Electronic Supporting Information

High-Density Insensitive Energetic Materials: 2,4,6-Tris(2-fluoro-2,2-dinitroethoxy)-1,3,5-triazine

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Table 1S. Selected torsion angles (°) in compound 1 in comparison with those of three symmetrically independent molecules A, A', A'' of compound 5.

Torsion angle	fluorodinitroethoxy-triazine **5**		trinitroethoxy-triazine **5**		
	A	A'	A	A'	A''
N1-C1-O1-C4	175.78(14)		178.8(6)	-173.2(6)	-171.3(6)
C1-O1-C4-C5	-174.02(14)		129.9(6)	117.5(7)	113.7(7)
O1-C4-C5-N4	57.24(17)		40.4(7)	36.5(8)	41.6(8)
O1-C4-C5-N5(F1)	-64.36(17)		-80.2(7)	-83.2(7)	-80.3(7)
O1-C4-C5-N6	172.95(13)		159.8(5)	155.9(6)	161.3(6)
C4-C5-N4-O2	-136.77(15)		-131.3(7)	-127.4(7)	-121.1(7)
C4-C5-N5-O5			-139.5(7)	-141.9(9)	-151.5(7)
C4-C5-N6-O6	146.92(15)		-141.6(7)	-142.2(7)	-140.6(7)
N2-C2-O8-C6	-0.4(2)		172.7(6)	179.2(6)	-179.8(6)
C2-O8-C6-C7	161.21(14)		160.7(7)	161.4(6)	162.7(6)
O8-C6-C7-N7(F2)	-178.02(13)		46.8(9)	-50.0(7)	-50.2(7)
O8-C6-C7-N8	61.6(2)		-78.5(8)	73.6(7)	70.6(7)
O8-C6-C7-N9	-58.34(18)		166.1(6)	-167.2(5)	-168.5(5)
C6-C7-N7-O9			-114.3(10)	140.8(7)	143.7(7)
C6-C7-N8-O12	12.0(2)		-127.1(8)	137.6(7)	123.3(7)
C6-C7-N9-O13	83.6(2)		-157.7(8)	137.8(7)	144.5(7)
N3-C3-O15-C8	-170.52(15)		176.3(6)	179.7(6)	178.8(6)
C3-O15-C8-C9	-148.01(19)	-171.0(4)	-131.8(7)	-145.6(6)	-143.2(6)
O15-C8-C9-N10	-53.2(3)	52.4(7)	-45.8(8)	-42.2(8)	-42.6(8)
O15-C8-C9-N11(F3)	67.8(3)	-72.6(7)	77.0(8)	80.5(7)	78.0(8)
O15-C8-C9-N12	-168.5(2)	166.5(4)	-162.4(8)	-162.9(7)	-161.3(7)
C8-C9-N10-O17	133.0(5)	44.8(10)	137.1(8)	130.0(7)	127.9(7)
C8-C9-N11-O19			126.3(7)	146.2(7)	145.3(7)
C8-C9-N12-O20	-141.4(2)	-118.6(4)	133.4(7)	130.6(7)	133.4(7)

Table 2S. Pair intermolecular interaction energies (kcal/mol) and shortened contacts (Å) of of compound **1** with its closest environment in the crystal obtained at M052X/aug-cc-pvdz level of approximation.[a,b]

