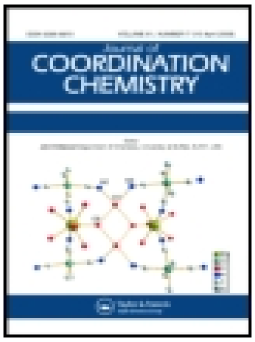


Taylor & Francis
Taylor & Francis Group

Journal of Coordination Chemistry

ISSN: 0095-8972 (Print) 1029-0389 (Online) Journal homepage: http://www.tandfonline.com/loi/gcoo20

A new coordination compound based on 4-amino-3-(tetrazol-5-yl)-furazan (HAFT): preparation, crystal structure, and thermal properties

Zi-Mei Ding, Wen-Li Cao, Xiao-Jing Hang, Xiao Ma, Hui Zheng, Kang-Zhen Xu & Jie Huang

To cite this article: Zi-Mei Ding, Wen-Li Cao, Xiao-Jing Hang, Xiao Ma, Hui Zheng, Kang-Zhen Xu & Jie Huang (2018): A new coordination compound based on 4-amino-3-(tetrazol-5-yl)-furazan (HAFT): preparation, crystal structure, and thermal properties, Journal of Coordination Chemistry, DOI: 10.1080/00958972.2018.1529308

To link to this article: https://doi.org/10.1080/00958972.2018.1529308

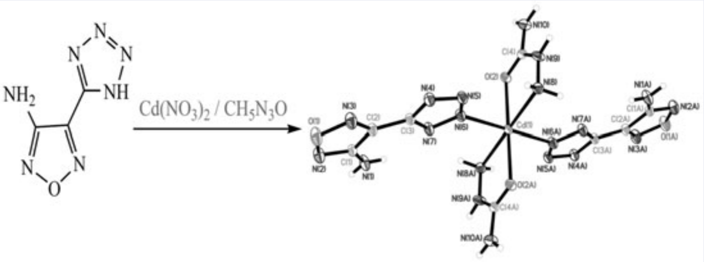
JOURNAL OF COORDINATION CHEMISTRY
https://doi.org/10.1080/00958972.2018.1529308

A new coordination compound based on 4-amino-3-(tetrazol-5-yl)-furazan (HAFT): preparation, crystal structure, and thermal properties

Zi-Mei Ding, Wen-Li Cao, Xiao-Jing Hang, Xiao Ma, Hui Zheng, Kang-Zhen Xu and Jie Huang

School of Chemical Engineering, Shaanxi Key Laboratory of Physico-Inorganic Chemistry, Northwest University, Xi'an, PR China

ABSTRACT
The green nitrogen-rich coordination compound $Cd(SCZ)_2(AFT)_2$ (**1**) (AFT =4-amino-3-(5-tetrazolate)-furazan and SCZ = semicarbazide) was first synthesized and characterized by EA and Fourier Transform Infrared (FT-IR). The single crystal was cultivated and determined with X-ray diffraction. It revealed that **1** crystallizes in the monoclinic space group $P2_1/c$. A Cd^{2+} ion is coordinated by four N atoms and two O atoms to form a distorted octahedral structure. Among them, two nitrogen atoms are from the two AFT ions and the other four atoms are from two SCZ molecules. The thermal decomposition behavior of **1** was studied with DSC and TG-DTG methods. The apparent activation energy (E), thermal stability, and safety parameters (T_{SADT}, T_{TIT}, and T_b) were calculated for **1**. Moreover, entropy of activation ($\Delta S^{\neq}$), enthalpy of activation ($\Delta H^{\neq}$), free energy of activation ($\Delta G^{\neq}$), specific heat capacity (C_p), and impact sensitivity were also discussed in detail.



ARTICLE HISTORY
Received 18 April 2018
Accepted 17 August 2018

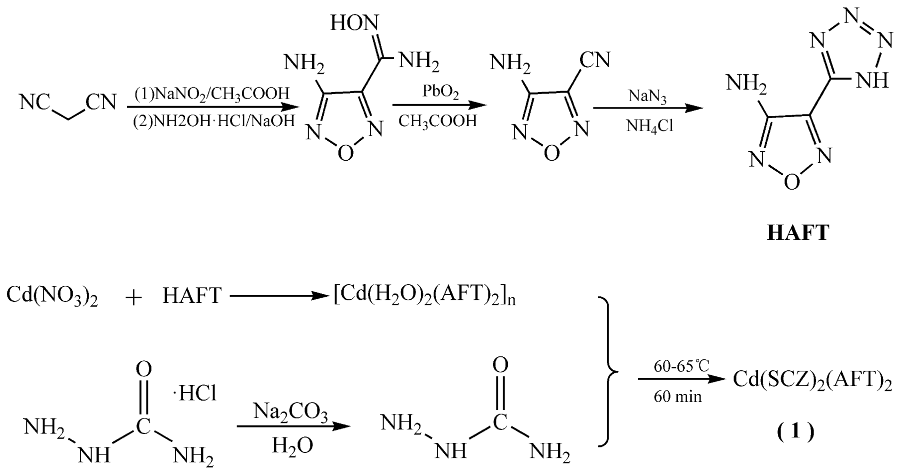
KEYWORDS
4-Amino-3-(tetrazol-5-yl)-furazan; cadmium complex; crystal structure; thermal properties; thermal safety

1. Introduction

In recent years, a series of energetic coordination compounds were synthesized using transition metal ions such as Cd^{2+}, Cu^{2+}, Zn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, and Mn^{2+} as central

CONTACT Jie Huang huangjie@nwu.edu.cn

Supplemental data for this article can be accessed https://doi.org/10.1080/00958972.2018.1529308.



