# Supplementary Material

## Matrix Isolation of Vapors from 1,2,4-Triazolium Salts: Exploring the Generation of *N*-Heterocyclic Carbenes

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# 1. Figures

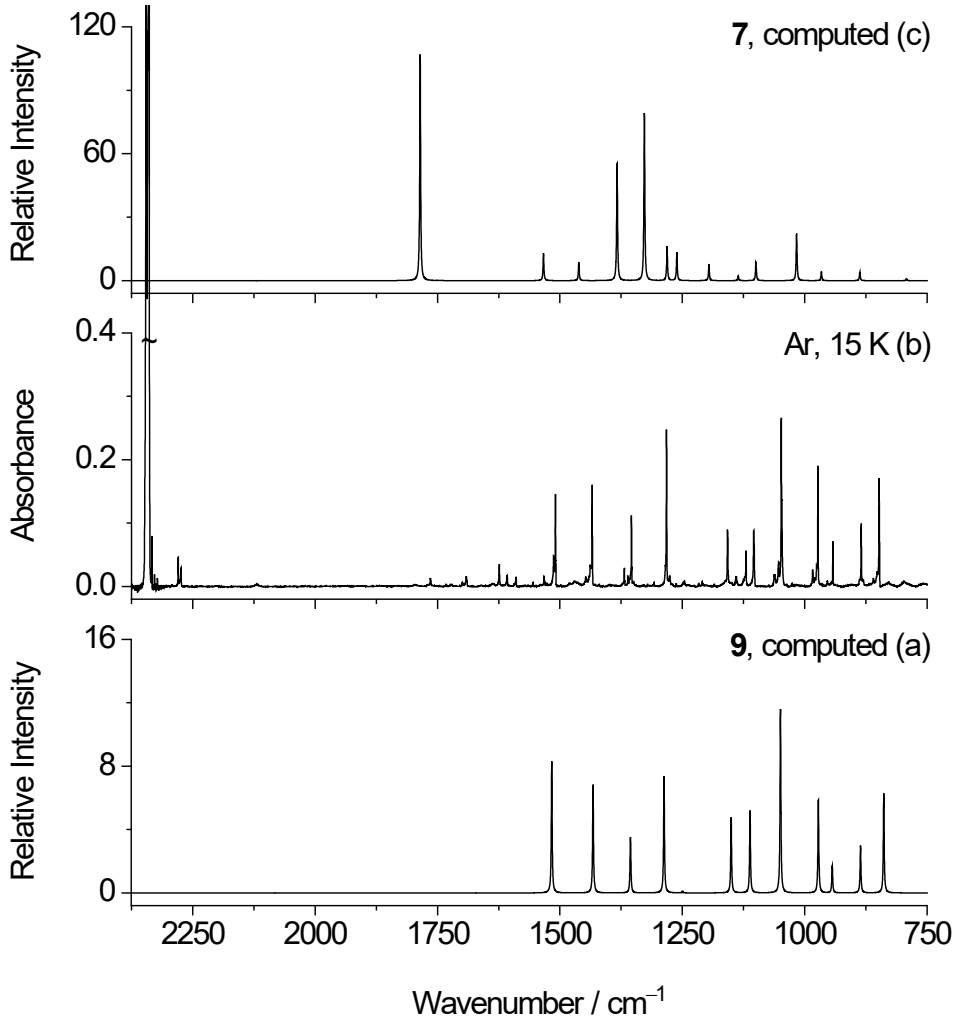


**Figure S1.** (b) Experimental IR spectrum recorded after trapping vapors of 1,2,4-triazole-3-carboxylic acid **7** in an Ar matrix at 15 K. Sublimation of the compound was achieved through heating the compound at ~338 K inside a miniature glass oven as described in the Materials and Methods section of this paper. The bands at 2345-2339 and 664-662 $cm^{-1}$, marked with an asterisk (*), are due to $CO_2$ trapped in the matrix. The experimental spectrum is compared with the B3LYP/6-311+G(2d,p) calculated IR spectra of (a) the most stable isomer of **7**, and of (c) 1,2,4-triazole **9** which nicely reproduces the experimental data. The calculated wavenumbers were scaled by 0.980. At the top of the figure, the thermal decomposition reaction of 1,2,4-triazole-3-carboxylic acid **7** is depicted, illustrating its conversion to 1,2,4-triazole **9** and $CO_2$.

