Synthesis and thermochemical properties of NF$_2$-containing energetic salts

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Abstract

Ammonium, 1,5-diamino-4-methyl-tetrazolium and 4-amino-1-methyl-triazolium salts of 5-difluoroaminodifluoromethyl-tetrazolate (TA-CF$_2$NF$_2$) were prepared by metathesis reactions of silver 5-difluoroaminodifluoromethyl-tetrazolate and the corresponding iodides. All are thermally stable to ~150 °C. The ammonium salt has a density of 1.88 g cm^{-3}. The combination of the CBS-4 method and isodesmic bond separation reactions was found to be an economical and reliable method to estimate heats of formation for polyfluorinated molecules. The standard heats of formation ($\Delta_f H_{298}^\circ$) of ammonium 5-difluoroaminodifluoromethyl-tetrazolate was calculated to be −53.13 kcal mol^{-1} using the CBS-4 method. While its detonation pressures (P) and velocities (D) were estimated using Cheetah 4.0: P = 28.78 GPa; D = 8490 m s^{-1}; detonation properties for 1,5-diamino-4-methyl-tetrazolium salts of 5-difluoroaminomethyltetrazolate (TA-CH$_2$NF$_2$), 5-difluoroaminotetrazolate (TA-NF$_2$) and 5-difluoroaminodinitromethyl-tetrazolate (TA-C(NO$_2$)$_2$NF$_2$) are also compared based on predicted densities and computed heats of formation.

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Keywords: Energetic materials; Fluorine; NF$_2$ compounds; Quantum chemical calculations

1. Introduction

During the past two decades, considerable effort has been focused on the development of high energy density materials (HEDM) with higher performance and/or enhanced insensitivity with respect to thermolysis, shock, friction, and electrostatic discharge [1–3]. These modern HEDMs derive most of their energy from: (1) oxidation of the carbon backbone, and (2) their very high positive heats of formation. Recently, using difluoramines as energetic materials, especially for weapon systems containing aluminum and boron appeared to offer intriguing possibilities [4]. Because on decomposition in the presence of a hydrogen source, the NF$_2$ compounds produce a larger number of moles of gas per gram, by releasing HF, than found for NO$_2$ compounds. In addition, the introduction of the dense NF$_2$ group (2.30 g cm^{-3} for NF$_2$ vs. 2.17 g cm^{-3} for NO$_2$)[5] would increase the density of an energetic material. Earlier calculations show that with similar structures, NF$_2$ compounds have higher impulse values than NO$_2$ compounds [6]. Currently, there are three main approaches to the synthesis of energetic difluoroamines: addition of NF$_2$ to alkene using N$_2$F$_4$ [7], difluoroamination of heterocyclic and dinitromethyl anions with NF$_2$OSO$_2$F [8] the formation of geminal difluoramino groups by reacting ketones with HNF$_2$ in fuming sulfuric acid [4a]. The three most promising of the known difluoramine candidates for use as energetic materials are 3,3,7,7-tetrakis(difluoramino)-octahydro-1,5-dinitro-1,5-diazocine (**1**, HNFX) [9], 1,1,3,5,5-pentanitro-1,5-bis(difluoramino)-3-azapentane (**2**) [10] and 1,1′-difluoramino-3,3′,4,4′-tetranitro-5,5′-bipyrazole (**3**) [11]. Although so far only one low-density polymorph of 1.807 g cm^{-3} was found for HNFX [4a], volume additivity calculations [5,12] predict a higher density of 1.914 or 1.919 g cm^{-3} for this compound. MOLPAK [13] also indicates that additional polymorphs with densities up to 2.03 g cm^{-3} may exist in a manner similar to HMX whose low-density polymorph (α-HMX, density = 1.84 g cm^{-3}) was first isolated. **2** has a density of 2.045 g cm^{-3} 3 which is extremely high for an acyclic compound, and **3** at 1.923 g cm^{-3} is also significant for an energetic material [10].