Scheme 1. Synthesis of HAFT and **1**.

metal cations [1–10]. In general, they can be easily prepared through coordination bonds between a metal center and organic linker. Thus, the synthesis of coordination polymer networks with these metal ions is of crucial importance [11]. These materials possess many advantages such as combined facile syntheses, structural versatility, unique properties, and applications as well as energetic properties [12, 13].

In the continuous research of new energetic materials, high-energy metal complexes are becoming more and more popular [14–18]. Energetic coordination complexes based on high nitrogen content ligands have obtained much attention due to their excellent energetic properties [19–21]. As we have noticed, based on the impact of energy and the environment, high energy ligands among the energetic compounds previously reported were primarily employing triazole/tetrazole/furazan/tetrazine and their derivatives [22–34].

Recently, nitrogen-rich energetic salts on account of 4-amino-3-(tetrazol-5-yl)-furazan (HAFT) have been reported, all of which are insensitive to impact, relatively high density, and thermally stable, with good detonation pressure and velocity [35, 36]. In previous work, Wu *et al.* reported energetic complexes $[Cd(H_2O)_2(AFT)_2]_n$ (**2**) [17, 18]. Afterward $[Cd(NH_2NH_2)_2(AFT)_2 0.7H_2O]_n$ (**3**) and $[Cd(NH_2NHCOCONHNH_2)_{1.5}(AFT)_2 5H_2O]_n$ (**4**) were also synthesized, in which coordination water molecules of **2** were replaced by NH_2NH_2 and $NH_2NHCOCONHNH_2$, but the structures of the above compounds contain free water molecules.

Herein, we report a coordination compound $Cd(SCZ)_2(AFT)_2$, with SCZ totally replacing coordination water molecules of **2**, which is prepared and characterized by X-ray single-crystal diffraction, EA, and Fourier Transform Infrared (FT-IR). The specific heat capacity (C_p) and mechanical sensitivity were investigated. The apparent activation energy (E), thermal stability, and safety parameters (T_{SADT}, T_{TIT}, and T_b) and thermodynamic functions ($\Delta S^{\neq}$, $\Delta H^{\neq}$, and $\Delta G^{\neq}$) for exothermic decomposition process were calculated and analyzed. This work will enrich the research on the coordination chemistry of HAFT.

2. Experimental

2.1. Materials and analysis

HAFT was prepared according to Andrianov and Eremeev [37] and the purity was over 99%. The synthesis route is shown in Scheme 1.

Sodium nitrite, ethyl acetate, sodium azide, ammonium chloride, sodium hydroxide, sodium carbonate, and cadmium nitrate were commercially available from Chinese Sinopharm Chemical Reagent Company and used as received. Other chemicals were purchased from Aladdin or Maclin chemical companies and used as received.

Elemental analyses (C, H, and N) were performed on a Vario EL III elemental analyzer (Elementar Co., Langenselbold, Germany). FT-IR spectra were determined as KBr pellet for solids using an EQUINX55 spectrometer in the range of 4000–500 cm^{-1}. Differential scanning calorimeter (DSC) tests were determined using a DSC-Q2000 apparatus (TA Instruments, New Castle, DE) under a nitrogen atmosphere at a flow rate of 50 $mL\cdot min^{-1}$; the heating rates (β) were 5, 10, 15, and 20 $°C\cdot min^{-1}$ from ambient temperature to 375 °C. The TG-DTG experiment was carried out with an SDT-Q600 apparatus (TA Instruments, New Castle, DE) under a nitrogen gas with a flow rate of 100 $mL\cdot min^{-1}$ at a heating rate of 10.0 $°C\cdot min^{-1}$. The specific heat capacity (C_p) was determined with a Micro-DSC III apparatus (SETARAM, Caluire-et-Cuire, France) with the operating temperature range of 283–333 K and the sample mass was 200 mg. The impact sensitivity was determined using a ZBL-B impact sensitivity instrument (Nachen Co., Beijing, China).