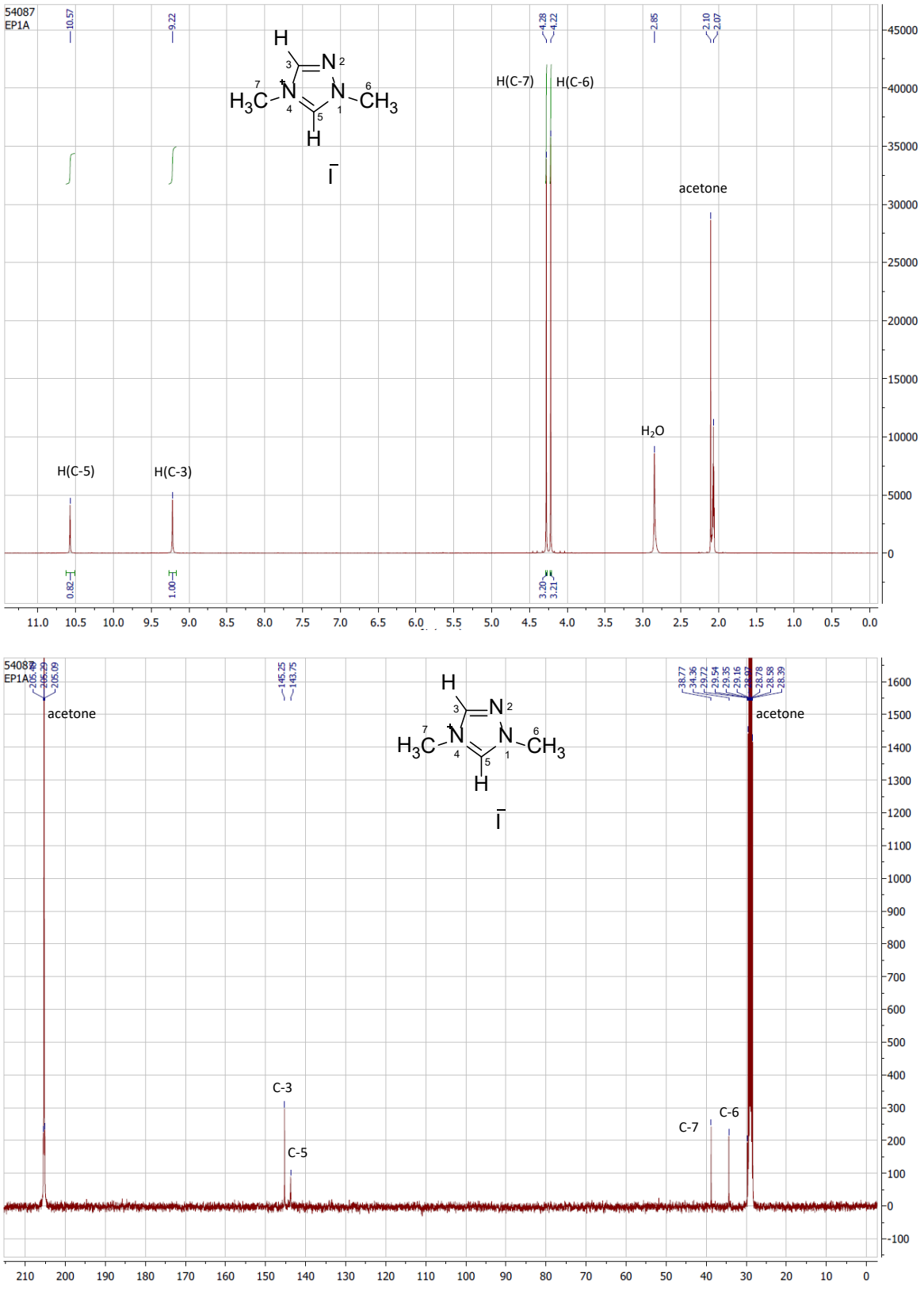


**Figure S2a.** $^{1}$H NMR (top) and $^{13}$C NMR (bottom) spectra of 1,4-dimethyl-1,2,4-triazolium iodide **[DMTrH$^{+}$][I$^{-}$]** (acetone-d$_6$).

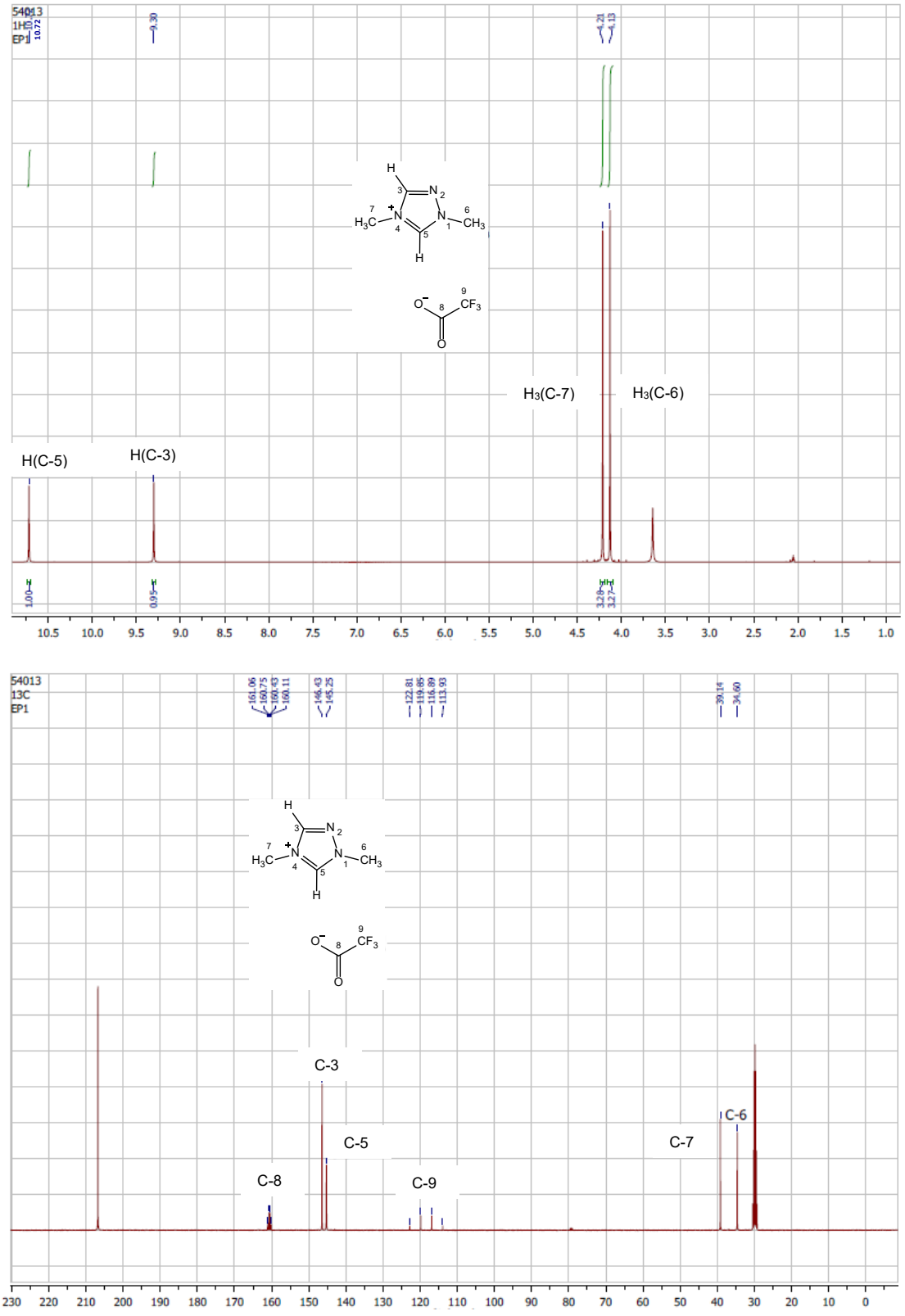


**Figure S2b.** $^{1}$H NMR (top) and $^{13}$C NMR (bottom) spectra of 1,4-dimethyl-1,2,4-triazolium trifluoroacetate **[DMTrH$^{+}$][TFA$^{-}$]** (acetone-$d_6$).

