Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information

Belonging to the manuscript

A thermally stable nitrogen-rich energetic material - 3,4,5-triamino-1-tetrazolyl-1,2,4-triazole (TATT)

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S2 *Ab initio* computational data.

S3-S8 X-ray crystallographic experimental detail and data of crystal TATT·HNO_3.

Table S1 Calculated (B3LYP/6-31+G**//MP2/6-311++G**) Total Energy (E_0), Zero-Point Energy (ZPE), Values of Thermal Correction (H_T), and Heats of Formation (HOF, gas) of the compounds.

Name	E_0 (au)	ZPE (au)	H_T (kJ/mol)	HOF (kJ/mol)
TATT	-663.7850126	0.137642	31.7	598.8
1,2,3,4-tetrazole	-257.6538704	0.046855	11.6	314.1
Guanidine	-204.8735031	0.075945	14.4	26.0
CH_4	-40.3796224	0.044793	10.0	-74.6[1]
CH_3NH_2	-95.59384	0.06403	11.5	-22.5[1]
NH_2NH_2	-111.5836915	0.05331	11.0	95.4[1]
NH_3	-56.4154647	0.034384	10.0	-45.9[1]
CH_2=NH	-94.3808863	0.039928	10.1	86.7

Geometry coordinates

B3LYP/6-31+G(d,p) optimized geometries (Å)

3,4,5-Triamino-1-tetrazolyl-1,2,4-triazole (TATT)

C	1.865698	-0.964459	-0.009536
N	1.993989	0.408111	-0.044825
N	2.965568	-1.771083	-0.052951
N	0.623382	-1.354618	-0.005449
C	0.720346	0.989725	-0.026780
N	-0.102576	-0.140135	-0.026403
C	-1.474645	-0.151648	-0.007716
N	3.200578	1.095764	0.054612
N	-2.226036	-1.289943	0.002742
N	-3.473663	-0.889166	0.017229
N	-3.440829	0.431296	0.015106
N	-2.213046	0.962129	0.000315
H	2.812682	-2.727191	0.234296
H	3.825834	-1.340184	0.259426
H	3.123083	1.753314	0.830976
H	3.324497	1.651520	-0.791144
H	-4.278648	0.997212	0.023513
N	0.527846	2.253362	-0.004673
H	-0.462320	2.483603	0.017218

References

[1] D. R. Lide, ed.,"Standard Thermodynamic Properties of Chemical Substances*" in CRC Handbook of Chemistry and Physics,Internet Version 2007, (87th Edition), <http:/www.hbcpnetbase.com>,* Taylor and Francis, Boca Raton, FL, 2007.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for crystal TATT·HNO_3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(5)	9105(1)	3093(1)	11171(2)	14(1)
C(7)	7705(1)	4296(1)	9226(2)	14(1)
C(11)	6848(1)	2587(1)	7982(2)	14(1)
N(1)	9661(1)	4092(1)	11863(1)	17(1)
N(2)	10448(1)	3501(1)	12945(1)	17(1)
N(3)	10379(1)	2252(1)	12921(1)	17(1)
N(4)	9504(1)	1956(1)	11775(1)	17(1)
N(6)	8184(1)	3220(1)	9902(1)	14(1)
N(8)	7976(1)	5485(1)	9625(1)	17(1)
N(9)	6853(1)	3905(1)	8002(1)	14(1)
N(10)	6068(1)	4643(1)	6985(2)	20(1)
N(12)	6108(1)	1924(1)	6887(2)	18(1)
N(13)	7654(1)	2122(1)	9119(1)	15(1)
N(14)	6239(1)	6970(1)	1417(1)	17(1)
O(1)	5972(1)	5830(1)	1120(1)	24(1)
O(2)	7049(1)	7235(1)	2588(1)	22(1)
O(3)	5719(1)	7847(1)	536(1)	26(1)
O(4)	7897(1)	9556(1)	10180(1)	19(1)

Table S3. Bond lengths [Å] and angles [°] for crystal TATT·HNO_3.

