Electronic Supplementary Material (ESI) for RSC Advances.

The novel compound Dimethylamine-5,5′-bistetrazole-1,1′-diolate: Crystal structure, Thermal investigation, Safety evaluation and Theoretical studies

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Figures

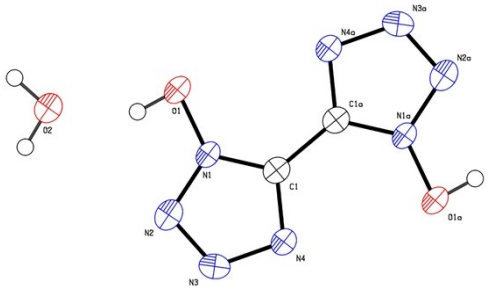

Fig. S1 The crystal structure of BTO (CCDC: 1532257)

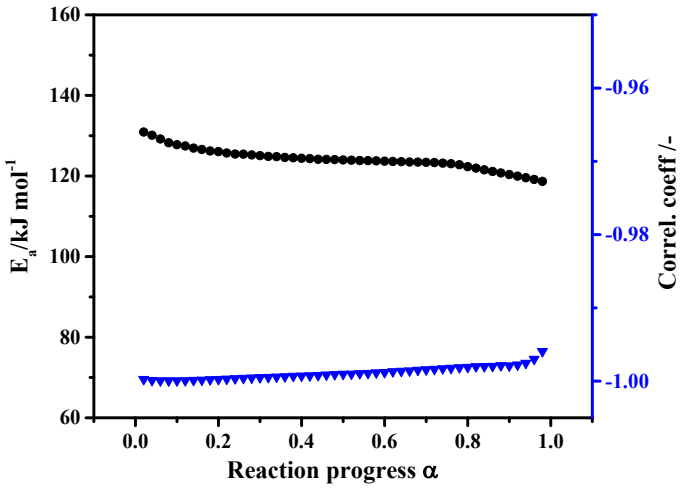

Fig.S2 Activation energy as a function of reaction progress of DMA-BTO by Friedman method of ATKS

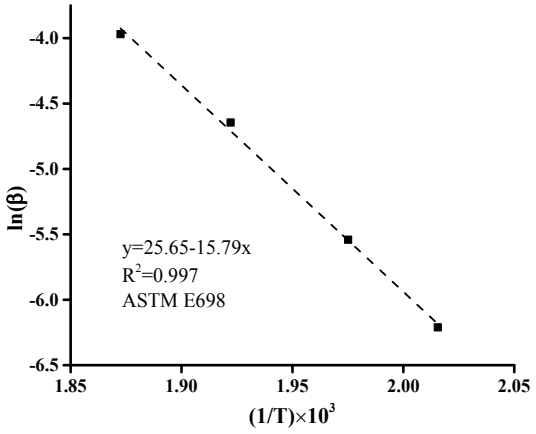

Fig.S3 lnβ versus 1/T for the decomposition of DMA-BTO by ASTM E698 method of AKTS

Tables

Table S1 crystal structure data for DMA-BTO and BTO

Formula	$C_6H_{16}N_{10}O_2$	$C_2H_6N_8O_4$
M_r(g mol^{-1})	260.29	206.15
Crystal size(mm^3)	0.65× 0.10×0.03	0.22× 0.20×0.18
Crystal group	Triclinic	Monoclinic
Space group	P-1	C2/m
a(Å)	5.571	7.752
b(Å)	7.293	6.391
c(Å)	8.500	8.702
α(deg)	109.868	90.00
β(deg)	102.043	116.05
γ(deg)	101.239	90.00
V(Å^3)	304.1	387.3
Z	1	2
D_{calcd}(g cm^{-3})	1.421	1.768
μ(Mokα)(cm^{-1})	1.12	1.62
F(000)(e)	138	212
hkl range	±7, -8→9, ±11	-9→6, -6→7, -9→10
$((\sin\theta)/\lambda)_{max}$(Å^{-1})	0.661	0.971
Refl. Measured/unique/R_{int}	3565/1437/0.0499	995/0.0388/0.0375
Parameter refined	85	49
R(F)/wR(F^2) (all reflexions)	0.1224/0.3422	0.1036/0.3191
GoF (F^2)^c	1.003	1.505
$\Delta\rho_{fin}$(max/min)(e Å^{-3})	0.660/-0.472	0.558/-0.605
CCDC	1447137	1532257