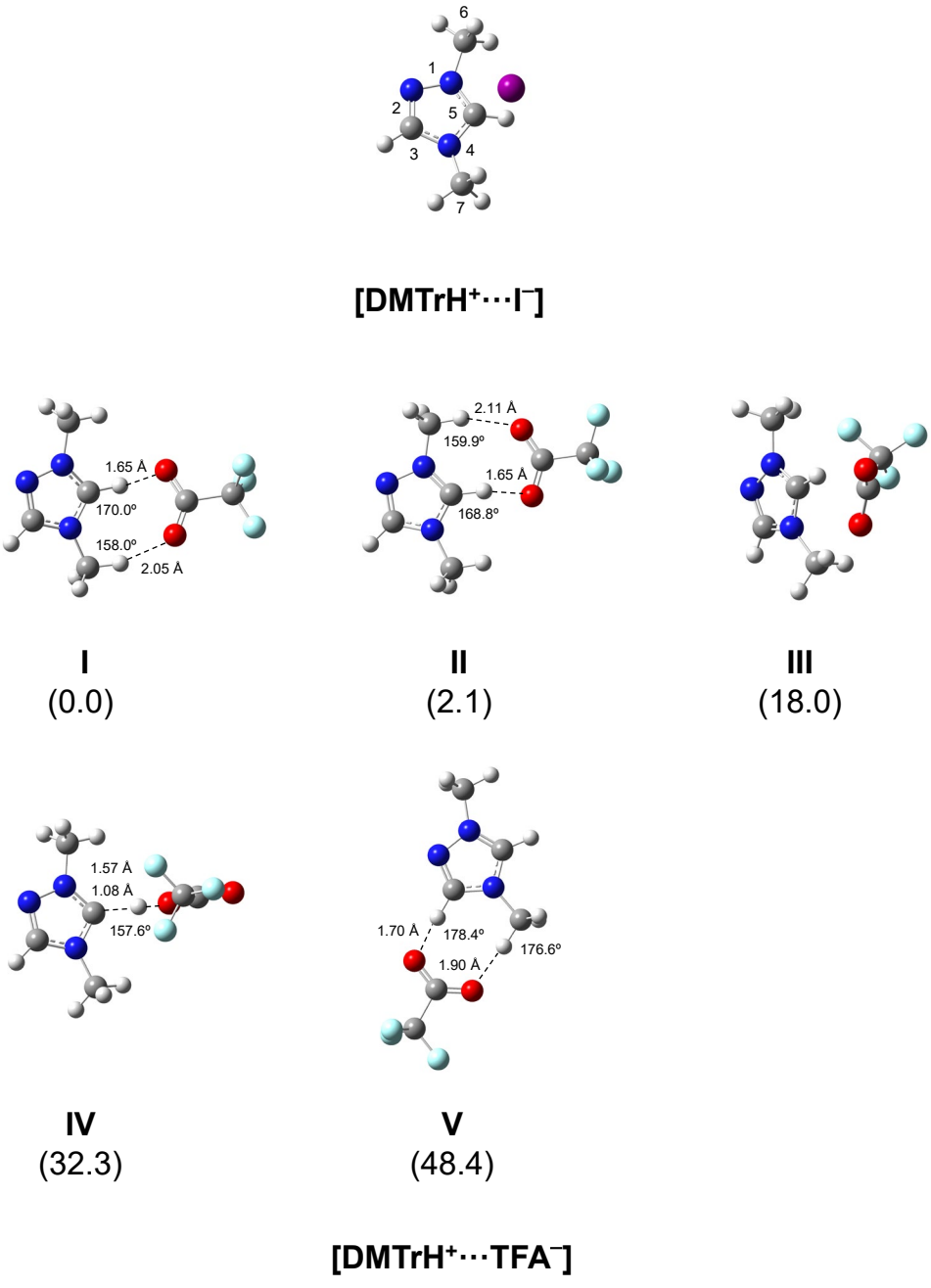


**Figure S3.** B3LYP/6-311+G(2d,p)[LANL2DZ]-GD3BJ optimized geometry of the **[DMTrH$^+$···I$^-$]** ion pair (atom numbering is given for the 1,2,4-triazolim cation) and B3LYP/6-311+G(2d,p)-GD3BJ optimized geometries of all minima exhibited by the **[DMTrH$^+$···TFA$^-$]** ion pair (values in square brackets are the relative Gibbs energies at 298.15 K in kJ mol$^{-1}$). The geometric parameters refer to H···O distances (Å) and C−H···O angles (º) characterizing the hydrogen bonds formed. In the specific case of structure **IV** of the **[DMTrH$^+$···TFA$^-$]** ion pair, the C5···H distance is also shown. Counterpoise correction was applied in all geometry optimizations.

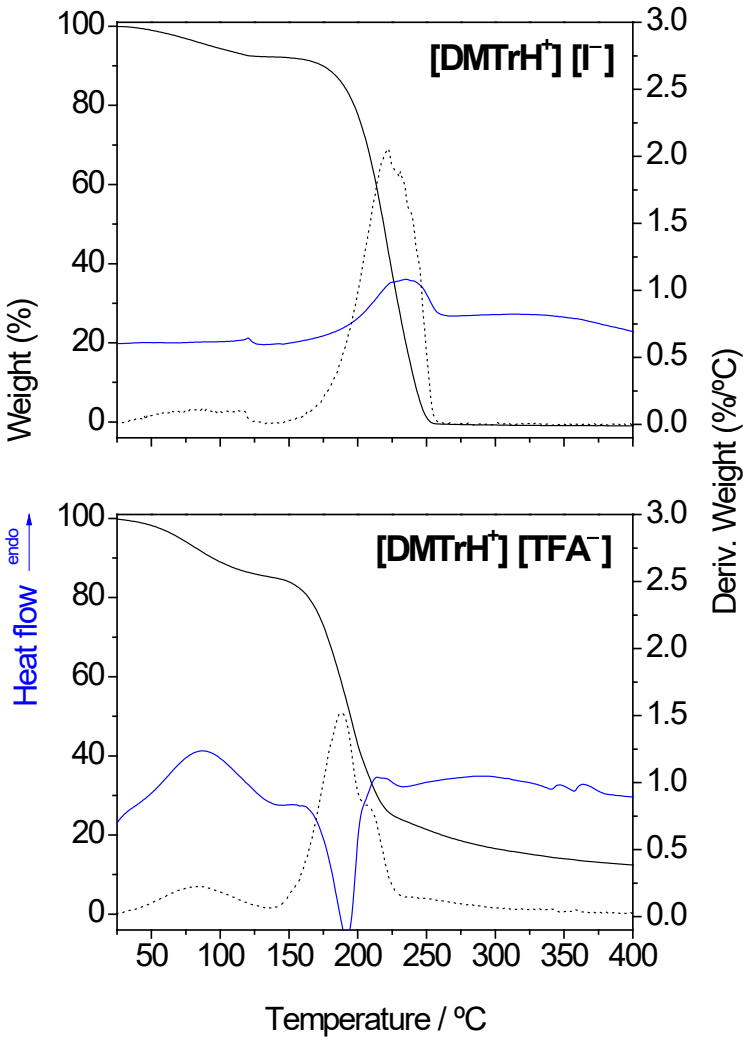


**Figure S4.** TG (black solid trace), DTG (dotted trace), and DSC (blue trace) curves for solid 1,4-dimethyl-4*H*-1,2,4-triazolium iodide **[DMTrH$^+$][TFA$^-$]** and liquid salt 1,4-dimethyl-4*H*-1,2,4-triazolium trifluoroacetate **[DMTrH$^+$][TFA$^-$]**.