2.2. Synthesis of $Cd(SCZ)_2(AFT)_2$\{bis((4-amino-3-(5-tetrazolate)-furazan)N)bis(semicarbazide-N,O)cadmium(II)\} (1)

1 was synthesized as follows: HAFT (2.5 mmol) was dissolved in distilled water (5 mL) and charged into a glass reactor with a water bath. It was kept under mechanical stirring and heated to 60 ~ 65 °C. A $Cd(NO_3)_2$ aqueous solution (0.25 mol L^{-1}, 5 mL) was added to the HAFT solution during 15 min with continuous stirring. Then, a solution containing SCZ (5 mmol) [SCZ (aq.): Semicarbazide hydrochloride (5 mmol) was dissolved in 5 mL distilled water. Using solid Na_2CO_3 in deionized water (5 mL) the solution pH was adjusted to value of 6–7] and the mixture was kept at 60 ~ 65 °C for 60 min. Afterward, the solution was cooled to room temperature, the resulting mixture was filtered and the filtrate allowed to evaporate in an undisturbed condition at ambient temperature. In the end, single crystals suitable for X-ray measurement was obtained by evaporation of the mother liquor at room temperature for one day. Yield: 70.8%. Anal. Calcd for $C_8H_{14}N_{20}O_4Cd$ (%): C, 16.95; H, 2.49; N, 49.43. Found: C, 16.93; H, 2.52; N, 49.40. IR (KBr, cm^{-1}): $\nu(-NH_2) = 3493$w, 3416w, $\nu(-NH) = 3294$w, 2974m, $\nu(-C=O) = 1644$m, $\nu(-C=N) = 1599$w, $\nu(N=N)$1547w, $\nu(-C-N) = 1396$m, 1207w, 1081s, $\gamma(-NH_2) = 763$w.

2.3. Crystal structure determination and refinement

Single crystals of the coordination compound were obtained by solvent evaporation at ambient temperature. X-ray diffraction data were collected [38] on a Bruker SMART

Table 1. Crystal data and structure refinement details of **1**.

Empirical formula	$C_8H_{14}N_{20}O_4Cd$
Formula weight ($g \cdot mol^{-1}$)	566.79
Temperature (K)	296(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	5.2047(11)
b (Å)	11.660(2)
c (Å)	16.019(4)
β (°)	97.882(3)
Volume (Å^3)	962.9(4)
Z	2
$D_{calc}/(g \cdot cm^{-3})$	1.955
F(000)	564
θ range/°	2.17–26.63
Goodness-of-fit on F^2	1.050
R_1 [$I > 2r(I)$]	0.0270
wR_2 [$I > 2r(I)$]	0.0609
R_1 (all data)	0.0364
wR_2 (all data)	0.0650
CCDC	1831044

APEX CCD X-ray diffractometer using graphite-monochromated Mo-Kα radiation ($\lambda = 0.71073$ Å). A semi-empirical absorption correction based on equivalent reflections was applied [39]. Data reduction was performed using the SAINT program from BRUKER AXS [40]. The structure was solved by direct methods (SHELXS-2014) [41] and refined by the full-matrix-block least squares method (SHELXL-2014) [41] on F^2 with anisotropic thermal parameters for all non-hydrogen atoms. H atoms could be generated from a difference Fourier map or the theoretical models (H1A and H1B could be generated from a difference Fourier map. Other H atoms could be generated from the theoretical models). Crystallographic data and refinement parameters are gathered in Table 1. Selected bond lengths and angles of **1** are listed in Table 2.

3. Results and discussion

3.1. Description of structure

Compound $Cd(SCZ)_2(AFT)_2$ crystallizes in the $P2_1/c$ space group and the unit cell is comprised of four molecules with the calculated density of 1.955 $g \cdot cm^{-3}$ at 296 K. As shown in Figure 1, a single molecule consisted of one Cd^{2+} ion, two SCZ molecules, and two AFT anions. The central Cd^{2+} ion is six-coordinate with four nitrogen atoms and two oxygen atoms to form an octahedral geometry, but the Cd^{2+} ion is seven-coordinate in energetic complex **4** [18]. Similarly, hydrazine molecules in **3** [18] and SCZ molecules in coordination compound **1** present typical bidentate coordination modes. The furazan-ring does not participate in these compounds. The tetrazole-ring presents a typical monodentate coordination mode in **1**, which is the same as that of **4**, but different in **2** and **3**. Compared with the above three cadmium salts, $Cd(SCZ)_2(AFT)_2$ is the salt with no crystallization water in its structure. The detailed geometry data for **1** (Table 2) show that the bond lengths of Cd–N are between 2.317(2) and 2.362(2) Å with an average value of 2.3402 Å and bond lengths of Cd–O is 2.3029(18) Å. The bond angles of N(6)–Cd(1)–N(8), O(2)–Cd(1)–N(6) and O(2)–Cd(1)–N(8) are 84.99(8)°, 90.43(8)° and 72.11(7)°, respectively. Cd^{2+} ion and SCZ

Table 2. Selected bond lengths (Å) and angles (°) of **1**.

Cd(1)–N(6)	2.317(2)	Cd(1)–N(8)	2.362(2)
Cd(1)–O(2)	2.3029(18)	Cd(1)–N(6A)#1	2.317(2)
Cd(1)–O(2A)#1	2.3029(18)	Cd(1)–N(8A)#1	2.362(2)
O(2)–Cd(1)–N(6)	90.43(8)	O(2)–Cd(1)–N(6A)#1	89.57(8)
O(2A)#1–Cd(1)–N(6)#1	89.57(8)	O(2A)#1–Cd(1)–N(6A)#1	90.43(8)
O(2)–Cd(1)–N(8)	72.11(7)	O(2)–Cd(1)–N(8A)#1	107.90(7)
N(6)–Cd(1)–N(8)	84.99(8)	N(6)–Cd(1)–N(8A)#1	95.01(8)

Symmetry transformations used to generate equivalent atoms: #1: $-x$, $2-y$, $1-z$.

