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Supporting Information

Trifluoromethyl- or pentafluorosulfanyl-substituted poly-1,2,3-triazole compounds as dense stable energetic materials

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Table of Contents

(Compounds are numbered as in article)

Table S1. Selected bond-lengths (Å) and bond angles (°) determined by X-ray diffraction of **3a**.

N(1)-C(24)	1.468(2)	N(1)-C(2)	1.471(2)
N(1)-C(13)	1.4738(19)	C(2)-C(3)	1.511(2)
C(3)-N(4)	1.4711(19)	N(4)-C(8)	1.341(2)
N(4)-N(5)	1.3473(18)	N(5)-N(6)	1.3140(19)
N(6)-C(7)	1.356(2)	C(7)-C(8)	1.367(2)
C(7)-C(9)	1.480(2)	C(8)-H(8)	0.9500
C(13)-C(14)	1.516(2)	C(14)-N(15)	1.4664(19)
N(15)-N(16)	1.3443(18)`	N(15)-C(19)	1.3457(19)
N(16)-N(17)	1.3166(19)	N(17)-C(18)	1.357(2)
C(18)-C(19)	1.368(2)	C(18)-C(20)	1.483(2)
C(19)-H(19)	0.9500	C(24)-C(25)	1.524(2)
C(25)-N(26)	1.466(2)	N(26)-C(30)	1.3460(19)
N(26)-N(27)	1.3477(19)	N(27)-N(28)	1.3141(19)
N(28)-C(29)	1.357(2)	C(29)-C(30)	1.363(2)
C(29)-C(31)	1.484(2)		
C(24)-N(1)-C(2)	110.33(12)	C(24)-N(1)-C(13)	110.77(12)
C(2)-N(1)-C(13)	109.77(12)	N(1)-C(2)-C(3)	113.17(13)
N(4)-C(3)-C(2)	112.57(13)	C(8)-N(4)-N(5)	111.16(13)
C(8)-N(4)-C(3)	127.62(13)	N(5)-N(4)-C(3)	120.74(13)
N(6)-N(5)-N(4)	107.26(12)	N(5)-N(6)-C(7)	108.15(13)
N(6)-C(7)-C(8)	109.25(14)	N(6)-C(7)-C(9)	121.27(14)
C(8)-C(7)-C(9)	129.41(16)	N(4)-C(8)-C(7)	104.17(14)
N(1)-C(13)-C(14)	112.99(12)	N(15)-C(14)-C(13)	112.54(13)
N(16)-N(15)-C(19)	111.02(13)	N(16)-N(15)-C(14)	119.66(12)
C(19)-N(15)-C(14)	129.28(13)	N(17)-N(16)-N(15)	107.58(12)
N(16)-N(17)-C(18)	107.87(13)	N(17)-C(18)-C(19)	109.45(14)
N(17)-C(18)-C(20)	121.03(14)	C(19)-C(18)-C(20)	129.52(15)
N(15)-C(19)-C(18)	104.07(14)	N(1)-C(24)-C(25)	112.72(13)
N(26)-C(25)-C(24)	112.17(13)	C(30)-N(26)-N(27)	111.08(13)
C(30)-N(26)-C(25)	128.29(14)	N(27)-N(26)-C(25)	120.59(13)
N(28)-N(27)-N(26)	107.44(12)	N(27)-N(28)-C(29)	107.82(13)
N(28)-C(29)-C(30)	109.79(14)	N(28)-C(29)-C(31)	121.56(15)
C(30)-C(29)-C(31)	128.65(15)	N(26)-C(30)-C(29)	103.87(14)

Table S2. Selected bond-lengths (Å) and bond angles (°) determined by X-ray diffraction of **4a.**