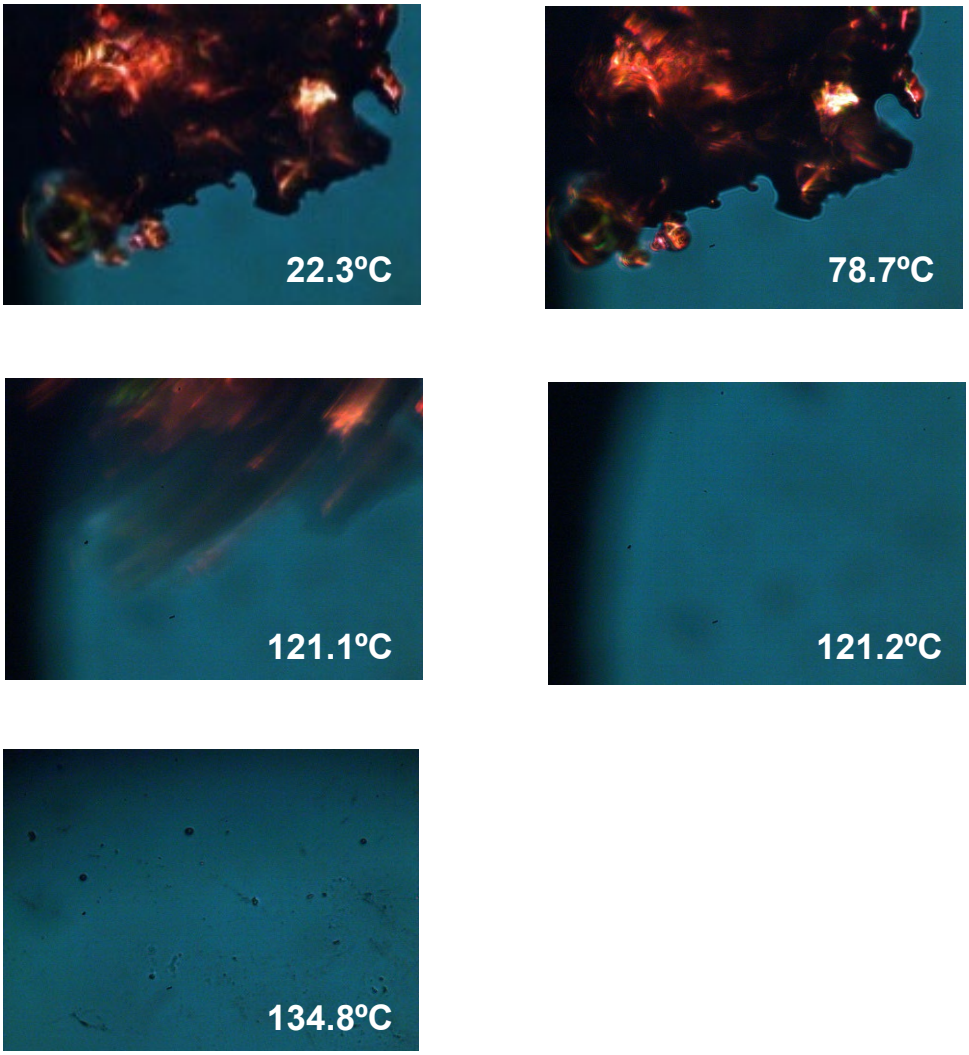


**Figure S5.** Polarized light thermomicroscopy images collected upon heating 1,4-dimethyl-4*H*-1,2,4-triazolium iodide **[DMTrH$^+$][I$^-$]** from 22 to 135 °C at a rate of 10 °C min$^{-1}$.

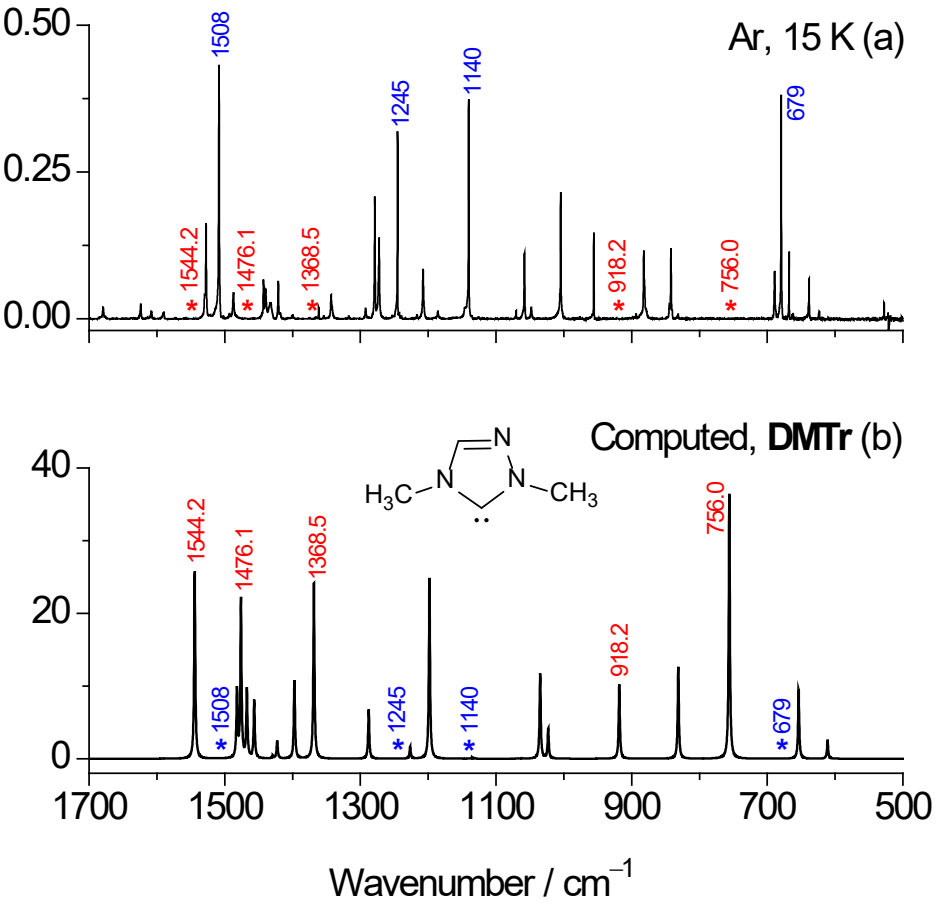


**Figure S6.** Spectral evidence for the non-formation of carbene 2,4-dimethyl-1,2,4-triazol-5-ylidene **DMTr** upon sublimation of 1,4-dimethyl-4*H*-1,2,4-triazolium iodide **[DMTrH$^+$][I$^-$]**. (a) Experimental IR spectrum of the vapors produced from the sublimation of the solid salt at ~ 363 K and trapped in solid Ar at 15 K. Red asterisks indicate predicted absorption positions for **DMTr** that lack correspondence in the experimental spectrum; (b) B3LYP/6-311+G(2d,p) calculated spectrum of **DMTr**. The wavenumbers were scaled by 0.98 and the the bands were simulated with Lorentzian functions with a full width at half-maximum (FWHM) of 2 cm$^{-1}$, with the band heights adjusted to match the calculated IR intensities Blue asterisks mark experimental band positions with no corresponding bands in the calculated spectrum.