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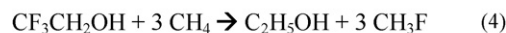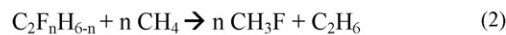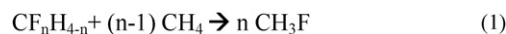
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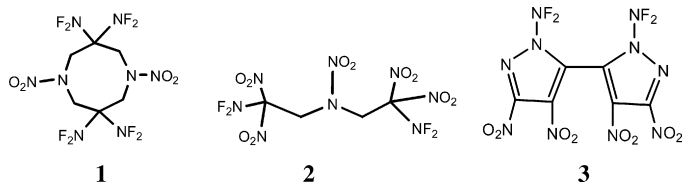
Ionic liquids/salts with high nitrogen content and high heats of formation were regarded as a new family of explosives or propellants, mainly because of their low vapor pressures, and adjustable properties brought about by changing the cation or anion counterparts, and because of their rather high densities. Here we report three typical energetic salts/liquid synthesized from 5-difluoroaminodifluoromethyl-tetrazole for which F_2NCF_2CN is the precursor [14].

2. Result and discussion

### 2.1. Preparation and characterization data for NF$_2$-containing energetic salts

Based on our earlier work [14], the ammonium 5-difluoroaminodifluoromethyl-tetrazolate (**5**) was readily obtained by a neutralization reaction. After being transformed into its silver salt, and followed by metathesis reaction with corresponding iodides, two ionic solid/liquid (**6**, **7**) were obtained in good yield (Scheme 1). Salts **5** and **6** are solids at room temperature, but **7** is a very non-viscous liquid with a density of 1.40 g cm^{-3} which may be attributed to the asymmetric character and lack of hydrogen bonding in the cation. The three compounds are thermally stable to ~150 °C. The ammonium salt (**5**) has a rather high density of 1.88 g cm^{-3}. The densities of the energetic salts were also predicted using our newly established volume parameters method for salts/liquids [15]. For **5** and **6**, the predicted densities are reasonably close to the experimental values.

$$CF_nH_{4-n}+ (n-1) CH_4 \rightarrow n\, CH_3F \qquad (1)$$

$$C_2F_nH_{6-n} + n\, CH_4 \rightarrow n\, CH_3F + C_2H_6 \qquad (2)$$

$$CF_3CN+ 3\, CH_4 \rightarrow CH_3CN + 3\, CH_3F \qquad (3)$$

$$CF_3CH_2OH + 3\, CH_4 \rightarrow C_2H_5OH + 3\, CH_3F \qquad (4)$$

$$CF_3CO_2H + 3\, CH_4 \rightarrow CH_3CO_2H + 3\, CH_3F \qquad (5)$$

Scheme 2. Isodesmic reactions for fluorinated compounds.

The heats of formation of the energetic salts were calculated using Gaussian 03 [16]. For fluorinated species, small basis sets may cause large deviations in these calculations. Initially, a comparison calculation was performed for 13 C1 and C2 fluorinated species by isodesmic reactions (Eqs. (1–5), Scheme 2) correlated to CH$_3$F (Scheme 1) (ΔH°_{298} (CH$_3$F, gas) = −56.5 kcal mol^{-1}) [17], using G2 [18], G3 [19], CBS-Q [20], CBS-4 [21], and B3LYP/6-311+G(3df,2p)// B3LYP/6-31g(d). Generally, due to a poor UHF/3-21G* geometry, the errors for the CBS-4M method are much larger than those found for G2, G3, CBS-Q, especially for a large system.