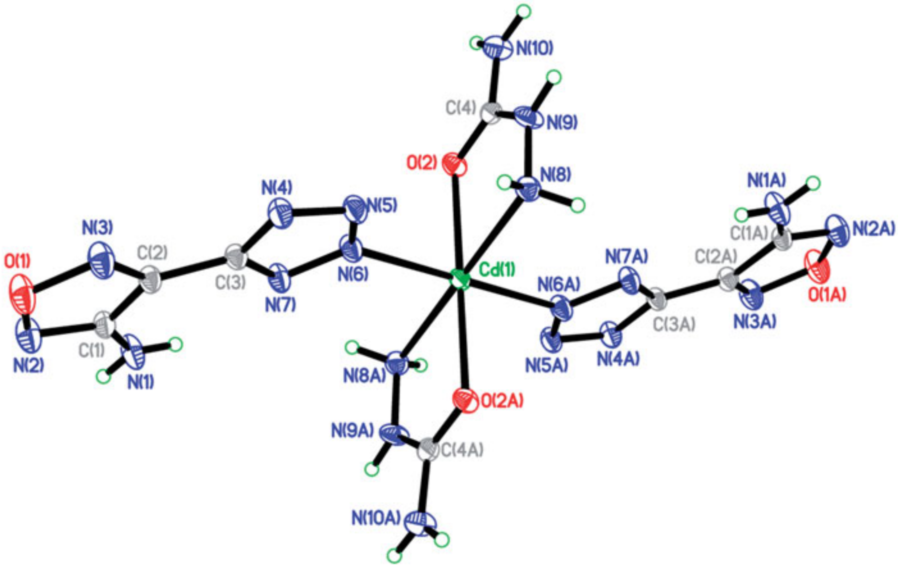


Figure 1. Molecular structure of **1**.

molecules are almost in the same plane (bond angles of two N and O atoms from SCZ and Cd^{2+} cation are 180.00°). Ring Cd(1)–O(2)–C(4)–N(9)–N(8)–N(10) constitutes the plane (A): $-2.2902x + 8.0430y - 8.1558z = 4.0163$ (mean deviation 0.410 Å). The bond angles of two N atoms (contraposition AFT groups) and Cd^{2+} cation are 180.00°. Ring atoms Cd(1)–C(3)–N(4)–N(5)–N(6)–N(7) are almost in coplanar in another plane (B): $3.1666x + 6.8784y + 7.0872z = 10.3308$ (mean deviation 0.829 Å). Planes A and B are nearly perpendicular to each other with a plane angle of 80.45°, which is benefiting to the stability of the structure. There are seven kinds of hydrogen-bond interactions in the crystal packing of **1** as shown in Table S1. Two kinds of hydrogen-bond interactions [N1 – H1···O2#1, N8 – H8···O2#3, symmetry transformation: #1: $-1-x$, $2-y$, $1-z$; #3: $1+x$, y, z] make $Cd(SCZ)_2(AFT)_2$ molecule form a 1D chain (Figure S1). The 2-D layer of $Cd(SCZ)_2(AFT)_2$ is constructed by two kinds of hydrogen-bond interactions (Figure S2) [N1 – H1···N2#2, N10 – H10···O1#5, symmetry transformation: #2: $-2-x$, $3-y$, $1-z$; #5: x, $-1+y$, z]. Three other kinds of N–H···N interactions [N1–H1···N2#4, N10–H10···N4#4, N10–H10···N5#4, symmetry transformation: #4: $-x$, $-0.5+y$, $0.5-z$] finally lead to the formation of a 3D network as shown in Figure 2. Those hydrogen bonds also play an important role in enhancing the stability of **1**.

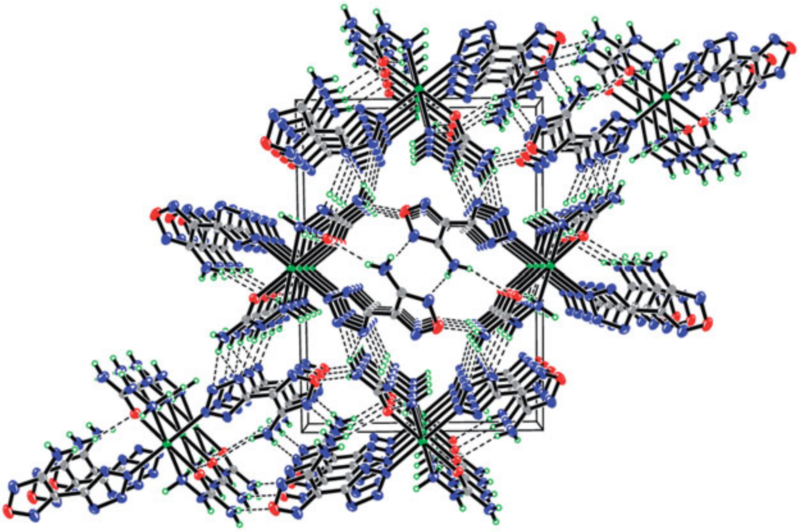


Figure 2. Packing structure of **1**.