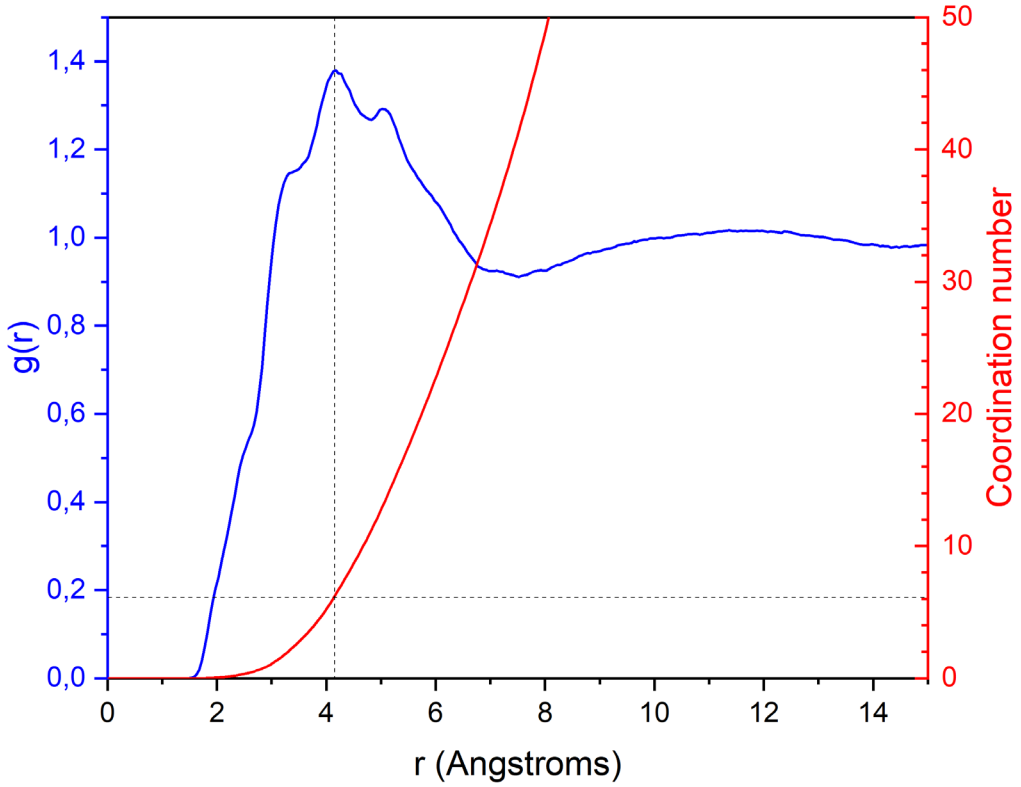


**Figure S7.** Radial distribution function (blue) and its integrated form (red), showing the number of anions around the cation moiety of the ionic liquid. The first "coordination sphere" contains 6 **TFA**$^{-}$ anions around 1 **DMTrH**$^{+}$ cation.

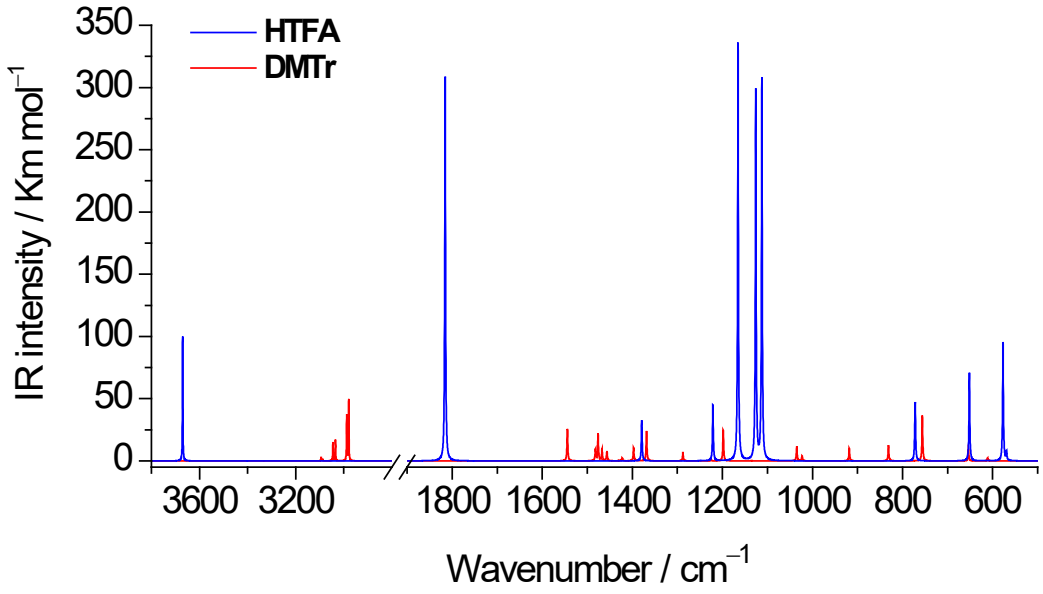


**Figure S8.** B3LYP/6-311+G(2d,p) spectra calculated for 1,4-dimethyl-1,2,4-triazol-5-ylidene **DMTr** (red trace) and for the most stable conformer of trifluoroacetic acid (**HTFA**, blue trace), highlighting the differences in band intensities between the two spectra. The wavenumbers were scaled by 0.980 and the the bands were simulated with Lorentzian functions with a full width at half-maximum (FWHM) of 2 $cm^{-1}$, with the band heights adjusted to match the calculated IR intensities.

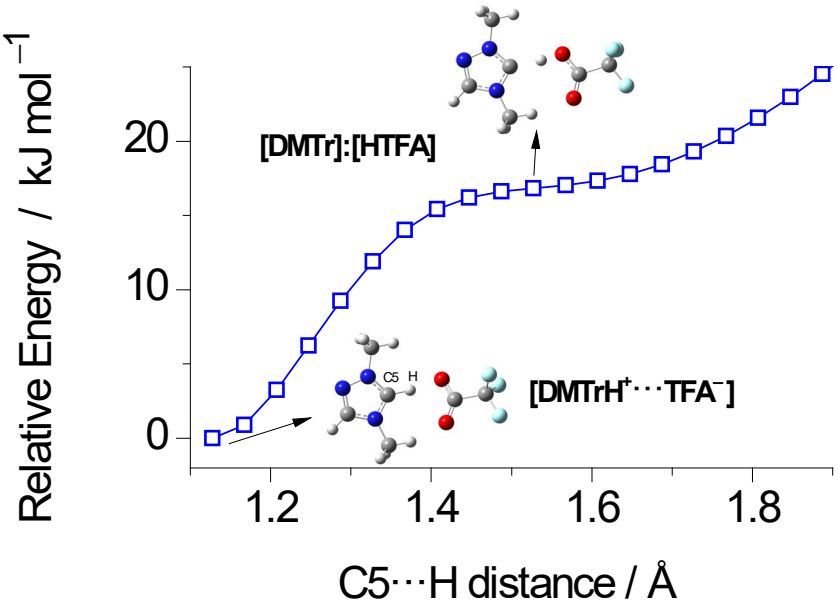


**Figure S9.** B3LYP/6-311+G(2d,p) relaxed potential energy scan as a function of the C5···H distance for the dissociation of the **[DMTrH$^+$···TFA$^-$]** ion pair. The minimum energy (C5···H = 1.13 Å) corresponds to the ion pair, while the flat region at C5···H = 1.57 Å represents the formation of the **[DMTrH$^+$]:[TFA$^-$]** complex which does not correspond to a true energy minimum.