However, the CBS-4 model is very much faster computationally. The errors of CBS-4 are systematic and may be greatly reduced by the use of isodesmic reactions [21]. These lend credibility to the investigation of large systems for which G2, G3 and CBS-Q methods are not feasible. As shown in Table 1, CBS-4 has a mean absolute deviation (MAD) of 0.95 kcal mol^{-1} for the 13 test sets which is comparable with results obtained when G2, G3, or CBS-Q is used and is much more accurate than a large basis set of 6–311+G(3df,2p) at B3LYP level on B3LYP/6-31g(d) geometry.
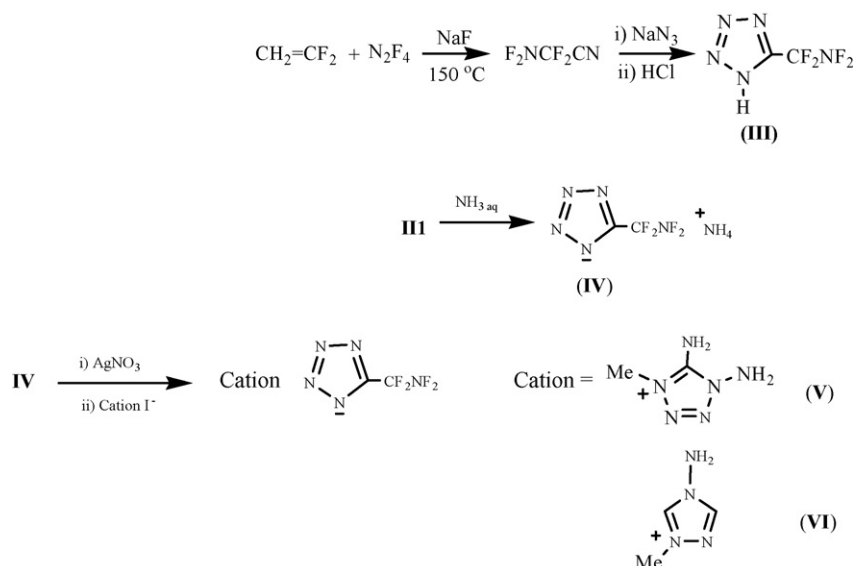
Scheme 1. Synthesis of NF$_2$-containing energetic salts.

Table 1
Calculated and literature heats of formation for fluorinated compounds[a]

Compound	$\Delta_f H^{\circ}_{298}$ Literature[a]	Deviation (literature–calculated)				
		G2	G3	CBS-Q	CBS-4M	DFT[b]
CH_2F_2	−108.10	−0.22	−0.12	0.03	0.00	−0.99
CHF_3	−166.20	0.41	0.52	0.75	0.74	−2.12
CF_4	−223.14	0.34	0.32	0.75	1.17	−4.67
CH_3COF	−105.66	−0.35	0.05	0.07	−0.21	−1.11
C_2H_5F	−65.78[c]	−0.52	−0.45	−0.40	−0.80	−0.79
CH_2F-CH_2F	−106.97[c]	−0.17	−0.01	0.10	−0.99	−1.00
CF_2H-CH_3	−118.79	1.95	2.12	1.38	1.61	0.38
CF_3CH_3	−178.20	2.54	2.98	3.20	2.50	−1.05
CF_2H-CF_2H	−211.11	0.72	0.97	1.36	−0.55	−2.89
C_2F_6	−321.27	2.37	2.33	2.61	1.07	−6.24
CF_3CN	−118.40	1.63	1.45	1.80	0.79	−2.46
CF_3CH_2OH	−212.33	−0.59	−0.50	−0.12	−1.29	−4.80
CF_3COOH	−246.51	0.55	0.51	0.67	−0.59	−3.62
Mean absolute deviation (MAD)		0.95	0.95	1.02	0.95	2.47

[a] From Ref. [22] unless otherwise stated.
[b] B3LYP/6-311+G(3df,2p)// B3LYP/6-31g(d).
[c] Ref. [23].

The heat of formation, $\Delta_f H^{\circ}_{298}$, for CH_3F, −56.5 kcal mol^{-1} used here is a calculated value [17] computed using complete basis set limit extrapolation where no empirical parameters are involved, because of the great uncertainty in the experimental value reported for its heat of formation. For example, in the JANAF tables [24] the value for $\Delta_f H^{\circ}_{298}$ (CH_3F, g) is given as −56 ± 6.9; −60 ± 3.5 kcal mol^{-1} (NIST benchmark database)[25]. Different calculation methods also lead to quite different results: −57.4 ± 1.2 kcal mol^{-1} (based on isogyric and hydrogenation reactions) [26]; −55.6 ± 2 kcal mol^{-1} [27]; and −55.9 ± 1 kcal mol^{-1} [28], −55.8 to −58.6 kcal mol^{-1} using atomization and isodesmic bond separation reactions when correlated to CF_4 using G2, G2(MP2), CBS-4, CBS-Q, CBS-APNO, BAC-MP4, etc. [29].