Entry	Close contact		Distance	Symmetry Code	Energy	Type of Interaction
1	O21	C2	2.992	1+x,y,z	-11.6	Nitro…Nitro O…π F…π
	O16	O3	2.898	1+x,y,z		
	O16	C1	2.955	1+x,y,z		
	F3'	**C1**	**3.005**	1+x,y,z		
2	O3	O16	2.898	-1+x,y,z	-11.6	Nitro…Nitro O…π F…π
	C1	O16	2.955	-1+x,y,z		
	C2	O21	2.992	-1+x,y,z		
	C1	**F3'**	**3.005**	**-1+x,y,z**		
3	O12	O6	3.009	1+x,y,1+z	-4.5	Nitro…Nitro
	O12	N4	3.003	1+x,y,1+z		
	O12	N6	3.012	1+x,y,1+z		
	N8	O3	2.934	1+x,y,1+z		
4	O3	N8	2.934	-1+x,y,-1+z	-4.5	Nitro…Nitro
	O6	O12	3.009	-1+x,y,-1+z		
	N4	O12	3.003	-1+x,y,-1+z		
	N6	O12	3.012	-1+x,y,-1+z		
5	O11	O7	3.029	x,y,1+z	-1.9	Nitro…Nitro
6	O7	O11	3.029	x,y,-1+z	-1.9	Nitro…Nitro
7	**F3**	**O16'**	2.928	1-x,1-y,1-z	-5.6	Nitro…Nitro F…Nitro
	O17	**O17'**	2.957	1-x,1-y,1-z		
	O16'	**F3**	2.928	1-x,1-y,1-z		
8	O14	H8B	2.428	1-x,1-y,2-z	-8.2	C-H…O
	H8B	O14	2.428	1-x,1-y,2-z		
	O14	**H8D**	2.359	1-x,1-y,2-z		
	H8D	**O14**	2.359	1-x,1-y,2-z		
9	N12	O17	3.018	2-x,1-y,1-z	-3.0	Nitro…Nitro F…Nitro
	O17	N12	3.018	2-x,1-y,1-z		
	O17	N10	2.913	2-x,1-y,1-z		
	N10	O17	2.913	2-x,1-y,1-z		
	O17	**F3'**	2.855	2-x,1-y,1-z		
	O16	**O16'**	2.976	2-x,1-y,1-z		
	F3'	**O17**	2.855	2-x,1-y,1-z		
	O16'	**O16**	2.976	2-x,1-y,1-z		
10	F2	O20	3.176	2-x,1-y,2-z	-1.1	
	O20	F2	3.176	2-x,1-y,2-z		
11	F1	O13	2.835	x,1/2-y,-1/2+z	-7.4	F…Nitro O…π
	C1	O12	2.957	x,1/2-y,-1/2+z		
12	O12	C1	2.957	x,1/2-y,1/2+z	-7.4	F…Nitro O…π
	O13	F1	2.835	x,1/2-y,1/2+z		
13	O2	O8	2.991	-1+x,1/2-y,-1/2+z	-4.4	Nitro…Nitro O…π
	O2	C2	2.921	-1+x,1/2-y,-1/2+z		
	O6	O15	2.851	-1+x,1/2-y,-1/2+z		
	O6	C3	2.926	-1+x,1/2-y,-1/2+z		
14	O8	O2	2.991	1+x,1/2-y,1/2+z	-4.4	Nitro…Nitro O…π
	O15	O6	2.851	1+x,1/2-y,1/2+z		
	C2	O2	2.921	1+x,1/2-y,1/2+z		
	C3	O6	2.926	1+x,1/2-y,1/2+z		

[a] Contacts given in bold correspond to interactions with minor part of the disordered fluorodinitroethoxy substituent

[b] Calculation was carried out by the Gaussian program [M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A., Jr. Montgomery, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J.

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Table 3S. Crystallographic data for low-temperature (100K) and room-temperature (298K) for compound **1**[c].[d]

Parameter	**1** (100K)	**1** (298K)
Empirical formula	$C_9H_6F_3N_9O_{15}$	$C_9H_6F_3N_9O_{15}$
Fw	537.23	537.23
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
a, Å	7.3284(6)	7.4308(4)
b, Å	22.5119(17)	22.8382(12)
c, Å	11.7209(9)	11.8801(6)
β, deg.	107.3420(10)	107.5930(10)
V, Å^3	1845.8(2)	1921.83(17)
Z	4	4
d_{calc}, g·cm^{-3}	1.933	1.857
μ, mm^{-1}	0.201	0.193
F(000)	1080	1080
θ range, deg.	1.81 – 30.00	1.81 – 30.00
independent reflections	5392	5601
R_{int}	0.0683	0.0275
reflections with $I>2\sigma(I)$	3520	3875
Completeness to theta θ, %	100	99.8
GOF (F^2)	1.007	1.036
$R_1(F)$ ($I>2\sigma(I)$)[a]	0.0440	0.432
$wR_2(F^2)$ (all data)[b]	0.0956	0.1224
Largest diff. peak/hole, e·Å^{-3}	0.389 / -0.273	0.275 / -0.265
№ CCDC	1507749	1507750

[a] $R_1 = \sum|F_o - |F_c||/\sum(F_o)$; [b] $wR_2 = (\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]^{1/2}$

[c] Difference in packing density upon going from 100 to 298K of compound **1** is 4.0%

[d] for data processing and crystal structure solution and refinement, the program packages APEX2 and SHELXTL were used [*APEX2*, Bruker AXS Inc., Madison, Wisconsin, USA, **2009**; Sheldrick, G.M. *Acta Cryst*, **2008**, *A64*, 112]