Table S2 Atomic coordinates of BTO

Atom	Site	*x*	*y*	*z*	Atom	Site	*x*	*y*	*z*
C(1)	m	-0.0206(10)	0	0.4103(8)	H(1O)	m	0.295(16)	0	0.333(7)
N(1)	m	0.1038(8)	0	0.3467(7)	H(1W)	m	0.356(18)	0	0.110(3)
N(2)	m	0.013(1)	0	0.1753(8)	H(2W)	m	0.532(8)	0	0.23(2)
N(3)	m	-0.1667(10)	0	0.1380(7)					
N(4)	m	-0.1979(8)	0	0.2809(6)					
O(1)	m	0.2951(7)	0	0.4303(7)					
O(2)	m	0.4180(8)	0	0.2177(6)					

Table S3 Selected bond lengths (Å), angles (deg), and torsion angles (deg) for DMA-BTO

Parameters	Experimental value	Parameters	Experimental value
Bond lengths (Å)		Bond angles (deg)	
O(1)-N(1)	1.322(6)	C(3)-N(5)-C(2)	113.4(5)
N(1)-C(1)	1.345(7)	N(4)-C(1)-N(1)	108.9(4)
N(1)-N(2)	1.363(7)	N(4)-C(1)-C(1)	127.7(6)
N(2)-N(3)	1.308(7)	N(1)-C(1)-C(1)	123.4(6)
N(3)-N(4)	1.336(7)	Torsion angles (deg)	
N(4)-C(1)	1.344(7)	O(1)-N(1)-N(2)-N(3)	178.7(5)
N(5)-C(3)	1.470(8)	C(1)-N(1)-N(2)-N(3)	0.6(6)
N(5)-C(2)	1.483(8)	N(1)-N(2)-N(3)-N(4)	-0.4(7)
C(1)-C(1)	1.469(10)	N(2)-N(3)-N(4)-C(1)	0.0(7)
Bond angles (deg)		N(3)-N(4)-C(1)-N(1)	0.4(6)
O(1)-N(1)-C(1)	129.6(5)	N(3)-N(4)-C(1)-C(1)	179.9(7)
O(1)-N(1)-N(2)	122.6(4)	O(1)-N(1)-C(1)-N(4)	-178.5(5)
C(1)-N(1)-N(2)	107.8(4)	N(2)-N(1)-C(1)-N(4)	-0.6(6)
N(3)-N(2)-N(1)	105.7(4)	O(1)-N(1)-C(1)-C(1)	2.0(10)
N(2)-N(3)-N(4)	112.4(5)	N(2)-N(1)-C(1)-C(1)	179.9(6)
N(3)-N(4)-C(1)	105.2(4)		

Table S4 Atomic coordinates of DMA-BTO

Atom	Site	*x*	*y*	*z*	Atom	Site	*x*	*y*	*z*
O(1)	1	0.1287(8)	0.2392(6)	0.5257(5)	H5A	1	-0.04640	0.14980	0.66040
N(1)	1	0.2515(9)	0.4359(7)	0.6031(6)	H5B	1	-0.19210	-0.01580	0.69800
N(2)	1	0.1994(10)	0.5650(8)	0.7420(7)	H2A	1	0.21360	0.31290	0.93280
N(3)	1	0.3593(10)	0.7440(8)	0.7860(7)	H2B	1	0.19340	0.07740	0.88540
N(4)	1	0.514(1)	0.7392(8)	0.6849(7)	H2C	1	0.02720	0.18270	1.00130
N(5)	1	-0.1139(9)	0.1221(7)	0.7426(6)	H3A	1	-0.37820	0.20410	0.86040
C(1)	1	0.4453(10)	0.5443(8)	0.5705(7)	H3B	1	-0.44630	0.18180	0.66110
C(2)	1	0.0981(12)	0.1786(9)	0.9042(8)	H3C	1	-0.22890	0.37680	0.81050
C(3)	1	-0.3080(12)	0.2302(10)	0.7710(9)					

