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A novel 3D energetic MOF of high energy content: synthesis and explosive performance of a silver nitrate compound with 4,4',5,5'-tetraamine-3,3'-bis(1,2,4-trazole)

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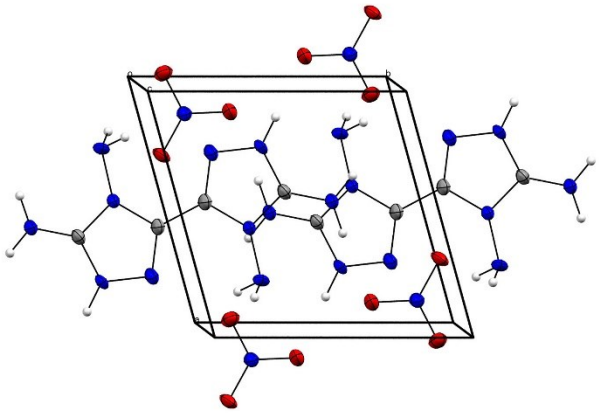

Fig. S1 Packing structure of $H_2(TABT)(NO_3)_2$

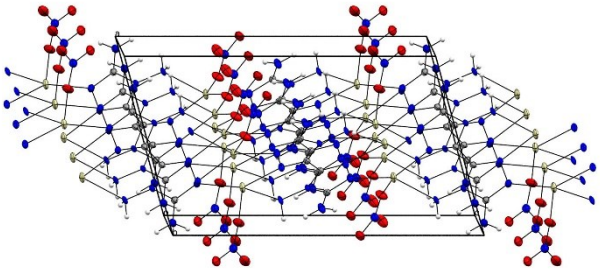

Fig. S2 Packing structure of $\{Ag_2(TABT)(NO_3)_2\}_n$

Table S1. Crystal properties of $H_2TABT(NO_3)_2$ and $Ag_2(TABT)(NO_3)_2$

Compound	$H_2TABT(NO_3)_2$	$Ag_2(TABT)(NO_3)_2$
Formula	$C_4H_{10}N_{12}O_6$	$C_2H_4AgN_6O_3$
Mw /g mol^{-1}	322.24	267.98
Crystal system	Triclinic	Monoclinic
Crystal group	*P*-1	$P2_1/c$
a/ Å	6.672(2)	8.9723(14)
b/ Å	6.9096(18)	5.0146(8)
c/ Å	6.992(2)	14.813(2)
α/°	73.521(12)	90
β/°	89.005(3)	105.854(2)
γ/°	75.832(5)	90
v/ Å^3	299.22(15)	641.14(17)
z	1	4
$\rho_{calc.}$ /g cm^{-3}	1.788	2.776
μ mm^{-1}	0.161	3.120
F(000)	166	516.0
2θ range /°	6.086-55.352	5.718-55.112
λ(Mokα)/Å	0.71073	0.71073
Temp. /K	100.15	100.15
Refl. collected	1823	3651
Refl. unique	1311	1467
R (int)	0.0138	0.0144
Data /rest. /param.	1311/0/101	1467/0/109
GOOF	1.132	1.077
R_1, wR_2 [$I>2\sigma(I)$]	R_1= 0.0433, wR_2= 0.1001	R_1=0.0183, wR_2=0.0402
R_1, wR_2 (all data)	R_1= 0.0550, wR_2= 0.1042	R_1=0.0233, wR_2=0.0423
Index range	-8⩽h⩽7, -9⩽k⩽7, -8⩽l⩽8	-11⩽h⩽9, -5⩽k⩽6, -18⩽l⩽19
Largest diff. peak/hole /e Å^{-3}	0.32/-0.32	0.43/-0.37
CCDC	2025060	2025062

