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Novel highly energetic pyrazoles: *N*-fluorodinitromethyl and *N*-[(difluoroamino)dinitromethyl] derivatives

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Treatment of 1,1-dinitro-1-(3,5-dinitropyrazol-1-yl)methanide with electrophilic fluorinating or difluoroaminating agents affords the corresponding fluorodinitromethyl or (difluoroamino)dinitromethyl pyrazole derivatives. Single crystal X-ray diffraction analysis shows a remarkable high density and DSC exhibits acceptable thermal stability of the compounds.

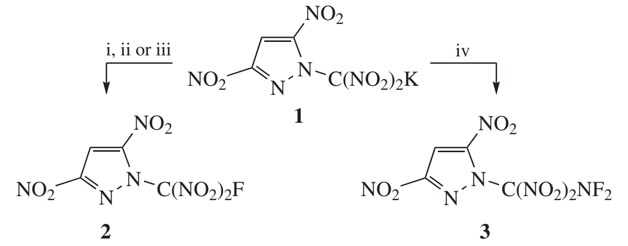
Fluorine and fluorinated functional groups are highly important substituents in the modern organic chemistry.[1] In particular, partially fluorinated nitro compounds find application in the field of energetic materials.[2] Fluorine- and oxygen-rich energetic compounds are promising ingredients of metallized formulations for composite propellants, explosives and pyrotechnics.

Molecules in which the fluorodinitromethyl moiety, $C(NO_2)_2F$, is attached *via* a carbon atom to an aliphatic, aromatic or heterocyclic backbone have been the subject of intensive investigation and useful energetic properties and stability have been found for such derivatives.[2(*a*),3] In contrast, less attention has been paid to compounds bearing the $C(NO_2)_2F$ moiety at the heterocyclic nitrogen atom.[4] Known 2-(fluorodinitromethyl)-5-nitrotetrazole[4(*c*)] is not stable. Energetic compounds containing (difluoroamino)dinitromethyl moiety, $C(NO_2)_2NF_2$, are more rare.[5] It is of note that incorporation of difluoroamino group, NF_2, is an effective tool in energetic compounds chemistry[6] since it brings a high energy content maintaining high density and acceptable thermal and processing properties. However, until now *N*-[(difluoroamino)dinitromethyl] heterocycles have not been reported.

In our studies, N-unsubstituted nitropyrazoles seemed suitable for the construction of a variety of energetic materials, in particular, N–F[7] and N–NF_2[8] derivatives. Here we report the synthesis of the first representatives of stable monocyclic azoles with $C(NO_2)_2F$ or $C(NO_2)_2NF_2$ moieties attached at the 1-position of the pyrazole ring.

Compounds bearing fluorodinitromethyl moiety are typically prepared from dinitromethane salts by an electrophilic fluorination. Traditionally,[3(*a*),9] powerful gaseous reagents such as elemental fluorine or $FClO_3$ are used. Moreover, solid reagents such as XeF_2,[10] MSO_4F,[11] RIF_2,[12] and 1-chloromethyl-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane bis(tetrafluoroborate) (Selectfluor®)[13] were proposed.

We explored the direct fluorination of potassium 1,1-dinitro-1-(3,5-dinitropyrazol-1-yl)methanide **1** using different electrophilic fluorinating agents (Scheme 1). Starting salt **1** was prepared following the literature procedure[14] from 1-acetonyl-3,5-dinitro-1*H*-pyrazole.[15] First experiments showed that fluorination of salt **1** in aqueous methanol with an excess of $FClO_3$ furnished the required fluorodinitromethyl compound **2** in 26% conversion at room temperature after 4 h. Prolongation of the reaction to 48 h did not improve the conversion. Changing the solvent for MeCN (48 h) afforded product **2** in 68% yield. On using Selectfluor® (MeCN, 20 °C), excellent conversion was achieved even in 2 h providing 84% yield.[†] When salt **1** was fluorinated with XeF_2 in MeCN at room temperature, the conversion was complete within 8.5 h to give product **2** in 89% yield.



Scheme 1 *Reagents and conditions*: i, $FClO_3$/MeCN, 20 °C; ii, Selectfluor®/MeCN, 20 °C; iii, XeF_2/MeCN, 20 °C; iv, F_2NOSO_2F/MeCN, –15 °C.

The discovery that F_2NOSO_2F[16] is an effective reagent for carrying out difluoroamination[17] of nitroalkane anions was a key factor in propelling the emerging field of synthetic organofluorine chemistry during the 1990s. In our experiments, salt **1** reacted with a slight excess of F_2NOSO_2F in MeCN at *ca.* –15 °C leading to difluoroamino derivative **3** in 75% yield.

[†] CAUTION! All compounds are potentially explosive and should be handled with appropriate precautions.