C(5)-N(1)	1.3259(14)	N(12)-C(11)-N(9)	121.98(9)
C(5)-N(4)	1.3432(14)	C(5)-N(1)-N(2)	100.07(9)
C(5)-N(6)	1.3884(14)	N(3)-N(2)-N(1)	114.14(9)
C(7)-N(8)	1.3143(14)	N(3)-N(2)-H(2)	121.2(12)
C(7)-N(6)	1.3406(14)	N(1)-N(2)-H(2)	124.5(12)
C(7)-N(9)	1.3585(13)	N(2)-N(3)-N(4)	107.08(9)
C(11)-N(13)	1.3127(14)	N(3)-N(4)-C(5)	103.79(9)
C(11)-N(12)	1.3308(14)	C(7)-N(6)-C(5)	128.18(9)
C(11)-N(9)	1.3820(14)	C(7)-N(6)-N(13)	112.11(9)
N(1)-N(2)	1.3326(13)	C(5)-N(6)-N(13)	119.68(9)
N(2)-N(3)	1.3134(14)	C(7)-N(8)-H(8A)	120.2(11)
N(2)-H(2)	1.00(2)	C(7)-N(8)-H(8B)	119.7(12)
N(3)-N(4)	1.3311(13)	H(8A)-N(8)-H(8B)	120.1(17)
N(6)-N(13)	1.4086(12)	C(7)-N(9)-C(11)	108.06(8)
N(8)-H(8A)	0.915(18)	C(7)-N(9)-N(10)	128.56(9)
N(8)-H(8B)	0.849(19)	C(11)-N(9)-N(10)	123.29(9)
N(9)-N(10)	1.3932(12)	N(9)-N(10)-H(10A)	107.7(11)
N(10)-H(10A)	0.890(18)	N(9)-N(10)-H(10B)	108.1(11)
N(10)-H(10B)	0.900(19)	H(10A)-N(10)-H(10B)	110.0(16)
N(12)-H(12A)	0.871(18)	C(11)-N(12)-H(12A)	119.1(12)
N(12)-H(12B)	0.897(18)	C(11)-N(12)-H(12B)	118.2(10)
N(14)-O(3)	1.2448(13)	H(12A)-N(12)-H(12B)	122.1(15)
N(14)-O(1)	1.2552(12)	C(11)-N(13)-N(6)	103.41(8)
N(14)-O(2)	1.2637(12)	O(3)-N(14)-O(1)	120.31(10)
O(4)-H(4A)	0.84(2)	O(3)-N(14)-O(2)	119.53(9)
O(4)-H(4B)	0.89(2)	O(1)-N(14)-O(2)	120.14(9)
		H(4A)-O(4)-H(4B)	102.4(18)
N(1)-C(5)-N(4)	114.92(10)		
N(1)-C(5)-N(6)	122.26(10)		
N(4)-C(5)-N(6)	122.82(10)		
N(8)-C(7)-N(6)	128.90(10)		
N(8)-C(7)-N(9)	125.99(10)		
N(6)-C(7)-N(9)	105.12(9)		
N(13)-C(11)-N(12)	126.71(10)		
N(13)-C(11)-N(9)	111.30(9)		

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for crystal TATT·HNO_3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(5)	14(1)	15(1)	14(1)	1(1)	2(1)	0(1)
C(7)	14(1)	13(1)	14(1)	1(1)	2(1)	0(1)
C(11)	16(1)	12(1)	15(1)	1(1)	4(1)	0(1)
N(1)	16(1)	15(1)	18(1)	1(1)	-1(1)	-1(1)
N(2)	16(1)	15(1)	18(1)	2(1)	-1(1)	-1(1)
N(3)	16(1)	15(1)	19(1)	1(1)	1(1)	-1(1)
N(4)	15(1)	15(1)	19(1)	1(1)	0(1)	1(1)
N(6)	13(1)	11(1)	16(1)	0(1)	0(1)	-1(1)
N(8)	18(1)	12(1)	20(1)	0(1)	-2(1)	0(1)
N(9)	14(1)	11(1)	16(1)	0(1)	0(1)	0(1)
N(10)	17(1)	15(1)	24(1)	2(1)	-4(1)	4(1)
N(12)	16(1)	12(1)	22(1)	0(1)	-2(1)	-1(1)
N(13)	15(1)	11(1)	18(1)	-2(1)	0(1)	-2(1)
N(14)	18(1)	12(1)	19(1)	-1(1)	1(1)	0(1)
O(1)	26(1)	11(1)	31(1)	-2(1)	0(1)	-4(1)
O(2)	20(1)	16(1)	26(1)	0(1)	-6(1)	-1(1)
O(3)	24(1)	14(1)	33(1)	1(1)	-8(1)	2(1)
O(4)	20(1)	13(1)	21(1)	1(1)	-3(1)	0(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for crystal TATT·HNO_3.

	x	y	z	U(eq)
H(2)	11059(14)	3940(20)	13670(30)	45(5)
H(4A)	7607(15)	9140(20)	9190(30)	43(5)
H(4B)	7897(13)	10340(20)	9730(30)	42(5)
H(8A)	8557(13)	5663(17)	10500(30)	34(4)
H(8B)	7621(13)	6088(19)	9040(20)	30(4)
H(10A)	5788(12)	5032(18)	7850(30)	35(4)
H(10B)	6319(13)	5225(18)	6290(30)	33(4)
H(12A)	5585(13)	2329(17)	6250(20)	30(4)
H(12B)	6131(12)	1071(17)	6970(20)	24(4)

Table S6. Torsion angles [°] for crystal TATT·HNO_3.