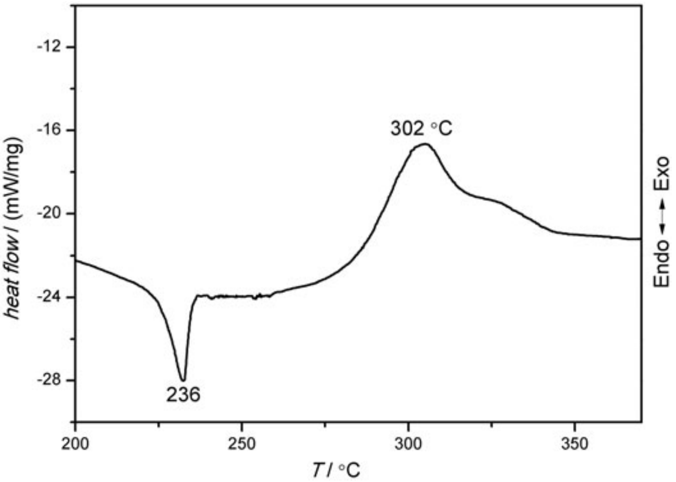


Figure 3. DSC curve of **1** at 10 °C·min^{-1}.

3.2. Thermal decomposition behavior

The DSC and TG-DTG data for **1** at heating rates of 10 °C min^{-1} are shown in Figures 3 and 4, respectively. As can be seen in Figure 3, the DSC curve of **1** consists of two stages. The first stage is an endothermic stage, which is a melting process and the melting point is 236 °C. It then starts to decompose at 269 °C, with continuous decomposition peaks at 302 °C. Corresponding to the process, there is a main mass loss of 38.01% in the TG-DTG curves. The decomposition temperature of $Cd(SCZ)_2(AFT)_2$ is higher than that of RDX and HMX [42] (219 and 275 °C, respectively), but slightly lower than that of **2** and **3** (318.2 and 320 °C, respectively) [17, 18]. Furthermore, using T_p as criterion, comparing with other coordination compounds such as $[Ni(SCZ)_3]TNR$ [43],

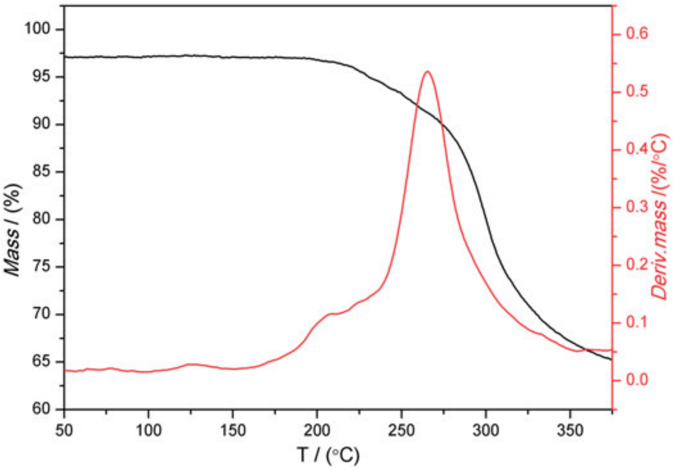


Figure 4. TG-DTG curves of **1** at 10 °C·min^{-1}.

$[Cd_2Cl_4(HATr)_3(H_2O)_2]$ [44], $[Mg(CHZ)_3](ClO_4)_4$ [45], $[Cu(DAT)_2(PA)_2]$ and $[Cu(DAT)_2(HTNR)_2]$ [46], $(NH_4)_2[Zn(BTA)_2(H_2O)]\cdot 2H_2O$, $(N_2H_5)_2[Zn(BTA)_2(H_2O)]\cdot 3H_2O$, and $(NH_3OH)_2[Zn(BTA)_2(H_2O)]\cdot 4H_2O$ [47] (The T_p at heating rates of 10 °C min^{-1} values are 216.8, 283.25, 284.85, 215.75, 246.05, 222.6, 219.5, and 227.6 °C, respectively.), **1** exhibits higher thermal stability. (HTNR =2,4,6-trinitroresorcinol), HATr =3-hydrazino-4-amino^{-1},2,4-triazole, CHZ =1,3-diaminourea, DAT =1,5-diaminotetrazole, PA = picric acid, BTA = N,N-bis(1H-tetrazol-5-yl)amine).

3.3. Non-isothermal kinetics analysis

In this work, based on the first exothermic peak temperatures measured at four different heating rates of 5, 10, 15, and 20 °C·min^{-1}, Kissinger's method [48] and Ozawa–Doyle's method [49] were applied to obtain the apparent activation energy (E), the pre-exponential factor (A), and linear correlation coefficients (r). The measured values of the extrapolated onset temperature (T_e) and peak temperature (T_p) of the exothermic decomposition reaction are listed in Table 3. The values of T_{e0} and T_{p0} in the stage corresponding to $\beta \rightarrow 0$ obtained by Equation (1) [50, 51] are also shown in Table 3.

$$T_{(e\ \text{or}\ p)i} = T_{(e0\ \text{or}\ p0)} + a\beta_i + b\beta_i^2 + c\beta_i^3 \qquad i = 1, 2, 3, 4 \qquad (1)$$

where a, b, and c are coefficients.

From Table 3, the apparent activation energy (E) obtained by the Kissinger method agrees well with that obtained by the Ozawa method, and the linear correlation coefficients are all very close to 1. Therefore, the results are credible. The Arrhenius equation has been obtained, expressed by using the calculated E_a (the average of E_k and E_o) and ln A_k as follows: $\ln k = 41.39 - 18.23 \times 10^3/RT$.