1-Fluorodinitromethyl-3,5-dinitropyrazole **2**. Selectfluor® (1 g, 2.82 mmol) was added to a suspension of potassium 1,1-dinitro-1-(3,5-dinitropyrazol-1-yl)methanide **1** (0.42 g, 1.4 mmol) in acetonitrile (10 ml) at room temperature followed by stirring for 2 h. The mixture was quenched with CH_2Cl_2 (60 ml) and filtered through a short layer of silica gel. The filtrate was concentrated *in vacuo*. The residue was recrystallized from hexane, affording product **2** as a colourless solid (0.33 g, 84%), mp 95–97 °C. ^{1}H NMR (DMSO-d_6) δ: 8.92 (s, 1H). ^{13}C NMR (DMSO-d_6) δ: 108.0 (C^4), 114.9 (d, CF, J_{CF} 313.3 Hz), 147.5 (C^5), 156.3 (C^3). ^{19}F NMR (DMSO-d_6) δ: –81.97. ^{14}N NMR (DMSO-d_6) δ: –33.5 (br. s). IR (KBr, ν/cm^{-1}): 3147, 1636, 1631, 1580, 1542, 1351, 1325, 1224, 1000, 977, 845, 825, 813, 793, 734. MS (EI), *m/z*: 234 $[M-NO_2]^+$, 188 $[M-2NO_2]^+$. Found (%): C, 17.41; H, 0.34; N, 31.25. Calc. for $C_4HFN_6O_8$ (%): C, 17.15; H, 0.36; N, 30.01.

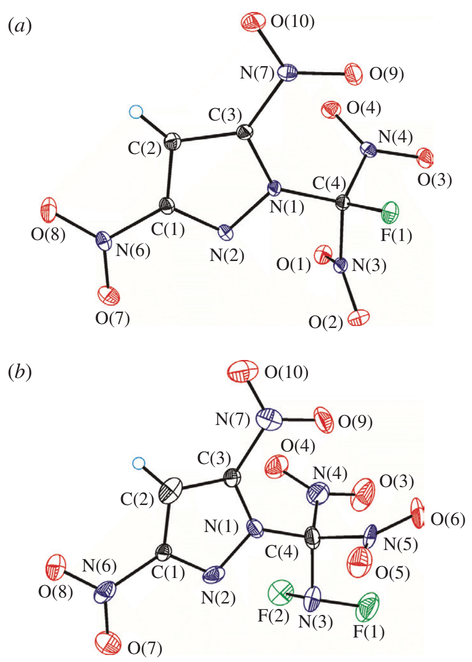


Figure 1 Molecular structures of compounds (*a*) **2** and (*b*) **3**. Displacement ellipsoids are drawn at the 50% probability level.

The structures of compounds **2** and **3** were estimated by elemental analysis, mass and NMR (^{1}H, ^{19}F, ^{14}N, ^{13}C) spectra† as well as single crystal X-ray diffraction (Figure 1).‡

The compounds show structural similarities, and their structures are also similar to that described for the trinitromethyl analogue, 1-(trinitromethyl)-3,5-dinitropyrazole **4**.[15] Both nitro groups at the pyrazole ring are coplanar to the ring and orientation of the fluorodinitromethyl and (difluoroamino)dinitromethyl moieties is similar to that of trinitromethyl moiety (see Online Supplementary Materials). An asymmetric unit cell of compound **2** contains one independent molecule and is characterized by high packing density due to numerous shortened intermolecular contacts which have also been observed in a series of polynitromethyl-containing compounds.[15,18] Difluoroamine **3** crystallizes as three independent molecules (A, A′, A″) in an asymmetric unit cell, and in the form of solvate with $CHCl_3$. The NF_2 group adopts pyramidal configuration (sums of bond angles at the N atom are 312.0(14), 312.1(15) and 311.0(15)°, for A, A′, A″, respectively).

Details of the crystal packing were estimated based on pair interaction energy estimation within M052X/6-311G(df,pd) level of theory[19] (see Online Supplementary Materials). It allows one to suggest that replacement of one nitro group in trinitromethyl moiety of compound **4** with fluorine (to compound **2**) or NF_2 (to compound **3**) substituent does not destroy the most energetically preferred chain formed along axis *a*, but it causes a relative reorientation of those chains in the crystal lattices. However, in the case of compound **2**, this does not significantly change both packing density and stabilization energy. Comparing compound **4** with **2**, the O···O and N···O shortened contacts are replaced with the F···O shortened contacts. For compound **3**, structural changes are more pronounced although not dramatic. The presence of solvent in the crystal structure of **3** does not allow for a direct comparison of the packing density. However, if a single crystal of $C(NO_2)_2NF_2$ derivative **3** without a solvent could be obtained, it would likely have a tighter intermolecular binding.

The estimated density of compound **2** at room temperature is 1.931 g cm^{-3}. This value was supported by our previous multi-temperature X-ray experiments[15,20] for nitro compounds, which showed that a decrease in the crystal packing density from 100 to 298 K varies from 3 to 4%. The density of compound **3** is 1.920 g cm^{-3} from gas pycnometer at 25 °C.