N(4)-C(5)-N(1)-N(2)	0.31(12)
N(6)-C(5)-N(1)-N(2)	-179.00(10)
C(5)-N(1)-N(2)-N(3)	-0.08(11)
N(1)-N(2)-N(3)-N(4)	-0.17(12)
N(2)-N(3)-N(4)-C(5)	0.33(11)
N(1)-C(5)-N(4)-N(3)	-0.42(12)
N(6)-C(5)-N(4)-N(3)	178.89(9)
N(8)-C(7)-N(6)-C(5)	-1.68(18)
N(9)-C(7)-N(6)-C(5)	178.39(10)
N(8)-C(7)-N(6)-N(13)	-179.63(10)
N(9)-C(7)-N(6)-N(13)	0.44(11)
N(1)-C(5)-N(6)-C(7)	-1.87(17)
N(4)-C(5)-N(6)-C(7)	178.87(10)
N(1)-C(5)-N(6)-N(13)	175.95(9)
N(4)-C(5)-N(6)-N(13)	-3.31(15)
N(8)-C(7)-N(9)-C(11)	-179.98(10)
N(6)-C(7)-N(9)-C(11)	-0.05(11)
N(8)-C(7)-N(9)-N(10)	-3.31(17)
N(6)-C(7)-N(9)-N(10)	176.62(10)
N(13)-C(11)-N(9)-C(7)	-0.39(11)
N(12)-C(11)-N(9)-C(7)	-179.04(9)
N(13)-C(11)-N(9)-N(10)	-177.27(9)
N(12)-C(11)-N(9)-N(10)	4.07(15)
N(12)-C(11)-N(13)-N(6)	179.19(10)
N(9)-C(11)-N(13)-N(6)	0.62(11)
C(7)-N(6)-N(13)-C(11)	-0.67(11)
C(5)-N(6)-N(13)-C(11)	-178.81(9)

Symmetry transformations used to generate equivalent atoms

Table S7. Hydrogen bonds for crystal TATT·HNO_3 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(4)#1	1.00(2)	1.62(2)	2.6146(12)	175.4(18)
O(4)-H(4A)...O(2)#2	0.84(2)	1.89(2)	2.7045(12)	160.7(19)
O(4)-H(4A)...N(14)#2	0.84(2)	2.67(2)	3.4908(13)	164.0(17)
N(8)-H(8A)...N(1)	0.915(18)	2.304(18)	2.8982(14)	122.3(14)
N(8)-H(8A)...N(3)#3	0.915(18)	2.335(18)	3.1366(13)	146.2(15)
N(10)-H(10A)...O(1)#4	0.890(18)	2.430(18)	3.2175(14)	147.7(14)
N(12)-H(12A)...O(3)#5	0.871(18)	2.027(18)	2.8800(13)	166.0(16)
O(4)-H(4B)...N(13)#6	0.89(2)	1.93(2)	2.7947(13)	165.8(16)
N(8)-H(8B)...O(2)#2	0.849(19)	2.101(19)	2.9349(13)	167.3(16)
N(8)-H(8B)...O(2)#2	0.849(19)	2.101(19)	2.9349(13)	167.3(16)
N(10)-H(10B)...O(3)#2	0.900(19)	2.204(19)	2.8273(13)	125.9(14)
N(10)-H(10B)...O(4)#7	0.900(19)	2.484(18)	3.1842(14)	135.0(15)
N(12)-H(12B)...O(1)#8	0.897(18)	2.079(18)	2.9371(13)	159.8(14)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y-1/2,-z+5/2 #2 x,-y+3/2,z+1/2 #3 -x+2,y+1/2,-z+5/2
#4 x,y,z+1 #5 -x+1,y-1/2,-z+1/2 #6 x,y+1,z
#7 x,-y+3/2,z-1/2 #8 x,-y+1/2,z+1/2