The mean absolute deviation (MAD) of the isodesmic reactions found using the four methods (G2, G3, CBS-Q and CBS-4) for the 13 fluorinated molecules listed in Table 1 is highly dependent on the heat of formation of CH_3F. As shown in Fig. 1, when values for $\Delta_f H^{\circ}_{298}$ (CH_3F) fall into the range of −56.4 ± 0.2 kcal mol^{-1}, the MAD for G2, G3, CBS-Q and CBS-4 isodesmic bond separation reactions approach the lowest point on the curves, and are less than 1.0 kcal mol^{-1}. Accordingly, a value of −56.4 ± 0.2 kcal mol^{-1} as the standard heat of formation for CH_3F at 298 K, and −54.5 ± 0.2 kcal mol^{-1} at 0 K can be derived based on the current method. This value agrees perfectly with the −56.5 ± 1.0 kcal mol^{-1} proposed by Dixon and co-workers [17]. This number further confirms that −56.5 kcal mol^{-1} used for heat of formation for CH_3F is very credible.

Considering that most of the errors in calculation of the heats of formation for energetic salts may derive from the estimation of lattice energy, CBS-4 is sufficient for the current purpose. Isodesmic bond separation reactions given below (Scheme 3) were used to compute the heats of formation of the NF_2-containing anions: TA-CF_2NF_2 (Eq. (6)), TA-CH_2NF_2 (Eq. (7)), TA-NF_2 (Eq. (8)), TA-$C(NO_2)_2NF_2$ (Eq. (9)) [30].

Standard heats of formation of the species involved in the isodesmic reactions are −17.83 kcal mol^{-1} for CH_4 [22], −20.08 kcal mol^{-1} for C_2H_6 [22], 47.9 kcal mol^{-1} for tetrazolate [31], −17.76 kcal mol^{-1} for CH_3NO_2 [22], while −23.44 kcal mol^{-1} was used as ΔH°_{298} for CH_3NF_2 which was calculated at G3 level of theory by isodesmic bond separation reaction (Eq. (10)).