## 2. Tables

**Table S1.** Experimental ATR IR spectrum of 1,4-dimethyl-4*H*-1,2,4-triazolium iodide [**DMTrH**$^+$] [**I**$^-$] at room temperature, B3LYP/6-311+G(2d,p)[LANL2DZ]-GD3BJ (including counterpoise correction) computed vibrational frequencies ($\tilde{\nu}$, cm$^{-1}$) and absolute intensities ($A^{th}$, km mol$^{-1}$), and approximate vibrational assignment for the **DMTrH$^+$···I$^-$** ion pair.

| Exp. (KBr pellet) [a] | | Calc. | | Approx. assignment [c] |
|---|---|---|---|---|
| $\tilde{\nu}$ | Int. | $\tilde{\nu}$ [b] | $A^{th}$ | |
| **1583**/1542 | s | 1561.4 | 65.2 | $\nu C_5N_4 - \nu C_3N_2$ |
| | | 1508.0 | 67.4 | $\nu C_5N_1 - \nu C_3N_2$ |
| 1452 | m, br | 1483.8 | 11.4 | $\delta(CH_3)$ as |
| | | 1472.1 | 11.7 | $\delta(CH_3)$ as |
| | | 1454.0 | 8.5 | $\delta CH_3$ as' |
| | | 1448.7 | 12.5 | $\delta CH_3$ as' |
| 1401 | | 1428.0 | 2.6 | $\delta CH_3$ s |
| 1389 | | 1410.3 | 3.6 | $\delta CH_3$ s |
| 1365 | m | 1377.9 | 78.0 | $\nu C_5N_4 + \nu C_5N_1 + \nu C_3N_2$ |
| | | 1363.3 | 13.6 | $\nu C_3N_4 - \nu C_6N_1$ |
| 1293 | w | 1275.4 | 3.5 | $\nu N_1N_2 + \nu C_5N_4$ |
| 1242 | w | 1228.4 | 6.8 | $\delta C_3H$ |
| 1178/**1166** | s | 1163.1 | 44.5 | $\delta C_5H$ |
| 1093 | w | 1126.2 | 5.0 | $\rho CH_3$ |
| 1077/**1070** | m | 1078.8 | 32.1 | $\rho CH_3'$; $\nu C_5N_1 + \nu C_5N_4$ |
| 988 | m | 1055.6 | 21.1 | $\nu C_3N_4$; $\delta N_1N_2C_3$; $\delta C_3N_4C_5$ |
| 900 | m | 960.5 | 20.0 | $\nu N_1N_2$; $\delta N_1N_2C_3$ |
| 854 | w | 832.2 | 4.4 | $\gamma C_3$; $\gamma C_3H$ |
| 740 | m | 738.9 | 9.4 | $\nu C_6N_1 - \nu C_4N_7$ |
| | | 718.4 | 79.0 | $\gamma C_5$ |
| 657/652 | m | 636.2 | 12.4 | $\gamma N_1 - \gamma N_2 + \gamma C_3 - \gamma N_4$ |
| | | 613.5 | 50.1 | $\nu C_6N_1 + \nu C_4N_7$ |
| 613/**605** | s | 571.6 | 160.1 | $\gamma N_1 + \gamma N_4 - \gamma C_5$ |

[a] Absorptions in the high frequency region, corresponding to CH and $CH_3$ stretching vibrations, were not analyzed. Experimental wavenumbers are given in cm$^{-1}$. For the multiplet bands, the most intense component is highlighted in bold. Abbreviations: br = broad. Experimental intensities (Int.) are expressed qualitatively: s = strong; m = medium; w = weak. [b] Calculated harmonic wavenumbers were multiplied by 0.980. [c] Abbreviations: ν, stretching; δ, in-plane bending; ρ, rocking; γ, out-of-plane bending. Signs "+" and "–" designate combination of vibrations occurring in the same phase and in the opposite phase, respectively.

## 3. Computational data

3.1. Cartesian coordinates for the optimized structures of the ion pairs and the species produced by evaporation of the studied salts

**[DMTrH$^+$···I$^-$]**

B3LYP/6-311+G(2d,p)[LANL2DZ]-GD3BJ (including counterpoise correction)

| | | | |
|---|---|---|---|
| N | -1.735535 | -1.043949 | 0.239226 |
| N | -2.434072 | -0.644759 | -0.870223 |
| C | -2.362234 | 0.651347 | -0.849287 |
| N | -1.648321 | 1.106164 | 0.228731 |
| C | -1.161397 | 0.001606 | 0.841529 |
| C | -1.353014 | -2.432823 | 0.405326 |
| C | -1.161829 | 2.459312 | 0.455387 |
| I | 1.647869 | -0.025447 | -0.101463 |
| H | -2.820526 | 1.302777 | -1.573747 |
| H | -0.656660 | -0.018626 | 1.787553 |
| H | -1.294187 | -2.665578 | 1.466912 |
| H | -2.109335 | -3.048667 | -0.072637 |
| H | -0.373458 | -2.577957 | -0.057186 |
| H | -1.727160 | 3.142748 | -0.173788 |
| H | -1.299943 | 2.732288 | 1.500154 |
| H | -0.099428 | 2.482848 | 0.198422 |

**[DMTr] (*C*$_s$)**

B3LYP/6-311+G(2d,p)

| | | | |
|---|---|---|---|
| N | 1.038698 | 0.140667 | 0.000000 |
| N | 0.708357 | -1.202380 | 0.000000 |
| C | -0.588229 | -1.175401 | 0.000000 |
| N | -1.053971 | 0.114895 | 0.000000 |
| C | 0.000000 | 0.993696 | 0.000000 |
| C | 2.441782 | 0.505104 | 0.000000 |
| C | -2.452826 | 0.511596 | 0.000000 |
| H | -1.214176 | -2.053655 | 0.000000 |
| H | 2.500531 | 1.590096 | 0.000000 |
| H | 2.932718 | 0.105710 | 0.888166 |
| H | 2.932718 | 0.105710 | -0.888166 |
| H | -2.960931 | 0.136045 | 0.889892 |
| H | -2.485880 | 1.597809 | 0.000000 |
| H | -2.960931 | 0.136045 | -0.889892 |

**[**1-methyl-1*H*-1,2,4-triazole **10] (*C*$_s$)**
B3LYP/6-311+G(2d,p)

| | | | |
|---|---|---|---|
| N | 0.000000 | 0.584470 | 0.000000 |
| N | -1.119685 | -0.179452 | 0.000000 |
| C | -0.629611 | -1.407568 | 0.000000 |
| N | 0.726833 | -1.482794 | 0.000000 |
| C | 1.085286 | -0.212503 | 0.000000 |
| C | -0.083902 | 2.030823 | 0.000000 |
| H | -0.614318 | 2.373183 | 0.888446 |
| H | -0.614318 | 2.373183 | -0.888446 |
| H | 0.925479 | 2.439222 | 0.000000 |
| H | -1.272618 | -2.273524 | 0.000000 |
| H | 2.095103 | 0.167867 | 0.000000 |

**[**4-methyl-1*H*-1,2,4-triazole **11] (*C*$_1$)**
B3LYP/6-311+G(2d,p)

| | | | |
|---|---|---|---|
| N | 1.495868 | -0.690780 | 0.008716 |
| N | 1.495869 | 0.690779 | 0.008716 |
| C | 0.247369 | 1.074709 | -0.005994 |
| N | -0.594622 | 0.000000 | -0.020547 |
| C | 0.247368 | -1.074709 | -0.005994 |
| C | -2.048095 | 0.000000 | 0.013455 |
| H | -2.423687 | 0.883510 | -0.500872 |
| H | -2.417717 | -0.000014 | 1.040400 |
| H | -2.423689 | -0.883495 | -0.500897 |
| H | -0.097281 | 2.096870 | -0.012817 |
| H | -0.097282 | -2.096870 | -0.012817 |