Table S2. Bond length of $H_2(TABT)(NO_3)_2$ and $Ag_2(TABT)(NO_3)_2$

	Atom	Length/Å	Atom	Length/Å
$H_2(TABT)(NO_3)_2$	N(1)–N(2)	1.375(2)	N(5)–C(2)	1.355(2)
	N(1)–C(1)	1.304(3)	C(1)–C(1)#1	1.454(4)
	N(2)–C(2)	1.332(2)	O(1)–N(6)	1.266(2)
	N(3)–C(2)	1.319(3)	O(2)–N(6)	1.240(2)
	N(4)–N(5)	1.405(2)	O(3)–N(6)	1.257(2)
	N(5)–C(1)	1.384(2)		
$Ag_2(TABT)(NO_3)_2$	Ag(1)–Ag(1)#1	3.3374(4)	N(2)–N(4)	1.407(2)
	Ag(1)–Ag(1)#2	3.3374(4)	N(2)–C(1)	1.366(3)
	Ag(1)–O(2)	2.5772(17)	N(2)–C(2)	1.373(3)
	Ag(1)–N(4)#3	2.4612(19)	N(3)–C(1)	1.328(3)
	Ag(1)–N(5)	2.1905(19)	N(5)–N(6)	1.400(3)
	Ag(1)–N(6)#1	2.2738(18)	N(5)–C(1)	1.331(3)
	O(1)–N(1)	1.250(3)	N(6)–C(2)	1.311(3)
	O(2)–N(1)	1.262(3)	C(2)–C(2)#2	1.455(5)
	O(3)–N(1)	1.253(3)		

Table S3. Bond angle of $H_2(TABT)(NO_3)_2$ and $Ag_2(TABT)(NO_3)_2$

	Atom	Angle/°	Atom	Angle/°
$H_2(TABT)(NO_3)_2$	C(1)–N(1)–N(2)	104.25(15)	N(5)–C(1)–C(1)#1	124.1(2)
	C(2)–N(2)–N(1)	111.93(15)	N(2)–C(2)–N(5)	106.05(16)
	C(1)–N(5)–N(4)	132.68(15)	N(3)–C(2)–N(2)	128.91(17)
	C(2)–N(5)–N(4)	120.81(15)	N(3)–C(2)–N(5)	125.04(17)
	C(2)–N(5)–C(1)	106.45(15)	O(2)–N(6)–O(1)	119.67(15)
	N(1)–C(1)–N(5)	111.31(16)	O(2)–N(6)–O(3)	121.10(16)
	N(1)–C(1)–C(1)#1	124.6(2)	O(3)–N(6)–O(1)	119.22(15)
$Ag_2(TABT)(NO_3)_2$	Ag(1)#1–Ag(1)–Ag(1)#2	97.401(15)	O(3)–N(1)–O(2)	119.4(2)
	O(2)–Ag(1)–Ag(1)#2	157.97(4)	C(1)–N(2)–N(4)	125.94(19)
	O(2)–Ag(1)–Ag(1)#1	68.68(4)	C(1)–N(2)–C(2)	106.93(18)
	N(4)#3-Ag(1)–Ag(1)#1	139.53(4)	C(2)–N(2)–N(4)	127.09(18)
	N(4)#3–Ag(1)–Ag(1)#2	89.63(5)	N(2)–N(4)–Ag(1)#4	127.28(14)
	N(4)#3–Ag(1)–O(2)	112.11(7)	N(6)–N(5)–Ag(1)	116.29(13)
	N(5)–Ag(1)–Ag(1)#1	88.70(5)	C(1)–N(5)–Ag(1)	135.32(16)
	N(5)–Ag(1)–Ag(1)#2	65.33(5)	C(1)–N(5)–N(6)	107.21(18)
	N(5)–Ag(1)–O(2)	96.41(7)	N(5)–N(6)–Ag(1)#2	115.14(13)
	N(5)–Ag(1)–N(4)#3	129.65(7)	C(2)–N(6)–Ag(1)#2	135.64(16)
	N(5)–Ag(1)–N(6)#1	145.84(7)	C(2)–N(6)–N(5)	108.05(18)
	N(6)#1–Ag(1)–Ag(1)#1	63.24(5)	N(3)–C(1)–N(2)	123.5(2)
	N(6)#1–Ag(1)–Ag(1)#2	97.65(5)	N(3)–C(1)–N(5)	127.6(2)
	N(6)#1–Ag(1)–O(2)	91.20(6)	N(5)–C(1)–N(2)	108.8(2)
	N(6)#1–Ag(1)–N(4)#3	76.35(6)	N(2)–C(2)–C(2)#5	124.5(2)
	N(1)–O(2)–Ag(1)	140.54(15)	N(6)–C(2)–N(2)	109.01(19)
	O(1)–N(1)–O(2)	120.2(2)	N(6)–C(2)–C(2)#5	126.5(3)
	O(1)–N(1)–O(3)	120.3(2)		