The heat of formation of 5-difluoroaminodifluoromethyl-tetrazolate (TA-CF_2NF_2) was found to be −75.71 kcal mol^{-1} (Eq. (6)) and its derivatives, e.g. 5-difluoroaminomethylte-trazolate (TA-CH_2NF_2), 5-difluoroaminotetrazolate (TA-NF_2) and 5-difluoroaminodinitromethyl-tetrazolate [30] (TA-$C(NO_2)_2NF_2$) have heats of formation of 23.02, 31.54, 27.28 kcal mol^{-1}, respectively (Table 2).
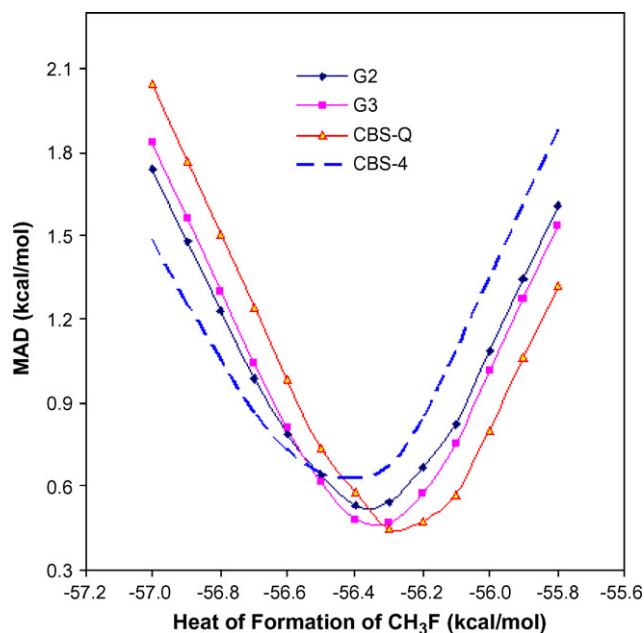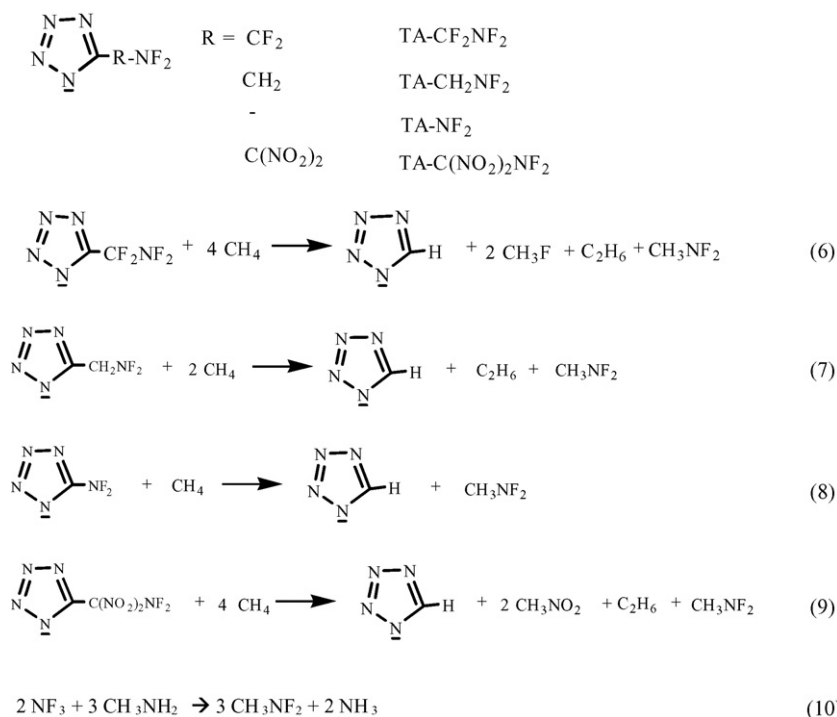

Fig. 1. MAD of 13 testing sets vs. ΔH°_{298} (CH_3F).

$$\text{TA-CF}_2\text{NF}_2 + 4\,\text{CH}_4 \longrightarrow \text{TA-H} + 2\,\text{CH}_3\text{F} + \text{C}_2\text{H}_6 + \text{CH}_3\text{NF}_2 \tag{6}$$

$$\text{TA-CH}_2\text{NF}_2 + 2\,\text{CH}_4 \longrightarrow \text{TA-H} + \text{C}_2\text{H}_6 + \text{CH}_3\text{NF}_2 \tag{7}$$

$$\text{TA-NF}_2 + \text{CH}_4 \longrightarrow \text{TA-H} + \text{CH}_3\text{NF}_2 \tag{8}$$

$$\text{TA-C(NO}_2)_2\text{NF}_2 + 4\,\text{CH}_4 \longrightarrow \text{TA-H} + 2\,\text{CH}_3\text{NO}_2 + \text{C}_2\text{H}_6 + \text{CH}_3\text{NF}_2 \tag{9}$$

$$2\,\text{NF}_3 + 3\,\text{CH}_3\text{NH}_2 \rightarrow 3\,\text{CH}_3\text{NF}_2 + 2\,\text{NH}_3 \tag{10}$$

Scheme 3. Isodesmic reactions for NF_2-containing anions.

