.795883209	238.90	320.9	2.80	-0.870
IV	-809.809225258	204.40	355.8	3.29	-0.838

Table S14. Mole fraction of carbon in EIL and in presence of oxidiser

Oxidiser	0.0%	10%	20%	30%	40%	50%	60%
$[EMIm]^+[tz]^-$	0.43	0.40	0.36	0.30	0.22	0.12	0.04
$[EMIm]^+[mtz]^-$	0.43	0.41	0.37	0.32	0.24	0.15	0.06
$[EMIm]^+[dc]^-$	0.50	0.47	0.42	0.35	0.27	0.17	0.07
$[EMIm]^+[CNtz]^-$	0.47	0.43	0.38	0.30	0.22	0.12	0.03
$[EMIm]^+[NH_2tz]^-$	0.39	0.37	0.34	0.28	0.20	0.11	0.03
$[EMIm]^+[trz]^-$	0.46	0.44	0.40	0.34	0.27	0.17	0.07
$[EMIm]^+[dtrz]^-$	0.32	0.25	0.18	0.11	0.05	0.00	0.00
$[EMIm]^+[dn]^-$	0.25	0.19	0.12	0.07	0.02	0.00	0.00
$[EMIm]^+[NO_2tz]^-$	0.37	0.31	0.25	0.17	0.09	0.03	0.00
$[EMIm]^+[NO_2Otz]^-$	0.32	0.26	0.19	0.12	0.05	0.00	0.00

Table S15. Isp values (in s) of EILs at various HAN concentration.

HAN (%)	$[EMIm]^+[tz]^-$	$[EMIm]^+[mtz]^-$	$[EMIm]^+[dc]^-$	$[EMIm]^+[CNtz]^-$	$[EMIm]^+[NH_2tz]^-$	$[EMIm]^+[trz]^-$	$[EMIm]^+[dtrz]^-$	$[EMIm]^+[dn]^-$	$[EMIm]^+[NO_2tz]^-$	$[EMIm]^+[NO_2Otz]^-$
0	221	213	208	221	219	207	241	252	239	246
10	229	222	218	228	227	217	246	256	244	251
20	236	230	226	235	235	225	250	260	249	255
30	243	238	234	242	242	234	258	272	254	260

40	249	245	242	249	248	242	273	286	263	274
50	257	252	250	257	257	249	291	301	281	291
60	277	271	267	278	279	266	305	312	299	306
70	301	297	294	302	302	292	315	319	313	316
80	317	315	314	316	317	314	307	308	315	310
90	296	299	299	293	294	301	278	279	284	280
100	238	238	238	238	238	238	238	238	238	238

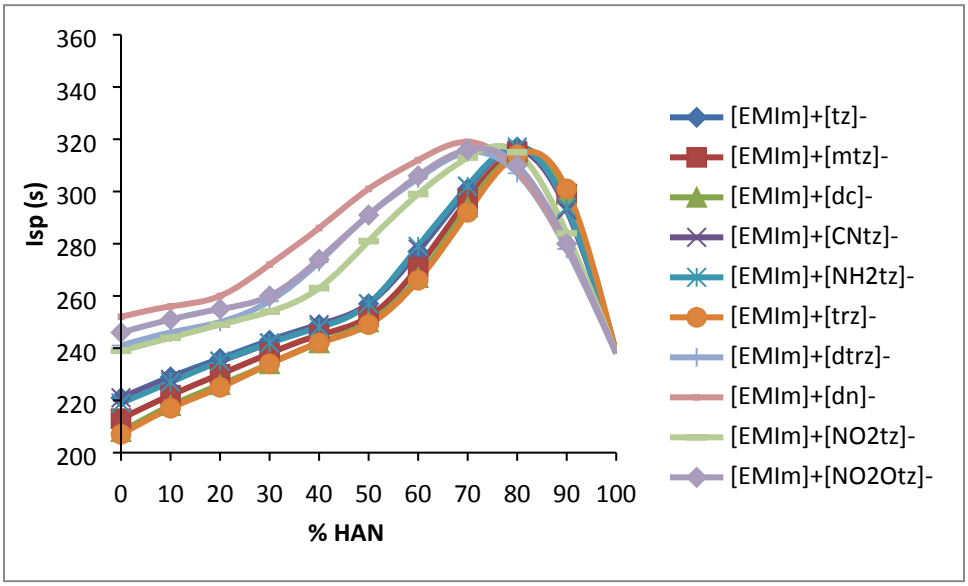


Figure S14: Plot showing the variation of Isp with respect to increasing concentration of HAN.