Table S4. Torsion Angle of $H_2(TABT)(NO_3)_2$ and $Ag_2(TABT)(NO_3)_2$

	Atom	Angle/°	Atom	Angle/°
$H_2(TABT)(NO_3)_2$	N(1)–N(2)–C(2)–N(3)	-179.7(2)	N(4)–N(5)–C(2)–N(3)	-2.7(3)
	N(1)–N(2)–C(2)–N(5)	-0.4(2)	C(1)–N(1)–N(2)–C(2)	0.2(2)
	N(2)–N(1)–C(1)–N(5)	0.1(2)	C(1)–N(5)–C(2)–N(2)	0.4(2)
	N(2)–N(1)–C(1)–C(1)#1	179.1(2)	C(1)–N(5)–C(2)–N(3)	179.73(19)
	N(4)–N(5)–C(1)–N(1)	-177.45(18)	C(2)–N(5)–C(1)–N(1)	-0.3(2)
	N(4)–N(5)–C(1)–C(1)#1	3.5(4)	C(2)–N(5)–C(1)–C(1)#1	-179.3(2)
	N(4)–N(5)–C(2)–N(2)	177.95(16)		
$Ag_2(TABT)(NO_3)_2$	Ag(1)–O(2)–N(1)–O(1)	148.63(19)	N(5)–N(6)–C(2)–N(2)	0.5(3)
	Ag(1)–O(2)–N(1)–O(3)	-32.5(3)	N(5)–N(6)–C(2)–C(2)#2	-179.3(3)
	Ag(1)–N(5)–N(6)–Ag(1)#1	-0.01(19)	N(6)–N(5)–C(1)–N(2)	-0.7(3)
	Ag(1)–N(5)–N(6)–C(2)	169.61(15)	N(6)–N(5)–C(1)–N(3)	-178.1(2)
	Ag(1)–N(5)–C(1)–N(2)	-167.26(17)	C(1)–N(2)–N(4)–Ag(1)#3	169.81(17)
	Ag(1)–N(5)–C(1)–N(3)	15.3(4)	C(1)–N(2)–C(2)–N(6)	-0.9(3)
	Ag(1)#1–N(6)–C(2)–N(2)	167.04(16)	C(1)–N(2)–C(2)–C(2)#2	178.9(3)
	Ag(1)#1–N(6)–C(2)–C(2)#2	-12.8(5)	C(1)–N(5)–N(6)–Ag(1)#1	-169.53(14)
	N(4)–N(2)–C(1)–N(3)	-3.8(4)	C(1)–N(5)–N(6)–C(2)	0.1(3)
	N(4)–N(2)–C(1)–N(5)	178.6(2)	C(2)–N(2)–N(4)–Ag(1)#3	-13.0(3)
	N(4)–N(2)–C(2)–N(6)	-178.5(2)	C(2)–N(2)–C(1)–N(3)	178.6(2)
	N(4)–N(2)–C(2)–C(2)#2	1.3(4)	C(2)–N(2)–C(1)–N(5)	1.0(3)

Table S5 Hydrogen bonding parameters of $H_2(TABT)(NO_3)_2$ and $Ag_2(TABT)(NO_3)_2$

	Bond	D–H···A/Å	d(H···A)/Å	d(D···A)/Å	∠DHA/º
$H_2(TABT)(NO_3)_2$	N(3)–H(3A)···O(2)	0.880	2.242	2.986	142.1
	N(3)–H(3A)···O(3)	0.880	2.342	3.045	136.9
	N(3)–H(3B)···O(1)	0.880	2.015	2.884	169.2
	N(2)–H(2)···O(1)	0.880	1.843	2.718	172.9
	N(4)–H(4A)···O(3)	0.821	2.213	3.020	167.8
	N(4)–H(4B)···O(2)	0.881	2.334	3.049	138.4
	N(4)–H(4A)···N(1)	0.821	2.756	3.016	100.6
	N(4)–H(4B)···N(1)	0.881	2.737	3.016	99.94
$Ag_2(TABT)(NO_3)_2$	N(3)–H(3A)···O(3)	0.880	2.085	2.875	148.9
	N(4)–H(4A)···O(2)	0.910	2.150	2.796	127.2
	N(4)–H(4B)···O(3)	0.910	2.017	2.870	155.5
	N(4)–H(4A)···O(1)	0.910	2.757	2.881	88.48
	N(4)–H(4B)···O(1)	0.910	2.518	2.881	104.3