Table 2
Heats of formation and detonation properties of NF_2-containing salts

Salts		$\Delta_f H^\circ_{298}$ (anion)	$\Delta_f H^\circ_{298}$ (cation)	Density[a] (g cm^{-3})	ΔH_L[b]	$\Delta_f H^\circ_{298}$	P (GPa)[c]	V (m s^{-1})[c]
Anion	Cation							
TA-CF$_2$NF$_2$	NH$_4^+$	−75.71	150.57[d]	1.90 (1.88)	127.99	−53.13	28.78	8490
TA-CF$_2$NF$_2$	DAMT[e]	−75.71	239.96	1.77 (1.69)	111.69	52.56	23.55	7905
TA-CH$_2$NF$_2$	DAMT[e]	23.02	239.96	1.636	114.65	148.33	24.82	8272
TA-NF$_2$	DAMT[e]	31.54	239.96	1.705	117.64	153.86	28.81	8752
TA-C(NO$_2$)$_2$NF$_2$	DAMT[e]	27.28	239.96	1.794	108.48	158.76	32.45	8582

$\Delta_f H^\circ_{298}$ and lattice enthalpy (ΔH_L), in kcal mol^{-1}.
[a] Predicted based on Ref. [15], experimental value listed in parenthesis.
[b] Predicted based on Ref. [33]. ΔH_L (kcal mol^{-1}) = 473.5 × $(W/\rho)^{1/3}$ + 26.0.
[c] Calculated using CHEETAH 4.0
[d] NIST web book, Ref. [31].
[e] DAMT: 1,5-diamino-4-methyl-tetrazolium.

It is likely that the stability of TA-C(NO$_2$)$_2$NF$_2$ would be low since –NO$_2$ and NF$_2$ on the same carbon tends to exert a destabilizing influence weakening both the C–NO$_2$ and C–NF$_2$ bonds. Actually, the ammonium and hydrazium salts of TA-C(NO$_2$)$_2$NF$_2$ have proven to be highly sensitive [30]. For TA-CH$_2$NF$_2$, there is a possibility of intramolecular elimination of HF, in comparison, salt **5** is quite stable and insensitive. The heat of formation of the cation 1,5-diamino-4-methyl-tetrazolium (DAMT) was calculated to be 239.96 kcal mol^{-1} based on the G3 electronic energetic reported by Klapötke et al. [32]. Thus, the heat of formation can be calculated by:

$$\Delta_f H^\circ_{298}(\text{salt}) = \Delta_f H^\circ_{298}(\text{cation}) + \Delta_f H^\circ_{298}(\text{anion}) - \Delta H_L,$$

where ΔH_L is the lattice enthalpy, for 1:1, non-linear, polyatomic salt, it was estimated by [33]

$$\Delta H_L\,(\text{kcal mol}^{-1}) = 473.5 \times \left(\frac{W}{\rho}\right)^{1/3} + 26.0$$

Detonation properties were also estimated using Cheetah 4.0 [34]. From Table 2, it can be seen that although the ammonium salt of TA-CF$_2$NF$_2$ has a low heat of formation, its detonation properties, e.g. detonation pressure (P) and detonation velocity (V) are comparable with those of TA-NF$_2$ salts, and are superior to those of TNT (P = 20.6 GPa, V = 6700 m s^{-1}). This is mainly due to the much higher density of **5**. The calculated

detonation velocity of compound **5**, and DAMT salt of TA-NF$_2$ are comparable with that of RDX ($P = 34.4$ GPa, $D = 8750$ m s^{-1}).

In summary, three NF$_2$-containing energetic salts/liquids were synthesized.

Each of these salts show moderate thermal stability to about 150 °C. The ammonium 5-difluoroaminodifluoromethyl-tetrazolate (**5**) has a rather high density of 1.88 g cm^{-3}. Their heats of formation were calculated using CBS-4 with isodesmic reactions. The results show that detonation properties of salt **5** are superior to those of TNT.

3. Experimental

3.1. General methods

^{1}H, ^{13}C NMR, and ^{19}F NMR spectra were recorded on a 300 MHz nuclear magnetic resonance spectrometer operating at 300.13, 75.48, and 282 MHz, respectively. Chemical shifts were reported relative to TMS or CFCl$_3$. Elemental analyses were measured with an Exeter Analytical CE-440 elemental analyzer. Gaseous N$_2$F$_4$ was purchased from Elf Atochem North America, Inc.