Table 3. The parameters determined by DSC curves at different heating rates (β) of **1.**

β/°C·min^{-1}	T_e /°C	T_p /°C	T_{e0} /°C	T_{p0} /°C	E_k /kJ·mol^{-1}	log A_k (s^{-1})	r_k	E_o/ kJ·mol^{-1}	r_o	$\bar{E}$/kJ·mol^{-1}
5.0	274.37	295.59	264.80	289.13	219.04	17.9761	0.9917	217.42	0.9924	218.23
10.0	283.94	302.05								
15.0	288.69	307.61								
20.0	292.93	312.34								

Subscript k, data obtained by Kissinger method; subscript o, data obtained by Ozawa method

3.4. Thermal stability and safety parameters and thermodynamic functions

Research focusing on energetic materials is not only for seeking high energy, but also for considering thermal safety. The self-accelerating decomposition temperature (T_{SADT} or T_{e0}), thermal ignition temperature (T_{TIT} or T_{be0}) and critical temperature of thermal explosion (T_b or T_{bp0}) are important parameters for evaluating their thermal stability. T_{TIT} and T_b can be obtained by Equations (2) and (3) [52], respectively. The values of T_{SADT}, T_{TIT}, and T_b are 264.80, 276.35, and 301.77 °C for **1**, respectively. The entropy of activation ($\Delta S^{\neq}$), enthalpy of activation ($\Delta H^{\neq}$), and free energy of activation ($\Delta G^{\neq}$) of the thermal decomposition reaction for **1** corresponding to T=T_{p0}, A=A_k, and E_a =E_k can be calculated by Equations (4)–(6) [53]. The values of $\Delta S^{\neq}$, $\Delta H^{\neq}$, and $\Delta G^{\neq}$ for **1** are 93.94 J·mol^{-1}·K^{-1}, 214.37 kJ·mol^{-1}, and 161.54 kJ·mol^{-1}, respectively,

$$T_{SADT} = T_{e0} \tag{2}$$

$$T_{be0(bp0)} = \left(E_O - \sqrt{E_O^2 - 4E_O R T_{e0(p0)}}\right)/2R \tag{3}$$

$$A = (k_B T/h)e^{\Delta S^{\neq}/R} \tag{4}$$

$$\Delta H^{\#} = E_a - RT \tag{5}$$

$$\Delta G^{\#} = \Delta H^{\#} - T\Delta G^{\#} \tag{6}$$

where k_B is the Boltzmann constant (1.381×10^{-23} J·K^{-1}) and h is the Planck constant (6.626×10^{-34} J·s).

From the results, T_{p0} and T_b for Cd(SCZ)$_2$(AFT)$_2$ show higher thermal stability than **3** (260.0 and 281.77 °C, respectively) and **4** [18] (289.13 and 301.77 °C, respectively). The thermal stability of **1** is similar to that of **2** [17] (296.4 and 300.23 °C).

3.5. Specific heat capacity

The continuous specific heat capacity of **1** was measured by Micro-DSC III, and the results are given in the Supplementary Material (Figure S3). The specific heat capacity equations of **1** have been obtained as follows: C_p (J·g^{-1}·K^{-1}) = $4.92483 \times 10 - 4.7294 \times 10^{-1}T + 1.5343 \times 10^{-3}T^2 - 1.6466 \times 10^{-6}T^3$ (283 K<T< 333 K), the molar heat capacity is 558.93 J·mol^{-1}·K^{-1} at 298.15 K. Specific heat capacity of **1** presents a good cubic relationship with temperature in determined temperature range.

3.6. Impact sensitivity

Impact sensitivity was determined using a ZBL-B impact sensitivity instrument. The coordination compound **1** (30 mg) was placed between two steel poles and hit by a 2.0 kg drop hammer at a height of 1.2 m. The test showed that the firing rate was 0% (>24 J), which was less sensitive to impact than TNT (15.0 J), RDX (7.5 J) and TKX-50 (20 J). In addition, the other three cadmium salt complexes [17, 18] are relatively less sensitive. Combining with their high nitrogen-content, these coordination compounds may have a possible application in the field of insensitive high explosive.

4. Conclusion

A new coordination compound based on HAFT was first synthesized and structurally characterized. The crystal belongs to monoclinic system with space group $P2_1/c$. The central Cd^{2+} ion is six-coordinate to form an octahedral geometry. The thermal decomposition behavior of **1** was researched. Results manifest that the decomposition peak temperature is 302 °C at the heating rate of 10 °C·min^{-1}, which is higher than that of RDX and HMX (219 and 275 °C, respectively) but slightly lower than that of **2** and **3** (318.2 and 320 °C, respectively). The non-isothermal kinetic parameters were also calculated through the Kissinger and the Ozawa methods, and the Arrhenius equation of **1** can be expressed as $\ln k = 41.39 - 218.23 \times 10^3/RT$. In addition, T_{SADT}, the thermal ignition temperature (T_{TIT}) and the critical temperature (T_b) of thermal explosion are 264.80, 276.35 and 301.77 °C, respectively. Moreover, $\Delta S^{\neq}$, $\Delta H^{\neq}$, and $\Delta G^{\neq}$ of the thermal decomposition reaction are 93.94 J·mol^{-1}·K^{-1}, 214.37 kJ·mol^{-1}, and 161.54 kJ·mol^{-1}, respectively. Besides, the specific heat capacity equation of **1** is C_p (J·g^{-1}·K^{-1}) $= 4.92483 \times 10 - 4.7294 \times 10^{-1}T + 1.5343 \times 10^{-3}T^2 - 1.6466 \times 10^{-6}T^3$ (283 K$<T<$ 333 K) and the molar heat capacity is 558.93 J·mol^{-1}·K^{-1} at 298.15 K. Coordination compound **1** has relatively less sensitive to impact (>24 J). This work has not only successfully produced a high-energy material, but also provided direction for the design and synthesis of a new generation of coordination compounds.