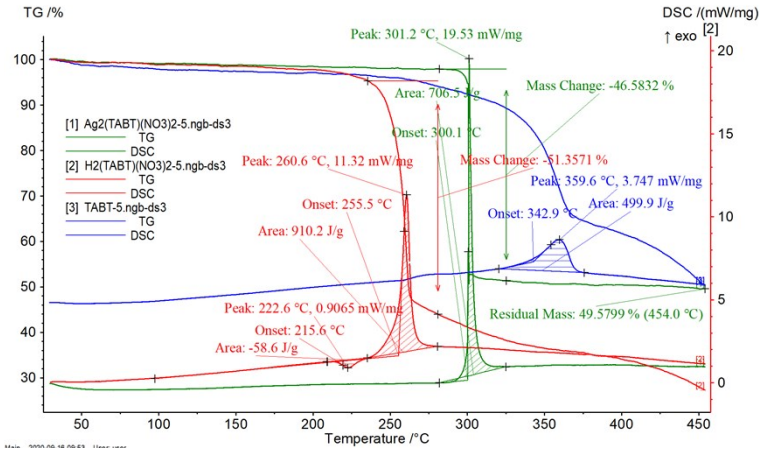

Fig. S3 DSC of TABT and its salts at the heating rate of 5 °C min^{-1}

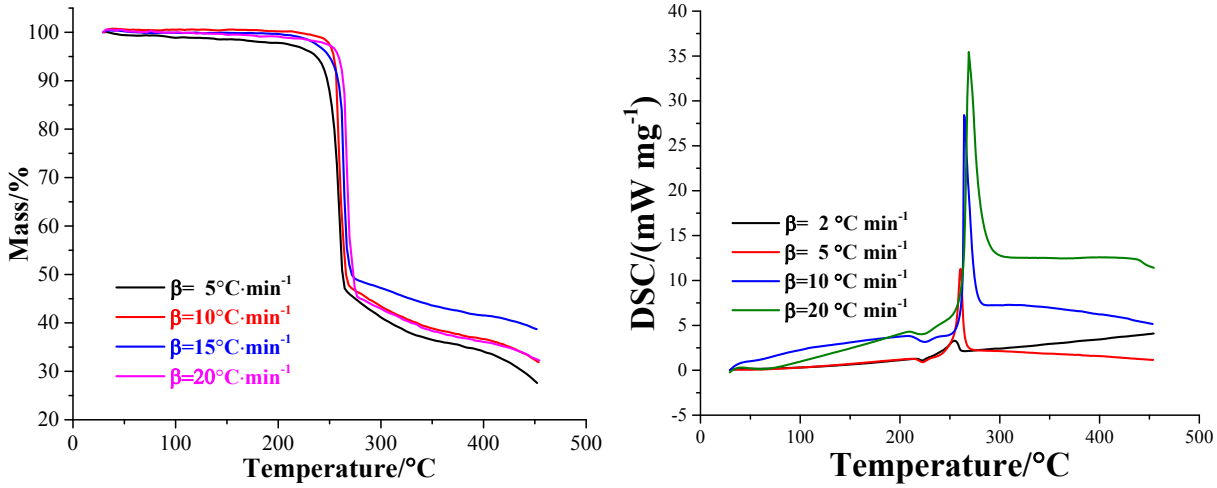

Fig. S4 TG-DSC curves of $H_2(TABT)(NO_3)_2$ under the different heating rates

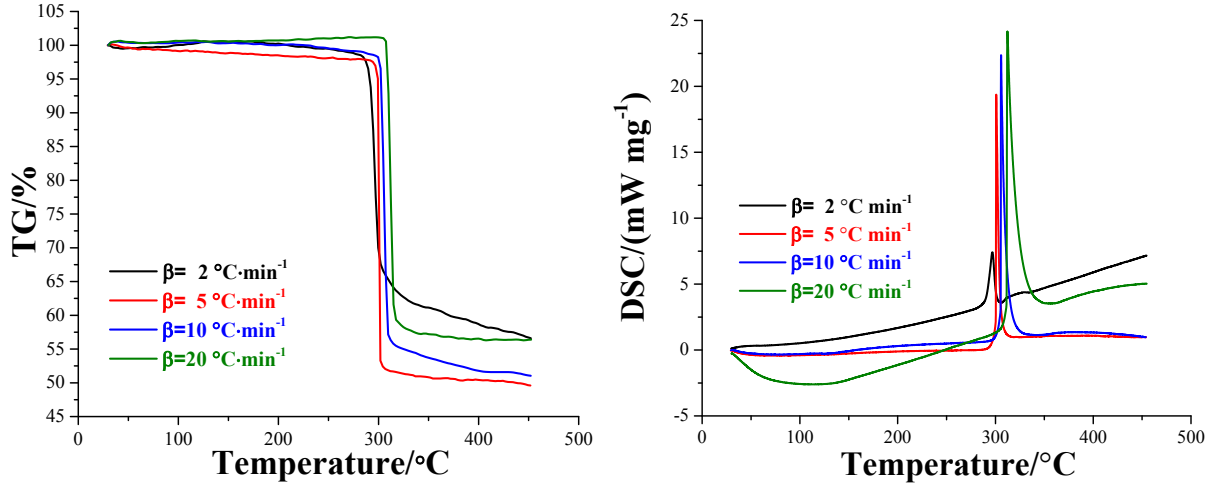

Fig. S5 TG-DSC curves of $Ag_2(TABT)(NO_3)_2$ under the different heating rates

Table S6 Thermo- kinetic parameters for $H_2(TABT)(NO_3)_2$ and $[Ag_2(TABT)(NO_3)_2]_n$

β	$C_4H_{10}N_{12}O_6$		$C_4H_8N_{12}O_6Ag_2$	
	*T*o	*T*p	*T*o	*T*p
2	245.5	253.8	290.8	296.5
5	256.3	260.6	299.4	301.2
10	259.0	264.5	304.9	306.2
20	264.0	269.0	311.1	312.2
E_k	368.6		392.7	
r_k	0.9992		0.9931	
A	3.295×10^{35}		1.140×10^{35}	
E_o	359.0		382.6	
r_o	0.9992		0.9935	
E_a	363.8		387.6	