3.2. Ammonium 5-difluoroaminodifluoromethyl-tetrazolate (5)

5-Difluoroaminodifluoromethyltetrazole (**4**) (0.1 g), which was prepared according to literature [14], was dissolved in 5 mL methanol, and 1 mL of 20% ammonia was added. After stirring for 20 min, the solvent was removed, and a colorless solid remained (0.11 g, yield 100%). m.p. 158 °C (dec.); ^{13}C NMR (CD$_3$CN): δ 120.2 (–CF$_2$NF$_2$, tt, $J = 264.8$, 14.0 Hz), 152.9 (t, C-CF$_2$NF$_2$, $J = 27.6$ Hz). ^{19}F NMR (CD$_3$CN): δ 18.54 (s, –CF$_2$NF_2, 2F), −100.6 (s, CF_2NF$_2$, 2F). Anal. calcd for C$_2$H$_4$F$_4$N$_6$ (M_W 188.09): C, 12.77; H, 2.14; N, 44.68; Found C 13.00; H 2.14; N 44.32.

3.3. 1,5-Diamino-4-methyl-tetrazolium 5-difluoroaminodifluoromethyl-tetrazolate (6)

Ammonium salt **5** (0.2 g) was dissolved in 5 mL water, and 0.18 g AgNO$_3$ in 5 mL water was added. After stirring for 20 min, the precipitate was filtered off and to the filtrate was added 1,5-diamino-4-methyl-tetrazolium iodide (0.26 g) [32a]. After stirring for 30 min at 25 °C, the yellow precipitate was filtered off. The solvent was evaporated, and the residue was recrystallized from alcohol/ether, to give a colorless solid, 0.26 g, yield 83%. m.p. 150 °C. (dec.). ^{1}H NMR (CD$_3$CN): δ 3.87 (s, 3H, CH$_3$), 7.03 (s, 2H, C-NH$_2$), 8.98 (s, 2H, N-NH$_2$); ^{13}C NMR (CD$_3$CN): δ 35.9 (–CH$_3$), 120.3 (–CF$_2$NF$_2$, tt, $J = 264.9$, 14.0 Hz), 149.5, 152.9 (t, C-CF$_2$NF$_2$, $J = 27.6$ Hz). ^{19}F NMR (CD$_3$CN): δ 18.6 (s, –CF$_2$NF_2, 2F), −100.7 (s, CF_2NF$_2$, 2F). Anal. calcd for C$_4$H$_7$F$_4$N$_{11}$ 1/4H$_2$O (M_W 289.67) C, 16.59; H, 2.61; N, 53.19; Found C 16.90; H 2.38; N 53.17.

3.4. 1-Methyl-4-amino-1,2,4-triazolium 5-difluoroaminodifluoromethyl-tetrazolate (7)

Compound **7** was prepared using the procedure above with 1-methyl-4-amino-1,2,4-triazolium iodide [35], colorless liquid, yield 99%. Glass transition temperature (T_g) −38 °C. Decomposition temperature (T_d) 151 °C. ^{1}H NMR (CD$_3$CN): δ 4.09 (s, 3H, CH$_3$), 6.80 (bs, 2H, N-NH$_2$), 8.82 (s, H, C-H); 9.84 (s, H, C-H); ^{13}C NMR (CD$_3$CN): δ 39.1 (–CH$_3$), 120.4 (–CF$_2$NF$_2$, tt, $J = 264.8$, 13.9 Hz), 143.2, 145.1, 153.1 (t, C-CF$_2$NF$_2$, $J = 27.6$ Hz). ^{19}F NMR (CD$_3$CN): δ 18.6 (s, –CF$_2$NF_2, 2F), −100.7 (s, CF_2NF$_2$, 2F). Anal. calcd for C$_5$H$_7$F$_4$N$_9$ (M_W 269.16) C, 22.31; H, 2.62; N, 46.83; Found C, 22.30; H, 2.62; N, 45.97.

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