Acknowledgments

The authors are very grateful for financial support.

Disclosure statement

No potential conflict of interest was reported by the authors.

Funding

This article received financial assistance from the National Natural Science Foundation of China (No. 21241003), the Education Committee Foundation of Shaanxi Province (No. 14JF025), and the Northwest University Graduate Innovation and Creativity Funds (No. YZZ17145).

References

[1] Y. Zhang, H. Wu, K.Z. Xu, W.T. Zhang, Z.Y. Ren, J.R. Song, F.Q. Zhao. *J. Phys. Chem. A.*, **118**, 1168 (2014).

[2] B.D. Wu, T.L. Zhang, L. Yang, J.G. Zhang, Z.N. Zhou. *Z. Anorg. Allg. Chem.*, **639**, 163 (2013).

[3] T.W. Myers, J.A. Bjorgaard, K.E. Brown, D.E. Chavez, S.K. Hanson, R.J. Scharff, S. Tretiak, J.M. Veauthier. *J. Am. Chem. Soc.*, **138**, 4685 (2016).

[4] B.D. Wu, Y.L. Li, F.G. Li, Z.N. Zhou, L. Yang, J.G. Zhang, T.L. Zhang. *Polyhedron*, **55**, 73 (2013).

[5] P.P. Sun, J.F. Dong, Y. Wang, Y.J. Liu, F. Sun, J.W. Yuan, G.W. Yang, Q.Y. Li. *Inorg. Chem. Commun.*, **73**, 77 (2016).

[6] X.B. Zhang, Y.H. Ren, W. Li, F.Q. Zhao, B.Z. Wang, J.R. Song. *Chem. Res. Chin. U.*, **29**, 627 (2013).

[7] S.S. Nagarkar, B. Joarder, A.K. Chaudhari, S. Mukherjee, S.K. Ghosh. *Angew. Chem. Int. Ed. Engl.*, **52**, 2881 (2013).

[8] O.S. Bushuyev, P. Brown, A. Maiti, R.H. Gee, G.R. Peterson, B.L. Weeks, L.J.H. Weeks. *J. Am. Chem. Soc.*, **134**, 1422 (2012).

[9] J.T. Wu, J.G. Zhang, X. Jin, X. Yin, T.L. Zhang. *J. Coord. Chem.*, **69**, 1236 (2016).

[10] X. Jin, C.X. Xu, X. Yin, P. He, J.G. Zhang. *J. Coord. Chem.*, **68**, 1913 (2015).

[11] N. Golovnev, M. Molokeev. *Acta Crystallogr. C.*, **69**, 704 (2013).

[12] G. Smith. *Acta Cryst. C.*, **69**, 1472 (2013).

[13] H.C. Kim, J.M. Gu, S. Hu, C.H. Yo, Y. Kim. *Acta Crystallogr. C. Struct. Chem.*, **71**, 929 (2015).

[14] K.A. McDonald, S. Seth, A.J. Matzger. *Cryst. Growth Des.*, **15**, 5963 (2015).

[15] V. Thottempudi, P. Yin, J.H. Zhang, D.A. Parrish, J.M. Shreeve. *Chemistry*, **20**, 542 (2014).

[16] J.M. Lin, Y.X. Qiu, W.B. Chen, M. Yang, A.J. Zhou, W. Dong, C.E. Tian. *CrystEngComm*, **14**, 2779 (2012).

[17] B.D. Wu, J. Liang, J.Y. Wang, C.W. An. *Main Group Chem.*, **1**, 67 (2017).

[18] B.D. Wu, X.Y. Li, J. Liang, X.H. Geng, H.S. Huang, H. Huang, J.Y Wang, W.H. Hu. *Polyhedron*, **139**, 148 (2018).

[19] B.D. Wu, F.G. Li, T.L. Zhang, L. Yang, Z.N. Zhou, J.G. Zhang. *Z. Anorg. Allg. Chem.*, **639**, 1248 (2013).

[20] W.C. Tong, L. Yang, B.D. Wu, T.L. Zhang. *Z. Anorg. Allg. Chem.*, **640**, 980 (2014).

[21] Q.H. Zhang, J.M. Shreeve. *Angew. Chem. Int. Ed.*, **10**, 2540 (2014).

[22] Y.C. Li, C. Qi, S.H. Li, H.J. Zhang, C.H. Sun, Y.Z. Yu, S.P. Pang. *J. Am. Chem. Soc.*, **132**, 12172 (2010).