Table S5 DTA Parameters of DMA-BTO

β (℃·min^{-1})	Endothermic peaks				Exothermic peaks			
	T_o(℃)	T_p(℃)	T_e(℃)	ΔH_1(kJg^{-1})	T_o(℃)	T_p(℃)	T_e(℃)	ΔH_1(kJg^{-1})
1	172.62	180.42	184.86	-1.12	205.39	221.71	236.50	11.43
2	175.54	188.80	194.91	-1.17	214.64	232.65	248.98	11.47
5	184.91	194.55	204.54	-1.21	226.86	246.94	262.76	11.49
10	287.56	204.40	215.44	-1.35	238.71	260.63	279.50	11.83

Table S6 Activation energy and pre-exponential factor evaluation by Kissinger method for thermal decomposition of DMA-BTO

β (℃·min^{-1})	log(β/T^2)	(1/T)×10^3	lnA	Arrhenius parameters		
				E_a(kJmol^{-1})	A (s^{-1})	r
1	-12.40	2.02	26.97	122.53	5.17×10^{11}	0.999
2	-11.75	1.97	26.97		5.19×10^{11}	
5	-10.89	1.92	27.03		5.52×10^{11}	
10	-10.25	1.87	26.95		5.06×10^{11}	

Table S7 Activation energy and pre-exponential factor evaluation by Ozawa method for thermal decomposition of DMA-BTO

β (℃·min^{-1})	log(β)	(1/T)×10^{-3}	lnA	Arrhenius parameters		
				E_a(kJmol^{-1})	A (s^{-1})	r
1	0	2.02	27.50	124.65	8.79×10^{11}	0.999
2	0.30	1.97	27.49		8.75×10^{11}	
5	0.69	1.92	27.54		9.16×10^{11}	
10	1.00	1.87	27.44		8.30×10^{11}	

Table S8 Calculated thermo-kinetic parameters of DMA-BTO byAKTS

samples	E_k/kJ mol^{-1}	Ln(A_k)/min^{-1}	R	E_o/kJ mol^{-1}	R
DMA-BTO	122.53	26.98	0.999	124.65	0.999

Table S9 The SADT of DMA-BTO by AKTS

storage mass/kg	1	10	30	50
SADT/℃	109	106	104	103

Table S10 Second-order perturbation theory analysis of the Fock matrix in NBO basis for DMA-BTO

Donor NBO	ED(i) (e)	Acceptor NBO	ED(i) (e)	$E^{(2)}$ (kJ mol^{-1})	ε_j-ε_i (a.u.)	F(i,j) (a.u.)
BD N(2)-N(3)	1.98735	BD* C(6)-C(34)	0.02956	3.59	1.33	0.062
BD N(3)-N(4)	1.98635	BD* O(1)-N(2)	0.02416	4.24	1.24	0.065
BD N(4)-N(5)	1.98257	BD* C(6)-C(34)	0.02956	5.08	1.31	0.073
		BD* O(1)-N(2)	0.02416	4.54	1.18	0.066
BD N(5)-C(6)	1.81802	BD* N(3)-N(4)	0.02183	23.45	0.29	0.080
		BD* N(33)-C(34)	0.53774	7.30	0.31	0.047
BD N(31)-N(32)	1.87991	BD* N(33)-C(34)	0.53774	11.66	0.33	0.062
BD N(33)-C(34)	1.98283	BD* O(29)-N(30)	0.02417	4.54	1.18	0.066

LP N(2)	1.41331	BD* N(3)-N(4)	0.02183	42.76	0.24	0.094
		BD* N(5)-C(6)	0.03284	58.39	0.26	0.111
BD* N(7)-H(9)	0.14140	BD* O(1)-N(2)	0.02416	5.69	0.03	0.040
BD* N(18)-H(20)	0.14125	BD* O(29)-N(30)	0.02417	5.71	0.03	0.040

Table S11 Mulliken charge population of atoms in DMA-BTO

Atom	Mulliken charge (e)	Natural charge (e)
O1	-0.493	-0.628
N2	-0.100	0.171
N3	-0.046	-0.093
N4	-0.105	-0.086
N5	-0.408	-0.409
C6	0.446	0.247
N7	-0.359	-0.606
C10	-0.195	-0.353
C14	-0.193	-0.354
H8	0.289	-0.461
H9	0.326	0.451
H11	0.133	0.191
H12	0.155	0.217
H13	0.136	0.195
H15	0.139	0.197
H16	0.144	0.208
H17	0.132	0.191