The difluoroamino derivative **3** possesses a positive oxygen balance (Ω_{CO_2} = +2.55), and compound **2** is oxygen-balanced (Ω_{CO_2} = 0), which are higher than that to RDX (Ω_{CO_2} = –21.6). The oxygen balance can be very useful in the processing of energetic materials formulations (*e.g.*, rocket propellants or mixtures of explosives).

The thermal stabilities of the compounds were determined by differential scanning calorimetric measurements (at a heating rate of 5 K min^{-1}). The difluoroamino compound **3** shows a relatively low thermal stability, decomposing at 113 °C (mp 38 °C), whereas fluorodinitromethyl derivative **2** is more thermally stable (mp 91 °C, bp 172 °C).

Previously it was reported that for nitropyrazoles[21] a simple prediction of the enthalpy of formation ($\Delta_f H^0$) can be performed with a good accuracy using the additive method based on the values of the group contribution and the intramolecular interaction.[22] The calculated $\Delta_f H^0$ value for compound **3** (+193 kJ mol^{-1}) involving N–F bonds is much greater than that for compound **2** (+1 kJ mol^{-1}) with C–F bond.

Calculation of detonation properties using SHOCK and DETONATION program[23] revealed that compound **3** has higher detonation pressure (P_{C-J} = 36.3 GPa) and velocity (D = 8721 m s^{-1}) than those of compound **2** (33.1 GPa, 8570 m s^{-1}). At the same time, the energetic performance of both compound are much superior to the common explosives TNT (19.5 GPa, 6860 m s^{-1}) and PETN (31.1 GPa, 8560 m s^{-1}), and only slightly lower than that of RDX (33.8 GPa, 8750 m s^{-1}). This makes them prospective compounds for further investigation as energetic materials.

In conclusion, for energetic materials designing, the pyrazole ring was N-functionalized with explosophore moieties such as (difluoroamino)dinitromethyl or fluorodinitromethyl. These novel compounds represent rare examples of functionalized nitro compounds, which can highlight fundamental scientific interest and practical applications.

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1-[(Difluoroamino)dinitromethyl]-3,5-dinitropyrazole **3**. A solution of salt **1** (1.45 g, 4.8 mmol) in acetonitrile (100 ml) was stirred at –17 °C under nitrogen while *N*,*N*-difluorohydroxylamine-*O*-fluorosulfonate (2.25 g, 14.9 mmol) was slowly added. After the yellow-orange solution became uncoloured (*ca.* 1.5 h), the mixture was allowed to warm to room temperature, and potassium fluorosulfate was filtered off. The filtrate was concentrated *in vacuo*. The residue was recrystallized from hexane affording product **3** as a colourless microcrystalline solid (1.13 g, 75%), mp 36 °C. ^{1}H NMR ($CDCl_3$) δ: 7.98 (s, 1H). ^{13}C NMR ($CDCl_3$) δ: 107.4 (C^4), 116.2 ($C–NF_2$), 148.8 (C^5), 157.2 (C^3). ^{19}F NMR ($CDCl_3$) δ: 43.5 (s, NF_2). ^{14}N NMR ($CDCl_3$) δ: –33.2, –38.0, –41.8. IR (KBr, ν/cm^{-1}): 3436, 3141, 1638, 1629, 1584, 1547, 1380, 1344, 1329, 1282, 1258, 1094, 1010, 983, 943, 927, 914, 867, 841, 823. Found (%): C, 15.41; H, 0.34; N, 31.25. Calc. for $C_4HF_2N_7O_8$ (313.09) (%): C, 15.35; H, 0.32; N, 31.32.

‡ *Single crystal X-ray study*. Compound **2**, $C_4HFN_6O_8$, at 100 K is monoclinic, space group $P2_1$, a = 6.2468(3), b = 10.0482(5) and c = 7.8737(4) Å, β = 110.6590(10)°, V = 462.44(4) Å^3, Z = 2, M = 259.15, d_{calc} = 2.012 g cm^{-3}, μ = 0.159 mm^{-1}, $F(000)$ = 280, wR_2 = 0.1252 calculated on F^2_{hkl} [GOF = = 1.018, R_1 = 0.0305 calculated on F_{hkl} using 2260 reflections with $I > 2\sigma(I)$].

Compound **3**, $C_4HF_2N_7O_8$ at 100 K, is triclinic, space group $P\bar{1}$, a = = 5.9779(12), b = 18.437(4) and c = 18.509(4) Å, α = 118.282(3)°, β = = 96.665(4)°, γ = 95.065(4)°, V = 1760.2(6) Å^3, Z = 6, M = 352.15, d_{calc} = 1.885 g cm^{-3}, μ = 0.303 mm^{-1}, $F(000)$ = 994, wR_2 = 0.2068 calculated on F^2_{hkl} [GOF = 1.099, R_1 = 0.0964 calculated on F_{hkl} using 3601 reflections with $I > 2\sigma(I)$].

CCDC 1410035 and 1410036 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* http://www.ccdc.cam.ac.uk.

Online Supplementary Materials

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.mencom.2015.11.010.

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