C(1)-C(2)#1	1.545(2)	C(1)-C(2)#2	1.545(2)
C(1)-C(2)#3	1.545(2)	C(1)-C(2)	1.545(2)
C(2)-N(3)	1.458(3)	C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800	N(3)-C(7)	1.349(3)
N(3)-N(4)	1.355(3)	N(4)-N(5)	1.309(4)
N(5)-C(6)	1.353(4)	C(6)-C(7)	1.360(4)
C(6)-C(8)	1.483(3)	C(7)-H(7)	0.9400
C(8)-F(11)	1.316(4)	C(8)-F(9)	1.332(4)
C(8)-F(10)	1.339(4)		
C(2)#1-C(1)-C(2)#2	112.23(10)	C(2)#1-C(1)-C(2)#3	112.23(10)
C(2)#2-C(1)-C(2)#3	104.09(19)	C(2)#1-C(1)-C(2)	104.09(19)
C(2)#2-C(1)-C(2)	112.23(10)	C(2)#3-C(1)-C(2)	112.23(10)
N(3)-C(2)-C(1)	114.94(18)	N(3)-C(2)-H(2A)	108.5
C(1)-C(2)-H(2A)	108.5	N(3)-C(2)-H(2B)	108.5
C(1)-C(2)-H(2B)	108.5	H(2A)-C(2)-H(2B)	107.5
C(7)-N(3)-N(4)	110.6(2)	C(7)-N(3)-C(2)	127.6(2)
N(4)-N(3)-C(2)	121.6(2)	N(5)-N(4)-N(3)	107.6(2)
N(4)-N(5)-C(6)	107.8(2)	N(5)-C(6)-C(7)	110.2(2)
N(5)-C(6)-C(8)	121.7(2)	C(7)-C(6)-C(8)	128.1(2)
N(3)-C(7)-C(6)	103.8(2)	N(3)-C(7)-H(7)	128.1
C(6)-C(7)-H(7)	128.1	F(11)-C(8)-F(9)	108.9(3)
F(11)-C(8)-F(10)	104.8(3)	F(9)-C(8)-F(10)	106.8(3)
F(11)-C(8)-C(6)	113.0(3)	F(9)-C(8)-C(6)	111.0(2)
F(10)-C(8)-C(6)	112.0(2)		

Symmetry transformations used to generate equivalent atoms:
#1 -x-1,-y,z #2 y-1/2,-x-1/2,-z-1/2 #3 -y-1/2,x+1/2,-z-1/2