**[DMTrH$^+$···TFA$^-$] –** Stucture **I (*C*$_1$)**
B3LYP/6-311+G(2d,p)-GD3BJ (including counterpoise correction)

| | | | |
|---|---|---|---|
| N | 2.382780 | -1.075048 | 0.084346 |
| C | 1.769039 | 0.110431 | 0.224769 |
| N | 2.691835 | 1.028927 | -0.014986 |
| C | 3.686422 | -0.807460 | -0.240784 |
| C | 2.500499 | 2.472566 | -0.005027 |
| C | 1.749357 | -2.389435 | 0.253454 |
| H | 0.683539 | 0.322053 | 0.443778 |
| H | 4.428010 | -1.567585 | -0.420239 |
| H | 1.449540 | 2.665791 | 0.198970 |
| H | 3.126438 | 2.913965 | 0.768273 |
| H | 2.776104 | 2.874172 | -0.978018 |
| H | 1.998248 | -2.787702 | 1.236118 |
| H | 0.671565 | -2.245159 | 0.150550 |
| H | 2.118093 | -3.055692 | -0.523806 |
| N | 3.905278 | 0.475581 | -0.310583 |
| C | -1.513441 | -0.157738 | 0.094600 |
| C | -3.042407 | 0.102732 | -0.068676 |
| O | -1.089736 | -1.273384 | -0.237198 |
| O | -0.877981 | 0.827819 | 0.547061 |
| F | -3.266217 | 1.105136 | -0.950323 |
| F | -3.715588 | -0.970090 | -0.510934 |
| F | -3.603291 | 0.470718 | 1.103926 |

**[DMTrH$^+$···TFA$^-$] –** Stucture **II (*C*$_s$)**
B3LYP/6-311+G(2d,p)-GD3BJ (including counterpoise correction)

| | | | |
|---|---|---|---|
| N | 1.186289 | 2.658554 | 0.000000 |
| C | 0.181186 | 1.767163 | 0.000000 |
| N | -0.936164 | 2.472691 | 0.000000 |
| C | 0.612977 | 3.903208 | 0.000000 |
| C | -2.301145 | 1.952300 | 0.000000 |
| C | 2.607692 | 2.306191 | 0.000000 |
| H | 0.332912 | 0.651862 | 0.000000 |
| H | 1.169283 | 4.825519 | 0.000000 |
| H | -2.229460 | 0.863081 | 0.000000 |
| H | -2.811379 | 2.313789 | 0.890727 |
| H | -2.811379 | 2.313789 | -0.890727 |
| H | 3.085294 | 2.707274 | 0.892273 |
| H | 2.680377 | 1.220759 | 0.000000 |
| H | 3.085294 | 2.707274 | -0.892273 |
| N | -0.686782 | 3.818049 | 0.000000 |
| C | -0.226922 | -1.524925 | 0.000000 |
| C | -0.072822 | -3.076537 | 0.000000 |
| O | -1.376260 | -1.066757 | 0.000000 |
| O | 0.869708 | -0.907511 | 0.000000 |
| F | 0.612977 | -3.495052 | 1.088101 |
| F | -1.247924 | -3.723081 | 0.000000 |
| F | 0.612977 | -3.495052 | -1.088101 |

**[DMTrH$^+$···TFA$^-$] –** Stucture **III (*C*$_1$)**
B3LYP/6-311+G(2d,p)-GD3BJ (including counterpoise correction)

| | | | |
|---|---|---|---|
| N | 2.247726 | 0.752334 | 0.061288 |
| C | 1.851857 | -0.262829 | 0.839394 |
| N | 1.705757 | -1.318625 | 0.055220 |
| C | 2.254245 | 0.265978 | -1.220424 |
| C | 1.111021 | -2.599345 | 0.402998 |
| C | 2.327212 | 2.155128 | 0.466106 |
| H | 1.723172 | -0.234217 | 1.903258 |
| H | 2.487385 | 0.867018 | -2.082133 |
| H | 1.217522 | -2.751668 | 1.474158 |
| H | 0.054102 | -2.575888 | 0.141312 |
| H | 1.628471 | -3.382589 | -0.145184 |
| H | 2.680284 | 2.207690 | 1.493131 |
| H | 3.030835 | 2.667716 | -0.186112 |
| H | 1.321778 | 2.569819 | 0.374091 |
| N | 1.938356 | -0.994200 | -1.254608 |
| C | -0.966020 | 0.745353 | 0.323975 |
| O | -0.536422 | 1.636983 | -0.418246 |
| O | -0.469787 | 0.252941 | 1.365595 |
| C | -2.294113 | 0.047146 | -0.111544 |
| F | -3.183010 | -0.045107 | 0.895601 |
| F | -2.021048 | -1.232693 | -0.512880 |
| F | -2.911717 | 0.647531 | -1.136904 |

**[DMTrH$^+$···TFA$^-$] –** Stucture **IV (*C*$_1$)**
B3LYP/6-311+G(2d,p)-GD3BJ (including counterpoise correction)

| | | | |
|---|---|---|---|
| N | -1.985481 | 1.073784 | 0.157797 |
| C | -1.270647 | -0.022304 | 0.526033 |
| N | -2.053388 | -1.028860 | 0.132555 |
| C | -3.149925 | 0.663830 | -0.437902 |
| C | -1.768852 | -2.446279 | 0.263063 |
| C | -1.541757 | 2.451819 | 0.326218 |
| H | -3.903052 | 1.330483 | -0.824432 |
| H | -0.819204 | -2.551784 | 0.779953 |
| H | -2.561742 | -2.927300 | 0.833916 |
| H | -1.704912 | -2.899043 | -0.725399 |
| H | -2.361060 | 3.059763 | 0.707818 |
| H | -0.723189 | 2.461209 | 1.040262 |
| H | -1.192373 | 2.856550 | -0.623311 |
| N | -3.225226 | -0.632318 | -0.467886 |
| O | 1.139090 | -0.062067 | 1.640984 |
| C | 2.210789 | -0.036879 | 0.898963 |
| H | 0.173011 | -0.056185 | 1.140993 |
| O | 3.348613 | -0.030360 | 1.287586 |
| C | 1.940148 | -0.011353 | -0.636344 |
| F | 1.216863 | 1.084865 | -0.982449 |
| F | 3.062582 | 0.006814 | -1.344260 |
| F | 1.222892 | -1.093406 | -1.023935 |

**[DMTrH$^+$···TFA$^-$] –** Stucture **V (*C*$_s$)**
B3LYP/6-311+G(2d,p)-GD3BJ (including counterpoise correction)

| | | | |
|---|---|---|---|
| N | -0.893870 | 2.171932 | 0.000000 |
| C | -0.791096 | 3.504544 | 0.000000 |
| N | 0.498378 | 3.795443 | 0.000000 |
| C | 0.389485 | 1.672902 | 0.000000 |
| C | 1.138846 | 5.101009 | 0.000000 |
| C | -2.140262 | 1.387848 | 0.000000 |
| H | 0.624771 | 0.578306 | 0.000000 |
| H | 0.370991 | 5.871322 | 0.000000 |
| H | 1.759723 | 5.190760 | 0.889212 |
| H | 1.759723 | 5.190760 | -0.889212 |
| H | -2.712286 | 1.631861 | 0.893758 |
| H | -2.712286 | 1.631861 | -0.893758 |
| H | -1.866962 | 0.322631 | 0.000000 |
| N | 1.253224 | 2.660181 | 0.000000 |
| O | -1.287456 | -1.482731 | 0.000000 |
| C | -0.089487 | -1.810646 | 0.000000 |
| H | -1.605995 | 4.207856 | 0.000000 |
| O | 0.937282 | -1.096859 | 0.000000 |
| C | 0.214741 | -3.342508 | 0.000000 |
| F | 0.937282 | -3.695233 | -1.088039 |
| F | 0.937282 | -3.695233 | 1.088039 |
| F | -0.891649 | -4.105138 | 0.000000 |

## 3.2. Force filed used in the Molecular Dynamics Simulations

Copy and paste the following data in a *.ff file.