T_{e0}	232.4		281.8	
T_b	238.5		288.7	

Table S7 Calculated parameters used in the isomeric reactions.

	H_0/Hartree	ΔH_f^θ(gas)/ (kJ mol^{-1})	ΔH_f^θ(gas)/ (kcal mol^{-1})	A/(Å^2)	v	σ^2_{tot}	$\Delta H^\theta_{f,sub}$/ (kcal mol^{-1})	$\Delta H^\theta_{f,sub}$/ (kJ mol^{-1})	$\Delta H^\theta_{f,solid}$/ (kJ mol^{-1})	$\Delta H^\theta_{f,solid}$/ (kcal mol^{-1})
TABT	-700.5564	472.0[a]	112.8	-	-	-		-	-	-
HNO_3	-279.2489	-134.41[b]	-32.11	-	-	-		-	-	-
$AgNO_3$	-5455.0253	284.9[b]	68.06	-	-	-		-	-	-
1	-1259.1179	**20.56**	4.912	306.0	0.2329	439.1	59.00	247.0	**-226.4**	**-54.09**
2	-11610.7603	**-179.7**	-42.93	332.5	0.2449	310.9	62.59	262.0	**-441.7**	**-105.5**

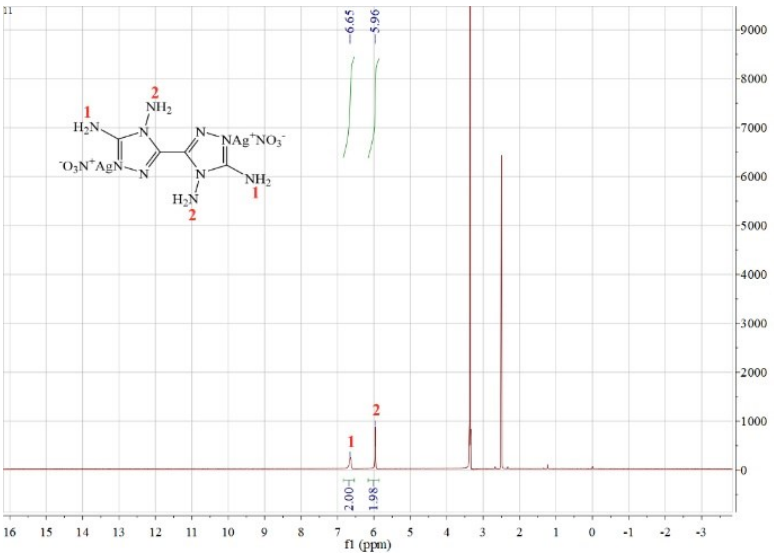

Fig. S6 ^{1}H of $\{Ag_2(TABT)(NO_3)_2\}_n$