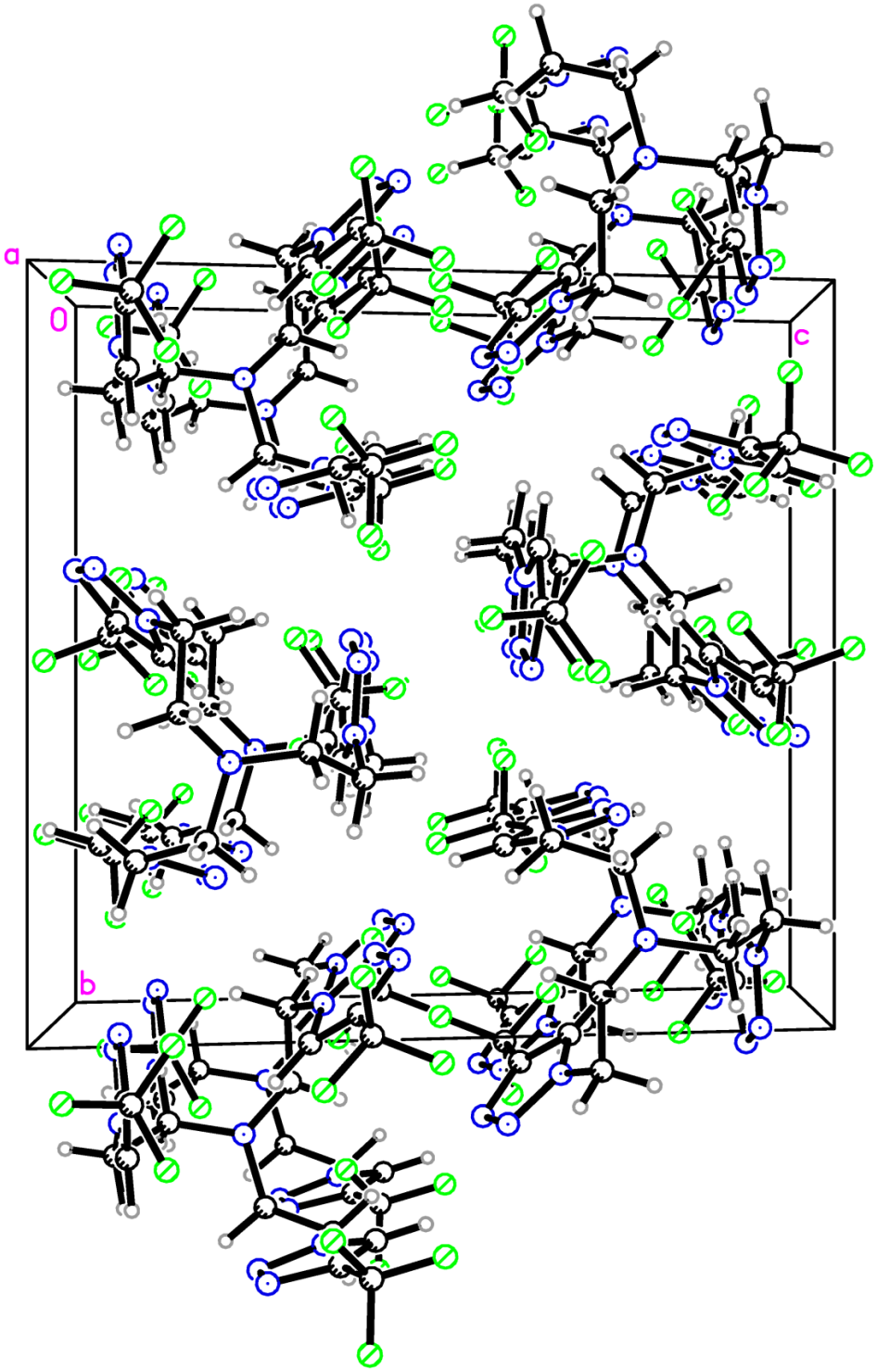

Figure S13. Packing diagram of **3a** with hydrogen atoms omitted for clarity.

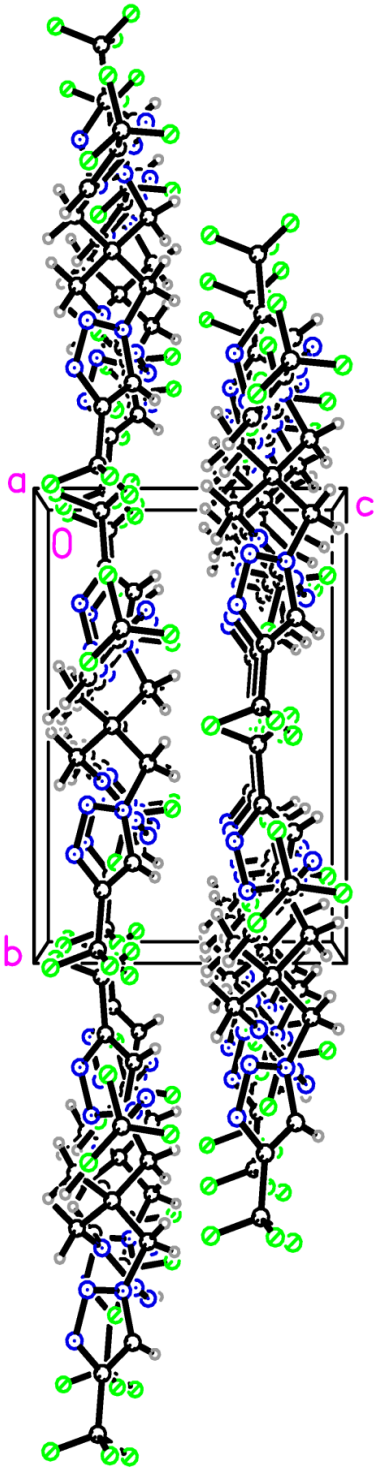

Figure 14. Packing diagram of **4a** with hydrogen atoms omitted for clarity.

Theoretical study

Computations were performed by using the Gaussian03 (Revision D.01) suite of programs.[1] The geometric optimization and the frequency analyses are carried out at the level of Becke three Lee-Yan-Parr (B3LYP) parameters up to 6-31+G(d,p) basis sets.[2] All of the optimized structures were characterized to be true local energy minima on the potential energy surface without imaginary frequencies. The enthalpy of reaction ($\Delta H_r^o 298$) is obtained by combining the MP2/6-311++G**[3] energy difference for the reaction, the scaled zero point energies, and other thermal factors. The heats of formation of the products were determined by using the method of isodesmic reactions (**Scheme 3**).[4] The *Ab Initio* computational data are listed below (**Table S1**).

TABLE S3. Calculated MP2/6-311++G**//B3LYP/6-31+G** Total Energies (E_0), Zero-Point Energies Correction (ZPE), Values of Thermal Correction (H_T), and Heats of Formation (HOF) of the compounds.

Name	E_0 (au)	ZPE (au)	H_T (kJ/mol)	HOF (kJ/mol)
1a	-790.0776109	0.19318	0.04594258	-412.1222322
2a	-1347.678735	0.19779	0.06357224	-1006.9089
3a	-2022.296927	0.339241	0.09875078	-1179.370148
4a	-2504.84247	0.338337	0.13015518	-1673.522392
5a	-967.0899587	0.141882	0.04218124	-251.546835
6a	-1488.750737	0.168206	0.02530108	-563.7279792
1b	-1348.937531	0.1957	0.04694924	-702.2252178
2b	-2465.391789	0.202599	0.05710782	-1564.856567
3b	-3698.867612	0.346181	0.09034406	-2019.678307
5b	-1525.947369	0.144333	0.04078124	-564.0311353
6b	-2606.463466	0.173037	0.01854284	-1120.904222

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