*ATOMS*
*#Unique_type, similar_type, m/u, q/e, pot, pars*
*#Trifluoroacetate*

| | | | | | | |
|---|---|---|---|---|---|---|
| *OFA* | *OFA* | *15.999* | *-0.7374* | *lj* | *2.960* | *0.8786* |
| *CO2* | *CO2* | *12.011* | *0.7390* | *lj* | *3.400* | *0.3598* |
| *CFA* | *CFA* | *12.011* | *0.5214* | *lj* | *3.400* | *0.4577* |
| *FA* | *FA* | *18.998* | *-0.2619* | *lj* | *3.118* | *0.2552* |
| *# 1,3,4 triazolium* | | | | | | |
| *HCR* | *HCR* | *1.008* | *0.2169* | *lj* | *2.420* | *0.1255* |
| *CR* | *CR* | *12.011* | *-0.0854* | *lj* | *3.550* | *0.2929* |
| *NA* | *NA* | *14.007* | *0.0847* | *lj* | *3.250* | *0.7113* |
| *CW* | *CW* | *12.011* | *0.2196* | *lj* | *3.550* | *0.2929* |
| *HCW* | *HCW* | *1.008* | *0.1808* | *lj* | *2.420* | *0.1255* |
| *NNC* | *NNC* | *14.007* | *-0.4067* | *lj* | *3.250* | *0.7113* |
| *C1* | *C1* | *12.011* | *-0.3669* | *lj* | *3.500* | *0.2761* |
| *H1* | *H1* | *1.008* | *0.1878* | *lj* | *2.500* | *0.1255* |
| *NNA* | *NNA* | *14.007* | *0.3972* | *lj* | *3.250* | *0.7113* |

*BONDS*

*# Atom i, Atom j, potential type, re/A , kr/kJmol-1*

*# Trifluoroacetate*

| | | | | |
|---|---|---|---|---|
| *CFA* | *CO2* | *harm* | *1.585* | *1700.40* |
| *CO2* | *OFA* | *harm* | *1.241* | *6298.38* |
| *CFA* | *FA* | *harm* | *1.359* | *3089.75* |

*# 1,3,4 triazolium*

| | | | | |
|---|---|---|---|---|
| *HCR* | *CR* | *harm* | *1.076* | *3521.92* |
| *NA* | *CR* | *harm* | *1.339* | *3971.86* |
| *NA* | *C1* | *harm* | *1.472* | *3084.99* |
| *C1* | *H1* | *harm* | *1.085* | *3294.54* |
| *NA* | *CW* | *harm* | *1.371* | *3084.99* |
| *CW* | *HCW* | *harm* | *1.076* | *3517.70* |
| *CW* | *NNC* | *harm* | *1.303* | *4418.36* |
| *NNC* | *NNA* | *harm* | *1.358* | *3842.65* |
| *NNA* | *CR* | *harm* | *1.323* | *4073.46* |
| *NNA* | *C1* | *harm* | *1.469* | *2843.61* |

*ANGLES*

*# Atom i, Atom j, Atom k, potential type, theta_e/deg, ka/kjmol-1*

*#trifluoroacetate*

| | | | | | |
|---|---|---|---|---|---|
| *CO2* | *CFA* | *FA* | *harm* | *114.126* | *440.26* |
| *FA* | *CFA* | *FA* | *harm* | *105.661* | *351.15* |
| *OFA* | *CO2* | *OFA* | *harm* | *132.906* | *494.48* |
| *CFA* | *CO2* | *OFA* | *harm* | *113.535* | *417.27* |

*# 1,3,4 triazolium*

| | | | | | |
|---|---|---|---|---|---|
| *NA* | *CR* | *HCR* | *harm* | *126.16* | *219.05* |
| *CR* | *NA* | *C1* | *harm* | *127.19* | *271.80* |
| *NA* | *C1* | *H1* | *harm* | *109.30* | *344.53* |
| *NA* | *CR* | *NNA* | *harm* | *107.39* | *288.57* |
| *NA* | *CW* | *NNC* | *harm* | *111.24* | *331.51* |
| *NA* | *CW* | *HCW* | *harm* | *123.97* | *234.53* |
| *NNA* | *NNC* | *CW* | *harm* | *104.74* | *385.76* |
| *NNA* | *CR* | *HCR* | *harm* | *126.44* | *220.22* |
| *CR* | *NA* | *CW* | *harm* | *105.72* | *282.62* |
| *CW* | *NA* | *C1* | *harm* | *127.08* | *266.71* |
| *CR* | *NNA* | *C1* | *harm* | *128.81* | *294.47* |
| *HCW* | *CW* | *NNC* | *harm* | *124.78* | *235.94* |
| *H1* | *C1* | *H1* | *harm* | *110.28* | *154.42* |
| *NNA* | *C1* | *H1* | *harm* | *108.70* | *348.75* |

*DIHEDRALS*

*# Atom i, Atom j, Atom k, Atom l, potential type, v1, v2, v3, v4*

*#trifluoroacetate*

*FA CFA CO2 OFA opls 0.0000 0.0000 0.00000 0.0000*
*# 1,3,4 triazolium*
*H1 C1 NA CR opls 0.0000 0.00000 -0.5816 0.0000*
*C1 NA CR HCR opls 9.6232 25.4764 0.0000 0.0000*
*HCN CW NA CR opls 9.6232 25.4764 0.0000 0.0000*
*NA CW NNC NNA opls 9.6232 25.4764 0.0000 0.0000*
*CW NA CR NNA opls 9.6232 25.4764 0.0000 0.0000*
*CW NA CR HCR opls 0.0000 20.5016 0.0000 0.0000*
*C1 NA CR NNA opls 0.0000 20.5016 0.0000 0.0000*
*C1 NNA CR NA opls 0.0000 20.5016 0.0000 0.0000*
*C1 NNA CR HCR opls 0.0000 20.5016 0.0000 0.0000*
*HCW CW NA CR opls 0.0000 0.0000 -0.5816 0.0000*
*HCW CW NA C1 opls 0.0000 0.0000 -0.5816 0.0000*
*NNC CW NA CR opls 9.6232 25.4764 0.0000 0.0000*
*NNC CW NA C1 opls 9.6232 25.4764 0.0000 0.0000*
*H1 C1 NA CW opls 0.0000 0.0000 -0.5816 0.0000*
*H1 C1 NNA CR opls 0.0000 0.0000 -0.5816 0.0000*

*IMPROPER*
*#triafluoroacetate*
*CFA OFA CO2 OFA opls 0.0000 0.0000 0.0000 0.0000*
*#1,3,4 triazolium*
*NA NNA CR HCR opls 0.0000 87.8640 0.0000 0.0000*
*CR CW NA C1 opls 0.0000 87.8640 0.0000 0.0000*
*NA HCW CW NNC opls 0.0000 87.8640 0.0000 0.0000*