[23] C. He, J.M. Shreeve. *Angew. Chem. Int. Ed. Engl.*, **54**, 6260 (2015).

[24] M.W. Schmidt, M.S. Gordon, J.A. Boatz. *J. Phys. Chem. A.*, **109**, 7285 (2005).

[25] Z. Zeng, H. Gao, B. Twamley, J.M. Shreeve. *J. Mater. Chem.*, **17**, 3819 (2007).

[26] M.H.V. Huynh, M.A. Hiskey, D.E. Chavez, D.L. Naud, R.D. Gilardi. *J. Am. Chem. Soc.*, **127**, 12537 (2005).

[27] H. Wei, H. Gao, J.M. Shreeve. *Chemistry*, **20**, 16943 (2014).

[28] D.E. Chavez, B.C. Tappan, M.A. Hiskey, S.F. Son, H. Harry, D. Montoya, S. Hagelberg. *Propellants Explos. Pyrotech.*, **30**, 412 (2005).

[29] N.P. Spiridonova, S.F. Melnikova, I.V. Tselinsky. *J. Heterocycl. Chem.*, **42**, 1237 (2005).

[30] D.A. Safin, A.P. Railliet, K. Robeyns, M.P. Mitoraj, P. Kubisiak, F. Sagan, Y. Garcia. *New J. Chem.*, **41**, 6210 (2017).

[31] Y.R. Yao, X. Chen, Y.P. Hu, B. Yan, Y.L. Guan, J.R. Song, H.X. Ma. *J. Chem. Thermodynamics*, **104**, 67 (2017).

[32] M.H. Keshavarz, K. Esmaeilpour, M. Oftadeh, Y.H. Abadia. *RSC Adv.*, **5**, 87392 (2015).

[33] H. Wei, J.H. Zhang, J.M. Shreeve. *Chem. Asian J.*, **10**, 1130 (2015).

[34] N.V. Palysaeva, K.P. Kumpan, M.I. Struchkova, I.L. Dalinger, A.V. Kormanov, N.S. Aleksandrova, V.M. Chernyshev, D.F. Pyreu, K.Y. Suponitsky, A.B. Sheremetev. *Org. Lett.*, **16**, 406 (2014).

[35] R. Wang, Y. Guo, Z. Zeng, B. Twamley, J.M. Shreeve. *Chemistry*, **15**, 2625 (2009).

[36] H. Wei, J. Zhang, C. He, J.M. Shreeve. *Chem. Eur. J.*, **21**, 8607 (2015).
[37] V.G. Andrianov, A.V. Eremeev. *Chem. Heterocycl. Compd.*, **30**, 608 (1994).
[38] Bruker. *SMART*, Bruker AXS, Madison, WI (2009).
[39] R. Blessing. *Acta Crystallogr. A. Found. Adv.*, **51**, 33 (1995).
[40] Bruker. *SAINT*, Bruker AXS, Madison, WI (2009).
[41] G.M. Sheldrick. *Acta Cryst.*, **C71**, 112 (2015).
[42] N. Radacsi, R.H. Bouma, E.L. Haye, J.H. Horst, A.I. Stankiewicz, A.E. Heijden. *Propellants Explos. Pyrotech.*, **38**, 761 (2013).
[43] W.C. Tong, R. Zhang, L.J. Xue, R. Xu, L.N. Zhang, T.L. Zhang, L. Yang. *Z. Anorg. Allg. Chem.*, **641**, 1550 (2015).
[44] C.X. Xu, J.G. Zhang, X. Yin, X. Jin, T. Li, T.L. Zhang, Z.N. Zhou. *J. Solid State Chem.*, **226**, 59 (2015).
[45] Z.M. Li, T.L. Zhang, L. Yang, Z.N. Zhou, J.G. Zhang. *J. Coord. Chem.*, **65**, 143 (2012).
[46] Y.G. Bi, Y.A. Feng, Y. Li, B.D. Wu, T.L. Zhang. *J. Coord. Chem.*, **68**, 181 (2015).
[47] F.G. Li, Y.G. Bi, W.Y. Zhao, T.L. Zhang, Z.N. Zhou, L. Yang. *Inorg. Chem.*, **54**, 2050 (2015).
[48] H.E. Kissinger. *Anal Chem.*, **29**, 1702 (1957).
[49] T. Ozawa. *Bull. Chem. Soc. Jpn.*, **38**, 1881 (1965).
[50] R.Z. Hu, S.L. Gao, F.Q. Zhao, Q.Z. Shi, T.L. Zhang, J.J. Zhang. *Thermal Analysis Kinetics (2th)*, Beijing Science Press, Beijing, China (2008).
[51] Q.L. Yan, S. Zeman, R. Svoboda, A. Elbeih, J. Málek. *J. Therm. Anal. Calorim.*, **112**, 823 (2013).
[52] W.L. Cao, J.J. Guo, X. Chen, Z.M. Ding, K.Z. Xu, J.R. Song, A. Fan, J. Huang. *J. Mol. Struct.*, **1147**, 754 (2017).
[53] T.L. Zhang, R.Z. Hu, Y. Xie, F.P. Li. *Thermochim. Acta*, **244**, 171 (1994).